Numerical Quadrature Methods
for
Singular and Nearly Singular Integrals

A thesis submitted to Brunel University
for the degree of Doctor of Philosophy
in the Faculty of Technology and Information Systems

by

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October 2001

Abstract

This thesis is concerned with the development, design, and analysis of simple and efficient numerical quadrature methods for integrals on finite intervals with endpoint singularities, for integrals on the real line of steepest descent type, for integrals on finite intervals with branch point singularities near the interval of integration, and for integrals on the real line of Laplace type with branch point singularities near the path of integration.

In Chapter 1 we develop and analyse a numerical quadrature method, known as *the variable transformation method*, for integrals on finite intervals with endpoint singularities. The idea of this variable transformation method is based on the Euler–Maclaurin formula, and seems to have been suggested first by Korobov in 1963. From the Euler–Maclaurin formula, it is obvious that the trapezium rule is an excellent numerical quadrature method for integrands that are periodic, and for integrands whose derivatives near the endpoints of the interval of integration decay rapidly. To make the integrands always satisfy these properties, the notion is to introduce a mapping function and substitute it into the integrals. This variable transformation method is also sometimes called a periodizing transformation.

For integrals on the real line of steepest descent type, integrals on finite intervals with branch point singularities near the interval of integration, and integrals on the real line of Laplace type with branch point singularities near the path of integration, we design numerical quadrature methods and analyses based on the numerical quadrature method for integrals on finite intervals with endpoint singularities via suitable substitutions.

These new numerical quadrature rules and analyses are illustrated and supported through numerical experiments. As larger applications we consider in Chapters 3 and 5 the problems of efficient evaluation of the impedance Green's function for the Helmholtz equation in a half-plane and half-space, important problems of acoustic propagation.

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Acknowledgements

I would like to deeply thank my supervisor, Dr Simon Chandler-Wilde, for his elaborate guidance, friendly encouragement and tolerance.

I am extremely grateful to the Ministry of University Affairs (Thailand) for providing me with a scholarship. I would also like to take this opportunity to thank the Department of Mathematics, King Mongkut's University of Technology, Thonburi, for permitting an extension to enable me to complete this thesis.

Last but not least, I wish to acknowledge here, all the support I have had from my family and friends. They have always been there for me, and made my research time enjoyable.

To mum and dad

Glossary of Symbols and Special Functions

Sets and Spaces

$\mathbb{N}$	set of natural numbers
$\mathbb{Z}$	set of integers
$\mathbb{R}$	set of real numbers
$\mathbb{C}$	set of complex numbers
$\|x\|$	absolute value of a real or complex number x
$C[a,b]$	space of real- or complex-valued continuous functions on the interval $[a,b]$
$C^m[a,b]$	space of m times continuously differentiable functions
$\{a_1,\ldots,a_m\}$	set of m elements $a_1,\ldots,a_m$
$U\backslash V$	difference set $U\backslash V := \{x \in U : x \notin V\}$ for two sets U and V
$F : X \to Y$	a mapping with domain X and range in Y

Norms

$\|\cdot\|$	norm on a linear space
$\|\cdot\|_1$	L_1 norm of a function
$\|\cdot\|_\infty$	maximum norm of a function

Special Functions

ζ	Riemann zeta function
Γ	gamma function

J_ν	Bessel function of the first kind of order ν
δ	delta function
erfc	complementary error function
$H_0^{(1)}$	Hankel function of the first kind of order zero
E_1	exponential integral

Miscellaneous

$\in$	element inclusion
$\subset$	set inclusion
$\cup$	union of sets
$\cap$	intersection of sets
$\approx$	approximately equal
$\sim$	asymptotically equal
Δ	Laplacian operator
max	maximum
sup	supremum
$\lfloor x \rfloor$	largest integer $\leq x$
exp	exponential function
$\mathrm{Re}\, z$	real part of z
$\mathrm{Im}\, z$	imaginary part of z
$\arg z$	argument of z
$\blacksquare$	end of proof

Main Assumptions in the Thesis

Assumption 1.1 *The function $w : [-1,1] \to [-1,1]$ is bijective, strictly increasing, and infinitely differentiable (i.e., $w \in C^\infty[-1,1]$). Further, w is an odd function with, for some integer $p \geq 2$,*

$$w^{(j)}(-1) = w^{(j)}(1) = 0, \qquad j = 1, 2, \ldots, p-1,$$

and

$$w^{(p)}(\pm 1) \neq 0.$$

Assumption 2.1 *For some $q \in \mathbb{N}$, $f \in C^q[0,\infty)$ and there exists $c > 0$ and $r > 1/2$ such that, for $n = 0, 1, \ldots, q$, it holds that*

$$|f^{(n)}(t)| \leq c(1+t)^{-r-n}, \qquad t \geq 0.$$

Assumption 2.1′ *For some $\varepsilon > 0$ and $\theta \in (0, \pi/2]$, the function f is analytic on $\mathcal{D}_{\varepsilon,\theta}$, where (see Figure 2.1)*

$$\mathcal{D}_{\varepsilon,\theta} := \Big\{ z \in \mathbb{C} : |\arg(z+\varepsilon)| < \theta \Big\}.$$

Further, for some $\widetilde{c} > 0$ and $r > 1/2$,

$$|f(z)| \leq \widetilde{c}(1+|z|)^{-r}, \qquad z \in \mathcal{D}_{\varepsilon,\theta}.$$

Assumption 4.1 *For some $q \in \mathbb{N}$ and b_r with $-1 < b_r < 1$ it holds that $f \in C^q(-1, b_r) \cap C^q(b_r, 1)$, and that there exist $c > 0$ and α with $0 < \alpha \leq 1$ such that, for $j = 0, 1, \ldots, q$,*

$$|f^{(j)}(t)| \leq \begin{cases} c\left[\dfrac{(1+t)|t-b_r|}{1+b_r}\right]^{\alpha-1-j}, & -1 < t < b_r, \\[2ex] c\left[\dfrac{(1-t)|t-b_r|}{1-b_r}\right]^{\alpha-1-j}, & b_r < t < 1. \end{cases}$$

Assumption 4.1′ *For some $\varepsilon > 0$, and $b = b_r + ib_i \in \mathbb{C}$ with $b_i \geq 0$, the function f is analytic in $\mathcal{D}_{\varepsilon,b}$, where (see Figure 4.1)*

$$\mathcal{D}_{\varepsilon,b} := \Big\{z \in \mathbb{C} : \mathrm{dist}(z, [-1,1]) < \varepsilon\Big\} \backslash \Big\{b_r + it : t \geq b_i\Big\}.$$

Further, for some $\widetilde{c} > 0$ and α with $0 < \alpha \leq 1$,

$$|f(z)| \leq \widetilde{c}\,|z - b|^{\alpha-1}, \qquad z \in \mathcal{D}_{\varepsilon,b}.$$

Assumption 5.1 *For some $q \in \mathbb{N}$ and $B_r > 0$, it holds that $f \in C^q[0, B_r) \cap C^q(B_r, \infty)$, and that there exist $\widehat{c} > 0$ and α with $0 < \alpha \leq 1$ such that, for $n = 0, 1, \ldots, q$,*

$$|f^{(n)}(t)| \leq \widehat{c}\,|t - B_r|^{\alpha-1-n}(1+t)^{-2\alpha}, \qquad t \in [0, B_r) \cup (B_r, \infty).$$

Assumption 5.1′ *For some $\varepsilon > 0$, $\theta \in (0, \pi/2]$, and $B = B_r + iB_i \in \mathbb{C}$ with $B_i \geq 0$, the function f is analytic in (see Figure 5.1)*

$$\mathcal{D}_{\varepsilon,\theta,B} := \mathcal{D}_{\varepsilon,\theta} \backslash \Big\{B_r + it : t \geq B_i\Big\},$$

where $\mathcal{D}_{\varepsilon,\theta}$ is defined by (see Figure 2.1)

$$\mathcal{D}_{\varepsilon,\theta} := \Big\{z \in \mathbb{C} : |\arg(z+\varepsilon)| < \theta\Big\}.$$

Further, for some $\widetilde{c} > 0$ and $\alpha > 0$,

$$|f(z)| \leq \widetilde{c}\,|z - B|^{\alpha-1}(1+|z|)^{-2\alpha}, \qquad z \in \mathcal{D}_{\varepsilon,\theta,B}.$$

Main Theorems and Corollaries in the Thesis

Theorem 1.3 *Suppose that w satisfies Assumption 1.1, $f \in S^{q,\alpha}$, for some $q \in \mathbb{N}$ and $\alpha > 0$, with $1 < \alpha p \leq q$. Then the error in the quadrature (1.26) can be bounded by*

$$|If - I_N f| \leq C\|f\|_{q,\alpha} N^{-\alpha p},$$

in the case $\alpha p \notin \mathbb{N}$, where the constant C depends only on q, α, and on the function w. If $\alpha p = q$, then

$$|If - I_N f| \leq c_\varepsilon C\|f\|_{q,\alpha} N^{\varepsilon - q}$$

for every $\varepsilon > 0$, where $c_\varepsilon > 0$ depends only on ε.

Theorem 2.5 *Suppose that w satisfies Assumption 1.1, f satisfies Assumption 2.1, and $1 < s < q$, where $s := (r - 1/2)p$. Then, for $s \notin \mathbb{N}$, the error in the quadrature (2.13) can be bounded by*

$$|Jf - J_N f| \leq c\, C(1 + \rho^q) N^{-s},$$

where the constant C depends only on q, r, and on the choice of the function w.

Corollary 2.1 *Suppose that w satisfies Assumption 1.1, f satisfies Assumption 2.1′, and $1 < s < q$, where $s := (r - 1/2)p$. Then, for $s \notin \mathbb{N}$, the error in the quadrature (2.13) can be bounded by*

$$|Jf - J_N f| \leq \frac{\tilde{c}\, C(1 + \rho^q)}{(\bar{\varepsilon} \sin\theta)^q} N^{-s},$$

where $\bar{\varepsilon} = \min\{\varepsilon, 1\}$ and the constant C depends only on q, r, and on the choice of the function w.

Theorem 4.1 *Suppose that w satisfies Assumption 1.1, f satisfies Assumption 4.1, $q \in \mathbb{N}$, and $1 < \alpha p \leq q$. Then, if $\alpha p \notin \mathbb{N}$, the error in the quadrature (4.9) can be bounded by*

$$|If - I_N \widetilde{f}\,| \leq c\,CN^{-\alpha p},$$

where the constant C depends only on q, α and on the function w. If $\alpha p = q$, then

$$|If - I_N \widetilde{f}\,| \leq c_\delta c\,CN^{\delta - q},$$

for every $\delta > 0$, where $c_\delta > 0$ depends only on δ.

Corollary 4.1 *Suppose that w satisfies Assumption 1.1, f satisfies Assumption 4.1′, $q \in \mathbb{N}$, and $1 < \alpha p \leq q$. Then, if $\alpha p \notin \mathbb{N}$, the error in the quadrature (4.9) can be bounded by*

$$|If - I_N \widetilde{f}\,| \leq \frac{\widetilde{c}\,C}{\widetilde{\theta}^q (1 - \widetilde{\theta}\,)^{1-\alpha}} N^{-\alpha p}$$

with

$$\widetilde{\theta} = \min\left\{\frac{\varepsilon}{R}, \frac{j}{j + 1 - \alpha}\right\},$$

where the constant C depends only on q, α and on the function w. If $\alpha p = q$, then

$$|If - I_N \widetilde{f}\,| \leq \frac{c_\delta \widetilde{c}\,C}{\widetilde{\theta}^q (1 - \widetilde{\theta}\,)^{1-\alpha}} N^{\delta - q},$$

for every $\delta > 0$, where $c_\delta > 0$ depends only on δ.

Theorem 5.1 *Suppose that w satisfies Assumption 1.1, f satisfies Assumption 5.1, $q \in \mathbb{N}$, and $1 < \alpha p < q$. Then, for $\alpha p \notin \mathbb{N}$, the error in the quadrature (5.12) can be bounded by*

$$|\bar{J} f - I_N \widetilde{F}\,| \leq \widehat{c}\,C(1 + \rho^q) N^{-\alpha p},$$

where the constant C depends only on q, α, and on the function w. If $\alpha p = q$, then

$$|\bar{J} f - I_N \widetilde{F}\,| \leq c_\delta \widehat{c}\,C(1 + \rho^q) N^{\delta - q},$$

for every $\delta > 0$, where $c_\delta > 0$ depends only on δ.

Corollary 5.2 *Suppose that w satisfies Assumption 1.1, f satisfies Assumption 5.1′, $q \in \mathbb{N}$, and $1 < \alpha p < q$. Then, for $\alpha p \notin \mathbb{N}$, the error in the quadrature (5.12) can be bounded by*

$$|\bar{J} f - I_N \widetilde{F}\,| \leq \frac{\widetilde{c}\, C(1+\rho^q)}{\widetilde{\omega}^q (1-\widetilde{\omega}\,)^{1-\alpha}}\, N^{-\alpha p}$$

with

$$\widetilde{\omega} = \min\left\{\frac{\eta}{R}, \frac{n}{n+1-\alpha}\right\}.$$

where the constant C depends only on q, α, and on the function w. If $\alpha p = q$, then

$$|\bar{J} f - I_N \widetilde{F}\,| \leq \frac{c_\delta \widetilde{c}\, C(1+\rho^q)}{\widetilde{\omega}^q (1-\widetilde{\omega}\,)^{1-\alpha}}\, N^{\delta - q},$$

for every $\delta > 0$, where $c_\delta > 0$ depends only on δ.

Chapter 0

Introduction

The main objective of this thesis is the development, design, and analysis of numerical quadrature methods suitable for integrals on finite intervals with endpoint singularities, for integrals on the real line of steepest descent type, for integrals on finite intervals with branch point singularities near the interval of integration, and for integrals on the real line of Laplace type with branch point singularities near the path of integration.

The problem of numerical quadrature is quite old, going back to the Greek quadrature of the circle by means of inscribed and circumscribed regular polygons, and is surveyed in the monographs by Davis and Rabinowitz [16], Engels [17], Smith [47], Krommer and Ueberhuber [34], and in numerous conference proceedings, e.g. Brass and Hämmerlin [9], Espelid and Genz [19]. A major area of theoretical work in numerical integration has occurred in the area of integral equations and the related boundary element method. Recent work has focussed on the development of efficient methods for treating different types of kernels (e.g. weakly singular, Cauchy singular, and hyper-singular kernels) that arise in applications. These applications include both evaluation of integrals arising when the boundary integral equations are discretised (see e.g. Kress [32], Hayami [21], Schwab and Wendland [44]) and evaluation of integral representation of fundamental solutions to the governing partial differential equations (see e.g. Chandler-Wilde and Hothersall [12], Hearn [22], Monacella [40], and Linton [35, 36]). Integrals of a sort arising in both these types of applications are addressed in this thesis.

In Chapter 1 we consider the evaluation of $\int_{-1}^{+1} f(t)\,dt$, where f may have endpoint singularities. This type of integral with specific weight functions containing the singularity of f can be numerically evaluated by a class of numerical quadrature rules collectively known as Gaussian quadrature rules, see e.g. Davis and Rabinowitz [16], Engels [17], Kress [33], Atkinson [3], Smith [47], Isaacson and Keller [28], and Blum [8]. Other methods for evaluating this type of integral include SINC quadrature, see e.g. Bialecki [6, 7], Lund and Bowers [38], and Stenger [48, 49].

A well-known method for this type of integral is a numerical quadrature method called *the variable transformation method.* The notion of this variable transformation method is to substitute $t = w(x)$ in $\int_{-1}^{+1} f(t)\,dt$, leading to the expression $\int_{-1}^{+1} w'(x) f(w(x))\,dx$, choosing $w : [-1,1] \to [-1,1]$ to be bijective, infinitely differentiable, and having all or many derivatives vanishing at ± 1. The idea of employing variable transformations, also called periodizing transformations [34], seems to have been suggested first by Korobov [31] in connection with the numerical approximation of integrals on the unit hypercube by lattice rules (cf. Sidi [46]). Since then, there are a number of transformation methods which have appeared in the literature with different transformations w, called mapping functions in this thesis. These transformations have been proposed by Korobov [31], Sag and Szekeres [43], Schwartz [45], Iri *et al.* [27], Takahasi and Mori [50], Mori [41], Hua and Wang [23], Sidi [46], and recently proposed by Kress [32, 33]. All variable transformation methods discussed by these authors are based on the Euler–Maclaurin formula [16], which shows that the trapezium rule is very accurate for evaluating the integral $\int_{-1}^{+1} g(t)\,dt$ when g is smooth and many derivatives of g vanish at the endpoints. In Chapter 1 we consider a numerical quadrature method, based on the Euler–Maclaurin formula, for integrals on finite intervals with endpoint singularities similar to the methods used by above authors. We develop an analysis of transformation methods suitable for the mapping functions proposed by Korobov [31], Sidi [46], and Kress [33]. Thus we can apply our analysis to the mapping functions given by these authors. Comparing this numerical quadrature with Gaussian quadrature, an advantage of this quadrature method is that weights and abscissae of this method are easily generated, leading to convenience of implementation. More crucially, these methods are robust with respect to the nature of the singularity which does not need to be known precisely as in Gaussian quadrature.

For integrals on the real line of steepest descent type in Chapter 2, integrals on finite intervals with branch point singularities near the interval of integration in Chapter 4, and integrals on the real line of Laplace type with branch point singularities near the path of integration in Chapter 5, we design numerical quadrature methods and analyses based on the numerical quadrature method for integrals on finite intervals with endpoint singularities contained in Chapter 1 via suitable substitutions.

As larger applications we consider in Chapters 3 and 5 the problems of efficient evaluation of the impedance Green's function for the Helmholtz equation in a half-plane and half-space, important problems of acoustic propagation. We would like to mention at this early state of the thesis that all numerical computations in this thesis are performed by using the interactive programming system, *Matlab*.

In summary, the numerical quadrature rule and analysis contained in Chapter 1 is the cornerstone of this thesis. It will be used and applied throughout the other chapters of this thesis to develop numerical quadrature methods for integrals on finite intervals with endpoint singularities, integrals on the real line of steepest descent type, integrals on finite intervals with branch point singularities near the interval of integration, and integrals on the real line of Laplace type with branch point singularities near the path of integration.

Chapter 1

A Numerical Quadrature Method for Integrals on Finite Intervals with Endpoint Singularities

We consider the problem of finding the numerical value of

$$If := \int_{-1}^{+1} f(t)\,dt, \tag{1.1}$$

where $f(t)$ may have singularities at $t = \pm 1$.

In the case that $f(t) = \rho(t)g(t)$ with $g \in \mathcal{C}^\infty[-1,1]$ and $\rho \geq 0$ a sufficiently simple function containing the singularity of f, the classical method for approximating the integral (1.1) is to use Gaussian quadrature for the weight function ρ, leading to approximations for If of the form

$$\sum_{i=1}^{N} a_i\, g(b_i). \tag{1.2}$$

In (1.2), $a_1, \ldots, a_N \in (0, \infty)$ and $b_1, \ldots, b_N \in (-1, 1)$ are, respectively, the weights and abscissae of the quadrature rule. For details of Gaussian quadrature, see e.g. Davis and Rabinowitz [16], Kress [33], Atkinson [3], Smith [47], Isaacson and Keller [28], and Blum [8]. These weights and abscissae are tabulated for certain functions ρ, e.g. $\rho(t) = (1+t)^a(1-t)^b$ for $a, b > -1$, in [1] or can be calculated by using standard subroutine libraries, e.g. [37]. Other methods for evaluating the integral (1.1) when f has singularities at ± 1 include SINC quadrature, see e.g. Bialecki [6, 7], Lund and Bowers [38], and Stenger [48, 49].

In this chapter, we consider a version of the quadrature method discussed in Korobov [31], Sag and Szekeres [43], Schwartz [45], Iri *et al.* [27], Takahasi and Mori [50], Mori [41], Hua and Wang [23], Sidi [46], and recently proposed by Kress [32, 33]. All quadrature methods discussed by these authors are based on the Euler–Maclaurin formula [16], which shows that the trapezium rule is very accurate for evaluating integrals of the form (1.1) when f is smooth and many derivatives of f vanish at ± 1. In these papers a variable transformation, sometimes called a periodizing transformation [34], of the form $t = w(x)$ is applied, leading to the expression

$$If = \int_{-1}^{+1} w'(x) f(w(x))\, dx. \tag{1.3}$$

In all the papers above, $w \in \mathcal{C}^\infty[-1,1]$ is injective and a large number or all derivatives of w vanish at ± 1. Sag and Szekeres [43] proposed the TANH transformations,

$$w(x) = \tanh\left(\frac{2cx}{1-x^2}\right), \tag{1.4}$$

for some $c > 0$. Iri *et al.* [27] proposed the so-called IMT transformations,

$$w(x) = \frac{\int_0^x \phi(s)\, ds}{\int_0^1 \phi(s)\, ds}, \tag{1.5}$$

with

$$\phi(x) = \exp\left(-\frac{c}{1-x^2}\right), \tag{1.6}$$

for some $c > 0$. Mori [41] proposed the Double Exponential transformations,

$$w(x) = \tanh\left(a \sinh\left(\frac{2bx}{1-x^2}\right)\right), \tag{1.7}$$

for $a, b > 0$. Note that the functions w given by (1.4), (1.5) with (1.6), and (1.7) all satisfy that $w \in \mathcal{C}^\infty[-1,1]$, and that all the derivatives of w vanish at ± 1.

The following are examples of functions $w \in \mathcal{C}^\infty[-1,1]$ with only derivatives up to a certain order vanishing at ± 1. Korobov [31] proposed the Polynomial transformations,

$$w(x) = \frac{\int_0^x (1-s^2)^{p-1}\, ds}{\int_0^1 (1-s^2)^{p-1}\, ds}, \qquad \text{for } p = 2, 3, \ldots. \tag{1.8}$$

Sidi [46] proposed the SINE transformations,

$$w(x) = \frac{\int_0^x \left(\cos\frac{\pi s}{2}\right)^{p-1} ds}{\int_0^1 \left(\cos\frac{\pi s}{2}\right)^{p-1} ds}, \qquad \text{for } p = 2, 3, \ldots. \tag{1.9}$$

In 1998 Kress [33] also suggested a new mapping function w, equations (1.31) and (1.33) of this thesis. All these mapping functions w are applied to one-dimensional integrals of the form (1.1) via the representation (1.3) by the authors above. However, Beckers and Haegemans [4] also consider a lattice rule for approximating multiple integrals, and apply this transformation method with w given by (1.4), (1.5) with (1.6), and (1.7).

In this chapter we will develop an analysis of transformation methods satisfying that $w \in \mathcal{C}^\infty[-1,1]$ with

$$w^{(j)}(\pm 1) = 0, \qquad j = 1, 2, \ldots, p-1, \quad \text{but} \quad w^{(p)}(\pm 1) \neq 0.$$

Thus our analysis can be applied to the functions w given by equations (1.8), (1.9), or (1.31) and (1.33). We consider the case discussed by Kress [33], where

$$|f^{(j)}(t)| \leq C(1-t^2)^{\alpha-1-j}, \qquad j = 0, 1, \ldots, q,$$

for some $q \in \mathbb{N}$ and α in the range $0 < \alpha \leq 1$. Our analysis follows closely that of Kress [33], but we generalise his results by considering the case $\alpha > 1$ as well as the case $0 < \alpha \leq 1$. More importantly, we sharpen his analysis considerably, establishing higher rates of convergence with the same assumptions on f. The rates of convergence we establish match those seen in the numerical experiments we carry out, in nearly all cases.

For $q \in \mathbb{N}$ and $\alpha > 0$, by $\mathcal{S}^{q,\alpha}[a,b]$ we denote the linear space of q-times continuously differentiable functions $f : (a,b) \to \mathbb{R}$ for which

$$\sup_{a<t<b} \left|f^{(j)}(t)\right| \left[(t-a)(b-t)\right]^{j+1-\alpha} < \infty, \qquad j = 0, 1, \ldots, q.$$

On $\mathcal{S}^{q,\alpha}[a,b]$ we define the norm

$$\|f\|_{q,\alpha,[a,b]} := \max_{j=0,\ldots,q} \sup_{a<t<b} \left|f^{(j)}(t)\right| \left[(t-a)(b-t)\right]^{j+1-\alpha}. \tag{1.10}$$

Then if $f \in \mathcal{S}^{q,\alpha}[a,b]$, it holds that, for $j = 0, 1, \ldots, q$,

$$\left|f^{(j)}(t)\right| \leq \|f\|_{q,\alpha,[a,b]} \left[(t-a)(b-t)\right]^{\alpha-1-j}, \qquad a < t < b. \tag{1.11}$$

We abbreviate $\mathcal{S}^{q,\alpha}[-1,1]$ and $\|\cdot\|_{q,\alpha,[-1,1]}$ by $\mathcal{S}^{q,\alpha}$ and $\|\cdot\|_{q,\alpha}$, respectively. Clearly, $\mathcal{S}^{q_2,\alpha_2} \subset \mathcal{S}^{q_1,\alpha_1}$ if $q_2 \geq q_1$ and $\alpha_1 \geq \alpha_2$ and $\|\cdot\|_{q_1,\alpha_1} \leq \|\cdot\|_{q_2,\alpha_2}$.

1.1 The Trapezium Rule

Our numerical quadrature method will be based on the trapezium rule, the error in which is quantified by the Euler–Maclaurin formula (e.g. Davis & Rabinowitz [16] and Kress [33]). As usual, given $a_0, a_1, \ldots, a_N \in \mathbb{C}$, we abbreviate the sum $\frac{1}{2}a_0 + a_1 + a_2 + \cdots + a_{N-1} + \frac{1}{2}a_N$ by $\sum_{j=0}^{N}{}'' a_j$ and we use the notation $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$. The following is the version of the Euler–Maclaurin formula that we require. We remind the reader that the Riemann zeta function is defined by

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}, \qquad s > 1.$$

Theorem 1.1 *Let $k \in \mathbb{N}_0$, $g \in C^k[a,b] \cap C^{k+1}(a,b)$ with*

$$\int_a^b \left|g^{(k+1)}(x)\right| dx < \infty, \tag{1.12}$$

and, in the case that $k \geq 1$,

$$g^{(m)}(a) = g^{(m)}(b) = 0, \qquad m = 1, 2, \ldots, k. \tag{1.13}$$

Define $h = (b-a)/N$, $x_j = a + jh$ for $j = 0, 1, \ldots, N$. Then

$$\int_a^b g(x)\, dx = h \sum_{j=0}^{N}{}'' g(x_j) + (-h)^{k+1} \int_a^b g^{(k+1)}(x) P_{k+1}\Big(\frac{x-a}{h}\Big)\, dx, \tag{1.14}$$

where, for $j = 1, 3, 5, \ldots$,

$$P_j(x) := (-1)^{\frac{j+1}{2}} \sum_{l=1}^{\infty} \frac{2\sin 2\pi l x}{(2\pi l)^j}, \qquad x \in \mathbb{R},$$

and, for $j = 2, 4, 6, \ldots$,

$$P_j(x) := (-1)^{\frac{j-2}{2}} \sum_{l=1}^{\infty} \frac{2\cos 2\pi l x}{(2\pi l)^j}, \qquad x \in \mathbb{R}.$$

Proof. We first prove the result under the assumption that $g \in C^{k+1}[a,b]$. Let $\lfloor x \rfloor$ denote the largest integer $\leq x$. It is easy to see that $P_1(x)$ is the Fourier series of the piecewise linear periodic function with period one, $x - \lfloor x \rfloor - 1/2$. Thus

$$P_1(x) = x - \lfloor x \rfloor - 1/2, \qquad x \in \mathbb{R}\backslash\mathbb{Z}. \tag{1.15}$$

Also

$$P_1'(x) = 1, \qquad x \in \mathbb{R}\backslash\mathbb{Z}. \tag{1.16}$$

and

$$P_1(1^-) = -P_1(0^+) = 1/2. \tag{1.17}$$

Clearly, for $n = 2, 3, 4, \ldots$,

$$P_n(0) = P_n(1) = (-1)^{\frac{n-2}{2}} 2(2\pi)^{-n}\zeta(n) =: b_{n-1}, \tag{1.18}$$

and

$$P_n'(x) = P_{n-1}(x), \qquad x \in \mathbb{R}\backslash\mathbb{Z}. \tag{1.19}$$

(This last equation holds for all $x \in \mathbb{R}$ for $n \geq 3$.) Suppose now that $G \in \mathcal{C}^{k+1}[0, N]$. By using (1.16), (1.17), and integration by parts,

$$\int_0^1 G(x)\,dx = \frac{1}{2}\big(G(0) + G(1)\big) - \int_0^1 G'(x)P_1(x)\,dx.$$

Hence, using (1.18), (1.19), integration by parts, and induction, we find that

$$\begin{aligned}\int_0^1 G(x)\,dx &= \frac{1}{2}\big(G(0) + G(1)\big) + \sum_{j=1}^{k}(-1)^j b_j \big(G^{(j)}(1) - G^{(j)}(0)\big) \\ &\quad + (-1)^{k+1}\int_0^1 G^{(k+1)}(x)P_{k+1}(x)\,dx.\end{aligned}$$

Thus, for $i = 1, 2, \ldots, N$,

$$\begin{aligned}\int_{i-1}^{i} G(x)dx &= \frac{1}{2}\big(G(i-1) + G(i)\big) + \sum_{j=1}^{k}(-1)^j b_j \big(G^{(j)}(i) - G^{(j)}(i-1)\big) \\ &\quad + (-1)^{k+1}\int_{i-1}^{i} G^{(k+1)}(x)P_{k+1}(x)dx.\end{aligned}$$

So

$$\begin{aligned}\int_0^N G(x)\,dx &= \sum_{i=1}^{N}\left[\int_{i-1}^{i} G(x)\,dx\right] \\ &= {\sum_{j=0}^{N}}'' G(j) + \sum_{j=1}^{k}(-1)^j b_j \big(G^{(j)}(N) - G^{(j)}(0)\big) \\ &\quad + (-1)^{k+1}\int_0^N G^{(k+1)}(x)P_{k+1}(x)\,dx. \end{aligned} \tag{1.20}$$

Substituting $x := hy + a$ in $\int_a^b g(x)\,dx$, we obtain

$$\int_a^b g(x)\,dx = h\int_0^N g(hy+a)\,dy$$

$$= h\sum_{j=0}^{N}{}'' g(x_j) + \sum_{j=1}^{k}(-1)^j b_j h^{j+1}\big(g^{(j)}(b) - g^{(j)}(a)\big)$$

$$+ (-h)^{k+1}\int_a^b g^{(k+1)}(x)P_{k+1}\Big(\frac{x-a}{h}\Big)\,dx,$$

where we have used the formula (1.20), which applies since $g \in \mathcal{C}^{k+1}[a,b]$ so that $G \in \mathcal{C}^{k+1}[0,N]$, where $G(y) := g(hy+a)$, $0 \le y \le N$. Applying (1.13), we get

$$\int_a^b g(x)\,dx = h\sum_{j=0}^{N}{}'' g(x_j) + (-h)^{k+1}\int_a^b g^{(k+1)}(x)P_{k+1}\Big(\frac{x-a}{h}\Big)\,dx.$$

If $g \in \mathcal{C}^k[a,b] \cap \mathcal{C}^{k+1}(a,b)$ and (1.13) holds then, for $0 < \varepsilon < (b-a)/2$, $g \in \mathcal{C}^{k+1}[a+\varepsilon, b-\varepsilon]$. Thus, where $\bar{x}_j = a + \varepsilon + j\bar{h}$, for $j = 0, 1, \ldots, N$, with $\bar{h} = (b-a-2\varepsilon)/N$, it holds that

$$\int_{a+\varepsilon}^{b-\varepsilon} g(x)\,dx = \bar{h}\sum_{j=0}^{N}{}'' g(\bar{x}_j) + (-\bar{h})^{k+1}\int_a^b G_\varepsilon(x)\,dx, \tag{1.21}$$

where

$$G_\varepsilon(x) := \begin{cases} g^{(k+1)}(x)P_{k+1}\Big(\dfrac{x-a-\varepsilon}{\bar{h}}\Big), & a+\varepsilon < x < b-\varepsilon, \\ 0, & \text{otherwise.} \end{cases}$$

Now, for $a < x < b$, $G_\varepsilon(x) \to g^{(k+1)}(x)P_{k+1}(\frac{x-a}{h})$ as $\varepsilon \to 0$ and $|G_\varepsilon(x)| \le |g^{(k+1)}(x)|\,\|P_{k+1}\|_\infty$. Thus, by the dominated convergence theorem, letting $\varepsilon \to 0^+$ in (1.21) we obtain (1.14). ■

Corollary 1.1 *If the conditions of Theorem 1.1 are satisfied, for some $k \in \mathbb{N}_0$, then*

$$\left|\int_a^b g(x)\,dx - h\sum_{j=0}^{N}{}'' g(x_j)\right| \le \frac{C_k}{N^{k+1}}\int_a^b \big|g^{(k+1)}(x)\big|\,dx,$$

where

$$C_k := \begin{cases} \dfrac{b-a}{2}, & k = 0, \\ \dfrac{2^{-k}(b-a)^{k+1}}{\pi^{k+1}}\zeta(k+1), & k \in \mathbb{N}. \end{cases}$$

Proof. From Theorem 1.1

$$\left| \int_a^b g(x)\,dx - h\sum_{j=0}^{N}{}'' g(x_j) \right| \le h^{k+1} \int_a^b \left| g^{(k+1)}(x) P_{k+1}\Big(\frac{x-a}{h}\Big) \right| dx$$

$$\le \|P_{k+1}\|_\infty h^{k+1} \int_a^b |g^{(k+1)}(x)|\,dx$$

$$= \frac{C_k}{N^{k+1}} \int_a^b |g^{(k+1)}(x)|\,dx,$$

where $C_k = \|P_{k+1}\|_\infty (b-a)^{k+1}$. From the definition of P_{k+1} and (1.15) it follows that $\|P_{k+1}\|_\infty = 1/2$ if $k = 0$ and $\|P_{k+1}\|_\infty \le \frac{1}{2^k \pi^{k+1}} \zeta(k+1)$, $k \in \mathbb{N}$. ■

Theorem 1.2 *Let $g \in \mathcal{S}^{k+2,\alpha}[a,b]$ with $k \in \mathbb{N}_0$ and $k+1 < \alpha < k+2$. Then*

$$\left| \int_a^b g(x)\,dx - h\sum_{j=0}^{N}{}'' g(x_j) \right| \le C\|g\|_{k+2,\alpha,[a,b]} N^{-\alpha},$$

where C is a constant dependent only on a, b, α, and k.

Proof. Throughout the proof, we let $C > 0$ denote a generic constant dependent only on a, b, α, and k. Since $g \in \mathcal{S}^{k+2,\alpha}[a,b]$ and $\alpha > k+1$, $g \in \mathcal{C}^k[a,b] \cap \mathcal{C}^{k+2}(a,b)$ with

$$\int_a^b |g^{(k+1)}(x)|\,dx \le \|g\|_{k+2,\alpha,[a,b]} \int_a^b \left[(x-a)(b-x)\right]^{\alpha-k-2} dx < \infty,$$

and, in the case that $k \in \mathbb{N}$,

$$g^{(m)}(a) = g^{(m)}(b) = 0, \qquad m = 1, 2, \ldots, k.$$

Thus the conditions of Theorem 1.1 are satisfied and, applying this theorem, we obtain that

$$\left| \int_a^b g(x)\,dx - h\sum_{j=0}^{N}{}'' g(x_j) \right| \le h^{k+1}\big(|I_1| + |I_2|\big), \tag{1.22}$$

where

$$I_1 = \int_a^{a+h} g^{(k+1)}(x) P_{k+1}\Big(\frac{x-a}{h}\Big)\,dx + \int_{b-h}^b g^{(k+1)}(x) P_{k+1}\Big(\frac{x-a}{h}\Big)\,dx,$$

and

$$I_2 = \int_{a+h}^{b-h} g^{(k+1)}(x) P_{k+1}\Big(\frac{x-a}{h}\Big)\,dx.$$

By (1.11),

$$|I_1| \leq C\|g\|_{k+2,\alpha,[a,b]}\int_a^{a+h} \left[(x-a)(b-x)\right]^{\alpha-k-2}\,dx$$

$$+ C\|g\|_{k+2,\alpha,[a,b]}\int_{b-h}^{b} \left[(x-a)(b-x)\right]^{\alpha-k-2}\,dx$$

$$\leq Ch^{\alpha-k-1}\|g\|_{k+2,\alpha,[a,b]}. \tag{1.23}$$

By integration by parts, and (1.11),

$$|I_2| = \left|\left[hP_{k+2}\Big(\frac{x-a}{h}\Big)g^{(k+1)}(x)\right]_{a+h}^{b-h} - h\int_{a+h}^{b-h} g^{(k+2)}(x)P_{k+2}\Big(\frac{x-a}{h}\Big)\,dx\right|$$

$$\leq Ch\left\{\left|g^{(k+1)}(a+h)\right| + \left|g^{(k+1)}(b-h)\right| + \int_{a+h}^{b-h}\left|g^{(k+2)}(x)\right|dx\right\}$$

$$\leq Ch\|g\|_{k+2,\alpha,[a,b]}\left\{h^{\alpha-k-2} + \int_{a+h}^{b-h}\left[(x-a)(b-x)\right]^{\alpha-k-3}dx\right\}$$

$$\leq Ch^{\alpha-k-1}\|g\|_{k+2,\alpha,[a,b]}. \tag{1.24}$$

(Note that this last step is where the condition that $\alpha < k+2$ is required.) So, combining (1.22), (1.23), and (1.24),

$$\left|\int_a^b g(x)\,dx - h\sum_{j=0}^{N}{}'' g(x_j)\right| \leq Ch^{\alpha}\|g\|_{k+2,\alpha,[a,b]}$$

$$\leq C\|g\|_{k+2,\alpha,[a,b]}N^{-\alpha}.$$

■

Remark 1.1 *If $g \in \mathcal{S}^{k+2,k+2}[a,b]$ then $g \in \mathcal{S}^{k+2,\alpha}[a,b]$ for $0 < \alpha < k+2$, so that, from Theorem 1.2 we deduce that*

$$\left|\int_a^b g(x)\,dx - h\sum_{j=0}^{N}{}'' g(x_j)\right| \leq C\|g\|_{k+2,k+2,[a,b]}N^{-\alpha}$$

for all $\alpha < k+2$, where C is a constant dependent only on a, b, α, and k.

Corollary 1.1 implies that the trapezium rule is very effective for the evaluation of (1.1) if f is smooth and many derivatives of f vanish at ± 1. To make use of this fact when $f \in \mathcal{S}^{q,\alpha}$ for some $q \in \mathbb{N}$ and $\alpha > 0$, we will make the substitution $t = w(x)$ in (1.1) where the function w satisfies the following assumptions.

Assumption 1.1 *The function* $w : [-1,1] \to [-1,1]$ *is bijective, strictly increasing, and infinitely differentiable (i.e.,* $w \in C^\infty[-1,1]$*). Further,* w *is an odd function with, for some integer* $p \geq 2$,

$$w^{(j)}(-1) = w^{(j)}(1) = 0, \qquad j = 1, 2, \ldots, p-1,$$

and

$$w^{(p)}(\pm 1) \neq 0.$$

Assuming that Assumption 1.1 holds, we will approximate the integral (1.1) by substituting $t = w(x)$ to obtain that

$$\int_{-1}^{+1} f(t)\, dt = \int_{-1}^{+1} g(x)\, dx,$$

where

$$g(x) := w'(x) f(w(x)), \tag{1.25}$$

and then apply the trapezium rule. Applying the trapezium rule with $2N+1$ points we get that, since $w'(-1) = 0 = w'(1)$,

$$If \approx I_N f := \sum_{k=1-N}^{N-1} a_k f(x_k), \tag{1.26}$$

where, for $k = 1-N, \ldots, N-1$,

$$a_k := \frac{1}{N} w'\left(\frac{k}{N}\right), \qquad x_k := w\left(\frac{k}{N}\right). \tag{1.27}$$

$I_N f$, given by (1.26), can be viewed as a new quadrature rule for $If = \int_{-1}^{+1} f(t)\, dt$, appropriate when f has endpoint singularities, with a_k and x_k the weights and abscissae of the quadrature rule, respectively. From the property of w in Assumption 1.1, it can be seen that a_k and x_k have the symmetry properties that

$$a_{-k} = a_k, \qquad x_{-k} = -x_k, \qquad k = 1-N, \ldots, N-1. \tag{1.28}$$

Further, it is obvious that if p increases, by Assumption 1.1 and Taylor's theorem applied to $w(k/N)$, the abscissae x_k and x_{-k} of the quadrature rule are graded more closely towards the endpoints 1 and -1, respectively.

Note that, if for some $a > 0$, $V : [-1,1] \to [0,a]$ is bijective, strictly increasing, and infinitely differentiable with, for some integer $p \geq 2$,

$$V^{(j)}(-1) = 0, \qquad j = 1, 2, \ldots, p-1, \tag{1.29}$$

and

$$V^{(p)}(-1) \neq 0, \tag{1.30}$$

then

$$w(x) := \frac{V(x) - V(-x)}{V(x) + V(-x)}, \qquad -1 \leq x \leq 1, \tag{1.31}$$

satisfies Assumption 1.1. In particular

$$w'(x) = 2\frac{V'(x)V(-x) + V'(-x)V(x)}{(V(x) + V(-x))^2} \geq 0, \qquad -1 \leq x \leq 1.$$

Clearly, if for some $b > 0$, $v : [-1,1] \to [0,b]$ is bijective, strictly increasing, and infinitely differentiable, with $v'(-1) \neq 0$, then $V(x) = [v(x)]^p$ satisfies (1.29) and (1.30). Thus, examples of functions satisfying (1.29) and (1.30) are

$$V(x) = \left(1 + x\right)^p, \qquad -1 \leq x \leq 1, \tag{1.32}$$

and, as suggested by Kress [33],

$$V(x) = \left[\left(\frac{1}{2} - \frac{1}{p}\right)x^3 + \frac{1}{p}x + \frac{1}{2}\right]^p, \qquad -1 \leq x \leq 1. \tag{1.33}$$

A further example, for which we will make calculations, is

$$V(x) = \begin{cases} \exp\left(-(1+x)^{-1}\right), & -1 < x \leq 1, \\ 0, & x = -1. \end{cases} \tag{1.34}$$

With V given by (1.34), w given by equation (1.31) does not satisfy Assumption 1.1, but $w : [-1,1] \to [-1,1]$ is bijective, strictly increasing, infinitely differentiable, an odd function, and

$$w^{(j)}(-1) = w^{(j)}(1) = 0, \qquad j \in \mathbb{N}.$$

The graphs of $w(x)$ and $w'(x)$ against x for each function V are depicted in Figures 1.1, 1.2 and 1.3, respectively. In Figure 1.2 it is seen that the choice (1.33), more sophisticated than (1.32), ensures that $w'(0) = V'(0)/V(0)$ is fixed, independent of p, which in turn ensures, from (1.27), that the density of quadrature points x_k around $x = 0$ remains fixed as p increases.

Through the remainder of this chapter, we assume that $f \in \mathcal{S}^{q,\alpha}$ for some $q \in \mathbb{N}$ and $\alpha > 0$, that w satisfies Assumption 1.1, and that g is given in term of f by (1.25).

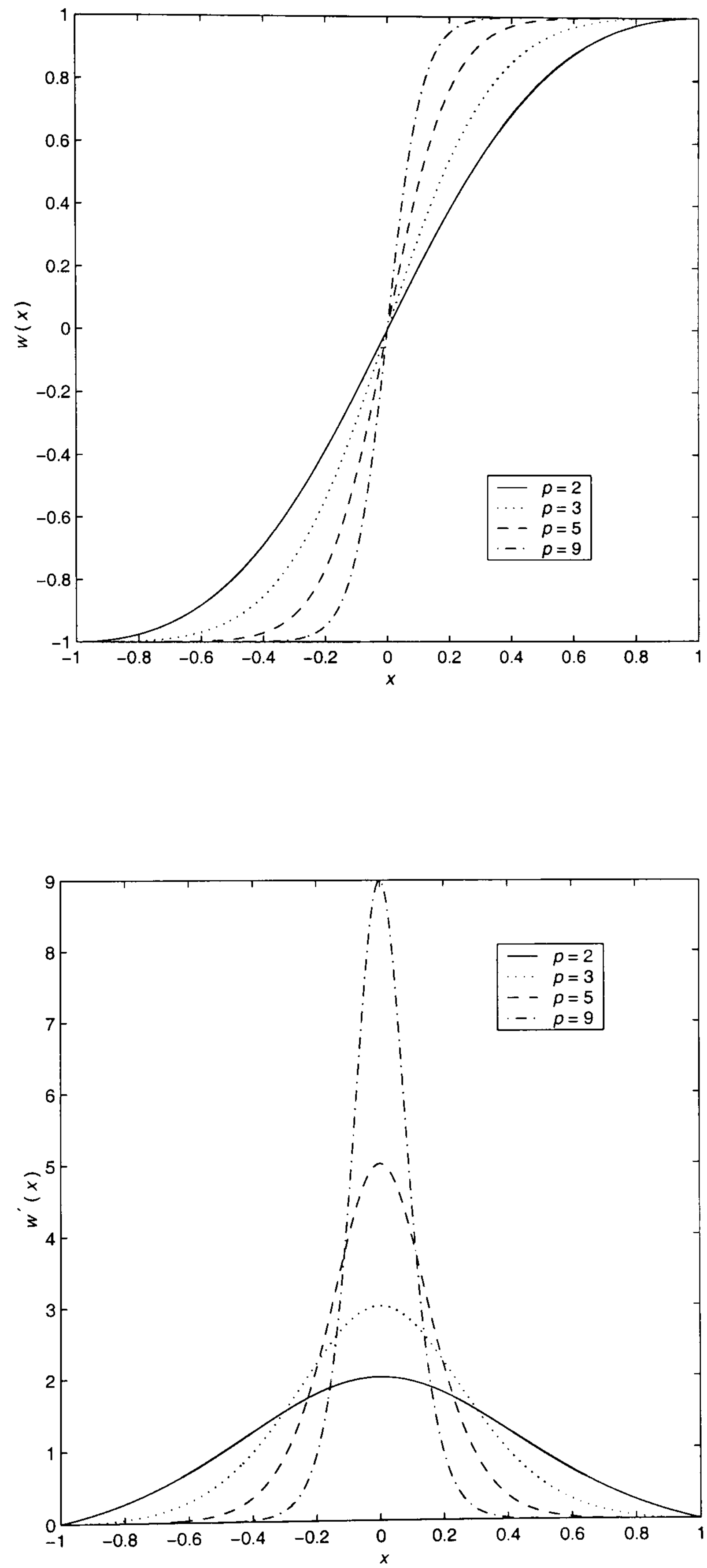


Figure 1.1: $w(x)$, $w'(x)$ vs. x, with w given by equations (1.31) and (1.32).

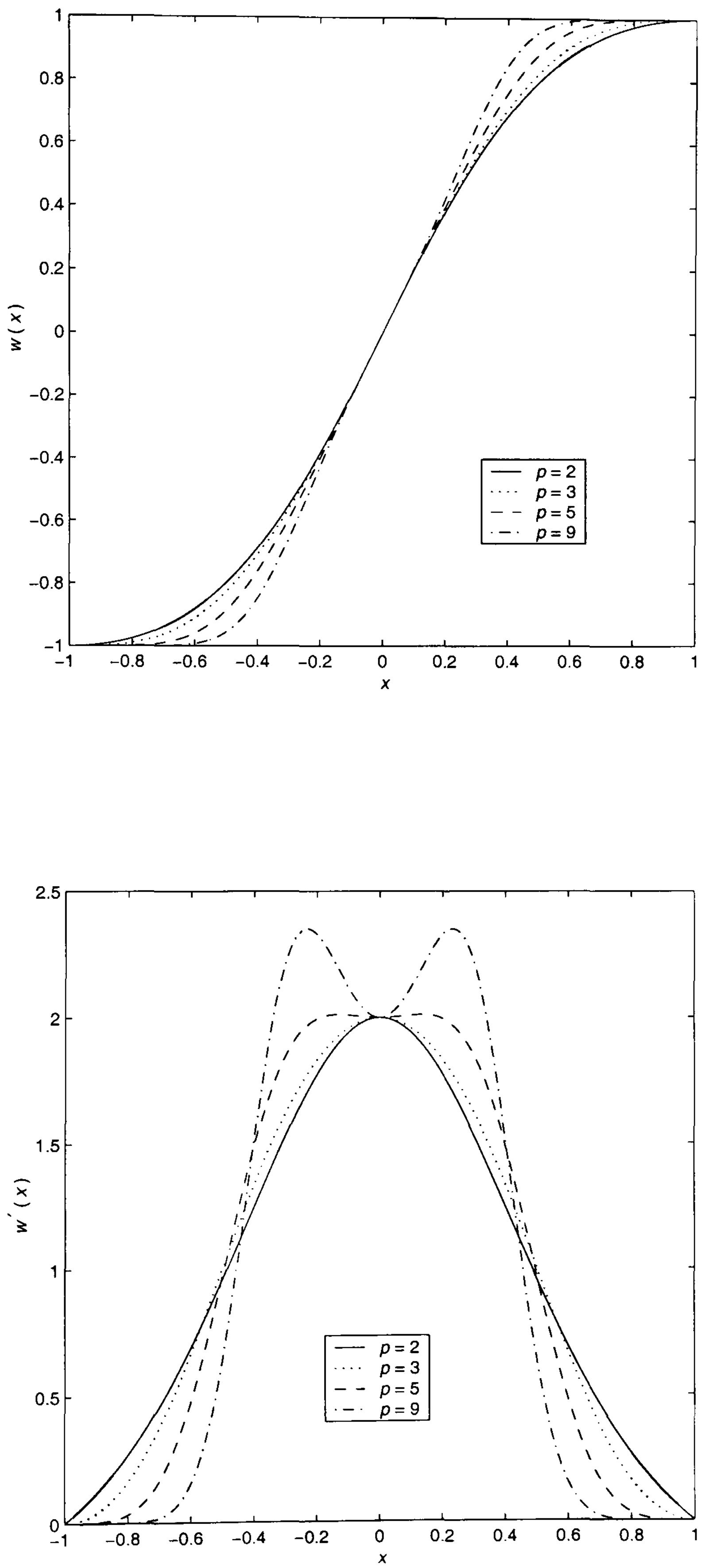


Figure 1.2: $w(x)$, $w'(x)$ vs. x, with w given by equations (1.31) and (1.33).

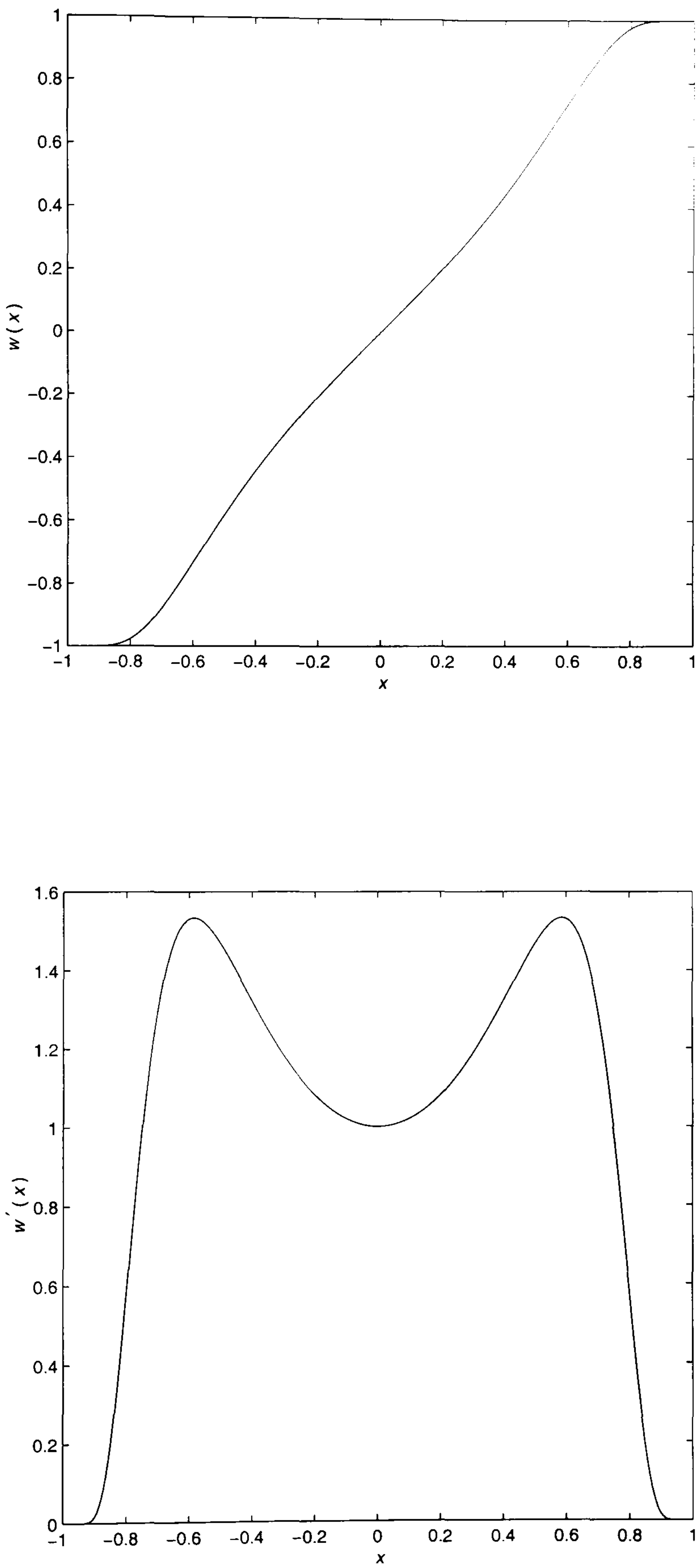


Figure 1.3: $w(x)$, $w'(x)$ vs. x, with w given by equations (1.31) and (1.34).

1.2 Error Analysis

Our error analysis will be based on an application of Corollary 1.1. Before applying Corollary 1.1, the following lemmas are needed to prove that the derivatives, up to a certain order, of $g(x) := w'(x)f(w(x))$ vanish at $x = \pm 1$. As usual, for $\phi \in \mathcal{C}[-1,1]$, we let $\|\phi\|_\infty := \max_{-1\le\zeta\le 1} |\phi(\zeta)|$ and, for $\phi \in \mathcal{C}(-1,1)$, let $\|\phi\|_1 := \int_{-1}^{+1} |\phi(t)|\, dt$, if the integral exists.

Throughout this section, we let $C, C' > 0$ denote generic constants, whose value depends at most on the values of q, α in $\mathcal{S}^{q,\alpha}$, p in Assumption 1.1, and on the choice of the function w.

Lemma 1.1 *If the conditions of Assumption 1.1 are satisfied, then*

$$C(1 \pm x)^p \le 1 \pm w(x) \le C'(1 \pm x)^p, \qquad -1 \le x \le 1$$

for some $0 < C < C'$ *dependent on the choice of function* w*, and* p *in Assumption 1.1.*

Proof. From Taylor's theorem and the assumptions on w, we obtain that, for $-1 \le x \le 1$,

$$1 + w(x) = \frac{w^{(p)}(\xi)(1+x)^p}{p!}$$

for some $\xi \in [-1, x]$. Thus

$$0 \le 1 + w(x) \le \frac{\left\|w^{(p)}\right\|_\infty (1+x)^p}{p!}, \qquad -1 \le x \le 1.$$

Further, since $w^{(p)}$ is continuous and $w^{(p)}(-1) \neq 0$, for some $\varepsilon > 0$,

$$\frac{|w^{(p)}(-1)|}{2} \le |w^{(p)}(x)|, \qquad -1 \le x \le -1 + \varepsilon.$$

Thus

$$C_1(1+x)^p \le 1 + w(x), \qquad -1 \le x \le -1 + \varepsilon,$$

where

$$C_1 := \frac{|w^{(p)}(-1)|}{2\,p!}.$$

It is also true that, for every $\varepsilon > 0$,

$$\frac{(1 + w(x))(1+x)^p}{2^p} \le 1 + w(x), \qquad -1 + \varepsilon < x \le 1.$$

Thus

$$C_2(1+x)^p \le 1 + w(x), \qquad -1+\varepsilon < x \le 1,$$

where

$$C_2 := 2^{-p} \min_{-1+\varepsilon<x\le 1} \{1 + w(x)\}.$$

So

$$C(1+x)^p \le 1 + w(x), \qquad -1 \le x \le 1,$$

with

$$C := \min\{C_1, C_2\}.$$

We argue in the same way for $1 - w(x)$, except that we use the fact that, for $-1 \le x \le 1$,

$$1 - w(x) = \frac{w^{(p)}(\xi)(1-x)^p}{p!}$$

for some $\xi \in [x, 1]$, that, for some $\varepsilon > 0$,

$$\frac{|w^{(p)}(1)|}{2} \le |w^{(p)}(x)|, \qquad 1-\varepsilon \le x \le 1,$$

and that, for every $\varepsilon > 0$,

$$\frac{\big(1 - w(x)\big)\big(1-x\big)^p}{2^p} \le 1 - w(x), \qquad -1 \le x \le 1 - \varepsilon.$$

■

Lemma 1.2 *If the conditions of Assumption 1.1 are satisfied, then for* $j = 1, 2, \ldots, p-1$,

$$|w^{(j)}(x)| \le C(1-x^2)^{p-j}, \qquad -1 \le x \le 1.$$

Proof. From Taylor's theorem, for $j = 1, 2, \ldots, p-1$ and $0 \le x < 1$ there exists $\xi \in (x, 1)$ such that

$$\begin{aligned} w^{(j)}(x) &= \sum_{n=j}^{p-1} \frac{w^{(n)}(1)(x-1)^{n-j}}{(n-j)!} + \frac{w^{(p)}(\xi)(x-1)^{p-j}}{(p-j)!} \\ &= \frac{w^{(p)}(\xi)(x-1)^{p-j}}{(p-j)!} \end{aligned}$$

by Assumption 1.1. Thus

$$|w^{(j)}(x)| \le \frac{\|w^{(p)}\|_\infty (1-x)^{p-j}}{(p-j)!}, \qquad 0 \le x \le 1$$

$$\le \|w^{(p)}\|_\infty (1-x)^{p-j}, \qquad 0 \le x \le 1.$$

It follows also that

$$|w^{(j)}(x)| = |w^{(j)}(-x)| \le C(1+x)^{p-j}, \qquad -1 \le x \le 0.$$

Thus, for $j = 1, 2, \ldots, p-1$,

$$|w^{(j)}(x)| \le C(1-x^2)^{p-j}, \qquad -1 \le x \le 1.$$

■

Lemma 1.3 *If $f \in \mathcal{S}^{q,\alpha}$ for some $\alpha > 0$ and $q \in \mathbb{N}$ and Assumption 1.1 holds then, for $j = 0, 1, \ldots, q$,*

$$|f^{(j)}(w(x))| \le C\|f\|_{q,\alpha}(1-x^2)^{(\alpha-1-j)p}, \qquad -1 < x < 1.$$

Proof. From (1.11),

$$|f^{(j)}(t)| \le \|f\|_{q,\alpha}(1-t^2)^{\alpha-1-j}, \qquad -1 < t < 1.$$

Since $w(x) \in (-1,1)$ for $x \in (-1,1)$, it follows using Lemma 1.1 that

$$|f^{(j)}(w(x))| \le \|f\|_{q,\alpha}\left[\left(1-w(x)\right)\left(1+w(x)\right)\right]^{\alpha-1-j}$$

$$\le \|f\|_{q,\alpha}[C(1-x)^p(1+x)^p]^{\alpha-1-j}$$

$$= C\|f\|_{q,\alpha}(1-x^2)^{(\alpha-1-j)p}.$$

■

The next few results are concerned with obtaining bounds for the derivatives of $g(x) := w'(x)f(w(x))$. For expressions for these derivatives we need the following.

For $r = 0, 1, \ldots, q$, and $j = 0, 1, \ldots, r$, let $u_j^r \in C^\infty[-1,1]$ be defined recursively by

$$u_0^0(x) = w'(x),$$

$$u_j^{r+1}(x) = \begin{cases} \dfrac{du_0^r(x)}{dx}, & \text{if } j = 0, \\ \dfrac{du_j^r(x)}{dx} + u_{j-1}^r(x)w'(x), & \text{if } j = 1, 2, \ldots, r, \\ u_r^r(x)w'(x), & \text{if } j = r+1. \end{cases}$$

Lemma 1.4 *If $f \in C^q(-1,1)$ and g is defined by (1.25) then $g \in C^q(-1,1)$ and. for $r = 0, 1, \ldots, q$,*

$$g^{(r)}(x) = \sum_{j=0}^{r} u_j^r(x) f^{(j)}(w(x)), \qquad -1 < x < 1.$$

Proof. For $r = 0$,

$$g^{(r)}(x) = g(x) = w'(x) f(w(x)) = u_0^0(x) f(w(x)).$$

If $r \in \{0, 1, \ldots, q-1\}$ and

$$g^{(r)}(x) = \sum_{j=0}^{r} u_j^r(x) f^{(j)}(w(x)), \qquad -1 < x < 1,$$

then

$$\begin{aligned} g^{(r+1)}(x) &= \sum_{j=0}^{r} \left[\frac{du_j^r(x)}{dx} f^{(j)}(w(x)) + u_j^r(x) w'(x) f^{(j+1)}(w(x)) \right] \\ &= \frac{du_0^r(x)}{dx} f(w(x)) + \sum_{j=1}^{r} \left[\frac{du_j^r(x)}{dx} + u_{j-1}^r(x) w'(x) \right] f^{(j)}(w(x)) \\ &\quad + u_r^r(x) w'(x) f^{(r+1)}(w(x)) \\ &= \sum_{j=0}^{r+1} u_j^{r+1}(x) f^{(j)}(w(x)). \end{aligned}$$

∎

Remark 1.2 *In the proof of the following lemma, we make use of the following elementary fact. If $F \in C^\infty[-1,1]$ and, for some $n \in \mathbb{Z}$,*

$$|F(x)| \le C(1-x^2)^n, \qquad -1 < x < 1,$$

then

$$|F'(x)| \le C'\left(1-x^2\right)^{n-1}, \qquad -1 < x < 1. \tag{1.35}$$

(This is clear from Taylor's theorem in the case $n > 1$. and in the case $n \le 1$ (1.35) holds automatically for all $F \in C^\infty[-1,1]$.)

Lemma 1.5 *If w satisfies Assumption 1.1 then, for $r = 0, 1, \ldots, q$, and $j = 0, 1, \ldots . r$.*

$$|u_j^r(x)| \le C(1-x^2)^{p-1+jp-r}, \qquad -1 < x < 1. \tag{1.36}$$

Proof. From Lemma 1.2

$$|u_0^0(x)| = |w'(x)| \le C(1-x^2)^{p-1}, \qquad -1 < x < 1, \tag{1.37}$$

so (1.36) holds for $r = 0$. If $r \in \{0, 1, \ldots, q\}$ and

$$|u_j^r(x)| \le C(1-x^2)^{p-1+jp-r}, \qquad j = 0, 1, \ldots, r, \qquad -1 < x < 1,$$

then

$$\left|u_0^{r+1}(x)\right| = \left|\frac{du_0^r(x)}{dx}\right| \le C(1-x^2)^{p-1-(r+1)},$$

and, for $j = 1, 2, \ldots, r$, using (1.37),

$$\begin{aligned} \left|u_j^{r+1}(x)\right| &\le \left|\frac{du_j^r(x)}{dx}\right| + \left|u_{j-1}^r(x)w'(x)\right| \\ &\le C(1-x^2)^{p-1+jp-(r+1)}, \end{aligned}$$

while

$$\begin{aligned} \left|u_{r+1}^{r+1}(x)\right| &= \left|u_r^r(x)w'(x)\right| \\ &\le C(1-x^2)^{p-1+(r+1)p-(r+1)}. \end{aligned}$$

Thus (1.36) holds with r replaced by $r+1$. By induction the result is established. ■

Lemma 1.6 *If $f \in S^{q,\alpha}$, for some $q \in \mathbb{N}$ and $\alpha > 0$, Assumption 1.1 holds, and g is defined by (1.25), then, for $r = 0, 1, \ldots, q$,*

$$|g^{(r)}(x)| \le C\|f\|_{q,\alpha}(1-x^2)^{\alpha p-1-r}, \qquad -1 < x < 1,$$

so that $g \in S^{q,\alpha p}$ with

$$\|g\|_{q,\alpha p} \le C\|f\|_{q,\alpha}.$$

Proof. From Lemma 1.3,

$$|f^{(j)}(w(x))| \le C\|f\|_{q,\alpha}(1-x^2)^{(\alpha-1-j)p},$$

and from Lemma 1.5,

$$\left|u_j^r(x)\right| \leq C(1-x^2)^{p-1+jp-r}.$$

Thus

$$\left|u_j^r(x)f^{(j)}(w(x))\right| \leq C\left\|f\right\|_{q,\alpha}(1-x^2)^{\alpha p-1-r}.$$

Using Lemma 1.4, we find that

$$|g^{(r)}(x)| \leq C\left\|f\right\|_{q,\alpha}(1-x^2)^{\alpha p-1-r},$$

and the result follows from (1.11). ■

The following theorem is the main result of this chapter, and will be used throughout the other chapters of this thesis.

Theorem 1.3 *Suppose that w satisfies Assumption 1.1, $f \in \mathcal{S}^{q,\alpha}$, for some $q \in \mathbb{N}$ and $\alpha > 0$, with $1 < \alpha p \leq q$. Then the error in the quadrature (1.26) can be bounded by*

$$|If - I_N f| \leq C\left\|f\right\|_{q,\alpha} N^{-\alpha p},$$

in the case $\alpha p \notin \mathbb{N}$, where the constant C depends only on q, α, and on the function w. If $\alpha p = q$, then

$$|If - I_N f| \leq c_\varepsilon C\left\|f\right\|_{q,\alpha} N^{\varepsilon - q}$$

for every $\varepsilon > 0$, where $c_\varepsilon > 0$ depends only on ε.

Proof. By Lemma 1.6, $g \in \mathcal{S}^{q,\alpha p}$, with $\|g\|_{q,\alpha p} \leq C\|f\|_{q,\alpha}$. Hence and by Theorem 1.2, if $\alpha p \notin \mathbb{N}$,

$$\begin{aligned} |If - I_N f| &\leq C\left\|g\right\|_{q,\alpha p} N^{-\alpha p} \\ &\leq C\left\|f\right\|_{q,\alpha} N^{-\alpha p}. \end{aligned}$$

In the case $\alpha p = q$, the result follows on noting Remark 1.1. ■

We finish this section with a comparison of this last theorem with results of previous authors. Theorem 1.3 is closest to Theorem 9.33 in Kress [33] who has considered the convergence of $I_N f$ under the same Assumption 1.1 on w, and with the same assumption that $f \in \mathcal{S}^{q,\alpha}$. Kress shows that

$$|If - I_N f| = O(N^{-q}) \text{ as } N \to \infty \tag{1.38}$$

in the case that q is an odd integer ≥ 3 with $q < \alpha p$. Sidi [46] also has a similar estimate. He makes a slightly stronger assumption than Assumption 1.1 on w, requiring additionally that $w'(x)$ has the asymptotic expansion

$$w'(x) \sim \sum_{j=0}^{\infty} \epsilon_j (1-x)^{p-1+2j} \quad \text{as} \quad x \to 1^-$$

with $\epsilon_0 > 0$. (The fact that w is odd implies a similar behaviour as $x \to -1^+$.) He restricts attention to two cases, that in which $f \in C^q[-1,1]$ for some sufficiently large q and that in which $f(x) = (1+x)^{\alpha-1}(1-x)^{\beta-1}g(x)$, where $\alpha > 0$, $\beta > 0$ are not integers and $g \in C^q[-1,1]$. In this latter case, he obtains that

$$|If - I_N f| = O(N^{-\omega}) \quad \text{as} \quad N \to \infty, \tag{1.39}$$

where

$$\omega = \min\{\,\alpha p, \beta p\,\},$$

provided q is sufficiently large.

The convergence rate predicted by Theorem 1.3 is greater than that predicted by (1.38), by as much as two for some values of αp (consider $\alpha p = 4.999$, for example, for which Kress predicts that (1.38) holds only for $q = 3$). The convergence rate predicted by (1.39) coincides with that predicted by Theorem 1.3, where they both apply, but Theorem 1.3 is a much more general result (for example the result of Sidi does not apply to $f(x) = \log(1-x^2)\sin x$, but Theorem 1.3 applies to this example since $f \in \mathcal{S}^{q,\alpha}$ for all $\alpha \in (0,1)$ and $q \in \mathbb{N}$).

1.3 Intervals Other Than $[-1, 1]$

The above sections consider the evaluation of $If = \int_{-1}^{+1} f(t)dt$ when $f \in \mathcal{S}^{q,\alpha}[-1,1]$. Clearly, by a simple linear transformation, we can apply the above method and analysis to evaluate, more generally,

$$\widetilde{I}f := \int_a^b f(t)\,dt,$$

where $f \in \mathcal{S}^{q,\alpha}[a,b]$. Precisely, if $f \in \mathcal{S}^{q,\alpha}[a,b]$ then

$$\begin{aligned}\widetilde{I}f &= \int_a^b f(t)\,dt \\ &= \int_{-1}^{+1} \widetilde{f}(x)\,dx = I\widetilde{f} \\ &\approx \widetilde{I}_N f := I_N\widetilde{f} = \sum_{k=1-N}^{N-1} a_k \widetilde{f}(x_k),\end{aligned} \tag{1.40}$$

where, for $k = 1-N, \ldots, N-1$,

$$a_k := \frac{1}{N} w'\left(\frac{k}{N}\right), \qquad x_k := w\left(\frac{k}{N}\right),$$

and

$$\widetilde{f}(x) := \left(\frac{b-a}{2}\right) f\left(\frac{(b-a)x+b+a}{2}\right).$$

Further, for $\widetilde{f} \in \mathcal{S}^{q,\alpha}[-1,1]$, it can be shown that

$$\|\widetilde{f}\|_{q,\alpha,[-1,1]} \le M \|f\|_{q,\alpha,[a,b]}, \tag{1.41}$$

where

$$M := \max\left\{ \left(\frac{b-a}{2}\right)^{2\alpha-1}, \left(\frac{b-a}{2}\right)^{2\alpha-1-q} \right\}.$$

Thus, applying Theorem 1.3, we obtain

Theorem 1.3′ *Suppose that w satisfies Assumption 1.1, $f \in \mathcal{S}^{q,\alpha}[a,b]$, for some $q \in \mathbb{N}$ and $\alpha > 0$, and $1 < \alpha p \le q$. Then the error in the quadrature (1.40) can be bounded by*

$$|\widetilde{I}f - \widetilde{I}_N f| \le CM \|f\|_{q,\alpha,[a,b]} N^{-\alpha p},$$

in the case $\alpha p \notin \mathbb{N}$, *where the constant* C *depends only on* q, α, *and on the function* w. *If* $\alpha p = q$, *then*

$$|\widetilde{I}f - \widetilde{I}_N f| \leq c_\varepsilon CM \|f\|_{q,\alpha,[a,b]} N^{\varepsilon - q}$$

for every $\varepsilon > 0$, *where* $c_\varepsilon > 0$ *depends only on* ε.

Proof. From $|\widetilde{I}f - \widetilde{I}_N f| = |I\widetilde{f} - I_N \widetilde{f}\,|$, the results follow from Theorem 1.3, and (1.41). ∎

1.4 Numerical Examples

Let

$$f(t) = (1-t^2)^{\alpha-1}\cos(nt) \tag{1.42}$$

for some $\alpha > 0$, and $n \geq 0$. As an example to illustrate the use of the quadrature rule (1.26), we will consider the problem of finding the numerical value of

$$If = \int_{-1}^{+1} f(t)\,dt, \tag{1.43}$$

for $n = 0, 4, 16$ and $\alpha = 0.5, 1.5$. Note that the exact value of the integral (1.43) is

$$If = \begin{cases} \dfrac{\sqrt{\pi}\,\Gamma(\alpha)}{\Gamma(\alpha+\frac{1}{2})}, & n = 0, \\[2ex] \dfrac{\sqrt{\pi}\,\Gamma(\alpha)}{(\frac{n}{2})^{\alpha-\frac{1}{2}}}\mathrm{J}_{\alpha-\frac{1}{2}}(n), & n > 0, \end{cases}$$

where J_ν denotes the Bessel function of the first kind of order ν. In particular, if $\alpha = 1/2$ then $If = \pi$ if $n = 0$, $\pi\mathrm{J}_0(n)$ if $n > 0$, and if $\alpha = 3/2$ then $If = \pi/2$ if $n = 0$, $\frac{\pi}{n}\mathrm{J}_1(n)$ if $n > 0$. For these values of n and α, the graphs of $f(x)$ against x are depicted in Figures 1.4 and 1.5. To see and appreciate the advantages of substituting the Kress form of the mapping function w, given by (1.31) and (1.33), into the integral If, we also depict the graphs of $g(x) = w'(x)f(w(x))$ against x for $\alpha = 0.5, 1.5$, $n = 4$ and, some values of p, in Figures 1.6 and 1.7, respectively. It can be observed qualitatively in these figures that the integrand $g(x)$ is smoother than $f(x)$, for the same choices of n and α, in particular near the endpoints ± 1, where this smoothness increases as p increases. Near ± 1, $g(x)$ is flatter as αp increases, in accordance with Lemma 1.6.

In the following results, the integral If is estimated by $I_N f$, the quadrature rule approximation (1.26), with $2N-1$ points. We note that, since f is even, and in view of the symmetry properties (1.28),

$$I_N f = a_0 f(x_0) + 2\sum_{k=1}^{N-1} a_k f(x_k), \tag{1.44}$$

where, for $k = 1, \ldots, N-1$,

$$a_k := \frac{1}{N}w'\left(\frac{k}{N}\right), \qquad x_k := w\left(\frac{k}{N}\right).$$

To enable comparison with the theoretical results of the error analysis, we will compute the Estimated Order of Convergence (EOC) for this quadrature rule, given by

$$\text{EOC} := \log_2\left(\frac{|If - I_N f|}{|If - I_{2N} f|}\right). \tag{1.45}$$

In this and all numerical examples in the thesis, we use the interactive programming system, *Matlab*, to carry out computations. We stop here to consider the effect of machine accuracy on our computations. From the quadrature rule approximation (1.44), we can see that the last abscissa

$$x_{N-1} = w\left(\frac{N-1}{N}\right) = w\left(1 - \frac{1}{N}\right).$$

In finite machine precision, this number will be indistinguishable from $w(1) = 1$ if N is large enough. Precisely, if w is calculated from (1.31), i.e., using

$$w(x) = \frac{V(x) - V(-x)}{V(x) + V(-x)}, \qquad -1 \le x \le 1,$$

then $w(x)$ will evaluate as 1 if $V(x) - V(-x)$ evaluates as the same number as $V(x) + V(-x)$. This will happen when $|V(-x)/V(x)| \le \varepsilon$, where ε is the smallest number such that $1 + \varepsilon$ is distinguishable from 1. Thus x_{N-1} will evaluate as 1 for $N \ge N_0$, where N_0 is the solution of

$$\frac{V\left(\frac{1-N_0}{N_0}\right)}{V\left(\frac{N_0-1}{N_0}\right)} = \varepsilon. \tag{1.46}$$

If $f(1)$ or $f(-1)$ are undefined, as is the case for f given by (1.42) for $\alpha < 1$, then, in finite machine arithmetic, $I_N f$ will be undefined for $N \ge N_0$. This can be fixed in part by redefining $f(\pm 1)$ to have the value zero or, equivalently, by replacing

$$I_N f := \sum_{k=1-N}^{N-1} a_k f(x_k) \tag{1.47}$$

by

$$I_N^{\square} f := \sum_{\substack{k=1-N \\ |\square x_k| < 1}}^{N-1} \square a_k f(\square x_k), \tag{1.48}$$

where $\square a_k$ and $\square x_k$ denote the machine values for a_k and x_k. However, by not placing any abscissae in the intervals $(-1, -1+\varepsilon)$ and $(1-\varepsilon, 1)$, it can be argued that the formula (1.48) ignores these parts of the integrals, making an error which may be estimated as

$$E_N^{\square} f = \int_{-1}^{-1+\varepsilon} f(t)\, dt + \int_{1-\varepsilon}^{+1} f(t)\, dt.$$

If $f \in \mathcal{S}^{q,\alpha}$ for some $\alpha > 0$ and $q \in \mathbb{N}$, this error is bounded by

$$\begin{aligned} \left|E_N^{\square} f\right| &\leq 2\|f\|_{q,\alpha} \int_{1-\varepsilon}^{+1} (1-t^2)^{\alpha-1} dt \\ &\approx 2^\alpha \|f\|_{q,\alpha} \int_0^\varepsilon u^{\alpha-1} du \\ &= \frac{2^\alpha \varepsilon^\alpha}{\alpha} \|f\|_{q,\alpha}. \end{aligned} \tag{1.49}$$

If $\alpha \geq 1$, this is of the same size as the machine precision but, if $0 < \alpha < 1$, ε^α can be appreciably bigger than ε. E.g. with f given by (1.42) with $n = 0$ and $\alpha = 0.5$,

$$E_N^{\square} f = 2 \int_{1-\varepsilon}^{+1} (1-t^2)^{-1/2} dt \approx 2^{3/2} \sqrt{\varepsilon}.$$

In our implementation of *Matlab*,

$$\varepsilon \approx 2.220 \times 10^{-16}, \tag{1.50}$$

so

$$E_N^{\square} f \approx 2^{3/2} \sqrt{\varepsilon} \approx 4.2 \times 10^{-8}. \tag{1.51}$$

We will see below that this is an approximate limit on the accuracy that can be obtained with (1.48) when $N \to \infty$.

From (1.46), we find that the analytic value of N_0 for equation (1.32) is

$$N_0 = \frac{1 + \varepsilon^{1/p}}{2\,\varepsilon^{1/p}} \approx \frac{1}{2\,\varepsilon^{1/p}}, \tag{1.52}$$

that the analytic value of N_0 for equation (1.33) is

$$\begin{aligned} N_0 &\approx \frac{(3p-4)(1+\varepsilon^{1/p}) + \sqrt{(3p-4)^2(1+\varepsilon^{1/p})^2 - 8p(3p-6)\varepsilon^{1/p}(1+\varepsilon^{1/p})}}{4\,p\,\varepsilon^{1/p}} \\ &\approx \frac{3p-4}{2\,p\,\varepsilon^{1/p}}, \end{aligned} \tag{1.53}$$

and that the analytic value of N_0 for equation (1.34) is

$$N_0 = \frac{1 - \ln\varepsilon - \sqrt{1 + \ln^2\varepsilon}}{2} \approx \frac{1 - 2\ln\varepsilon}{2}. \tag{1.54}$$

With ε given by (1.50), we tabulate values of N_0 obtained from equations (1.52), (1.53), and (1.54), in Table 1.11. Recall that for $N \geq N_0$, $I_N f$ is undefined if $f(\pm 1)$ is undefined.

In the tables of values of $I_N f$ and related errors we show below, whenever $I_N f$ evaluated as NaN (Not a Number), which we expect to occur for $N \geq N_0$, we replace the (unknown) value of $I_N f$ by that of $I_N^{\square} f$, given by (1.48), putting numerical values calculated using $I_N^{\square} f$ in brackets to distinguish them from values calculated using $I_N f$.

All numerical results in Tables 1.1–1.6 are evaluated using the mapping function w given by equations (1.31) and (1.33), suggested by Kress [33]. For comparison purposes, we also show results, in Tables 1.7–1.8, computed using the mapping function w given by equations (1.31) and (1.32), and results computed using the mapping function w given by equations (1.31) and (1.34), in Tables 1.9–1.10. Recall that we compute the error in estimating If with $I_N f$ given by (1.44). So we calculate and tabulate the EOC given by (1.45) in these tables. We also show at the top of each column the value of αp: recall that it has been shown in Theorem 1.3 that, as $N \to \infty$, $|If - I_N f| = O(N^{\varepsilon - \alpha p})$ for $\varepsilon = 0$ if $\alpha p \notin \mathbb{N}$, for every $\varepsilon > 0$ if $\alpha p \in \mathbb{N}$ with $\alpha p \geq 2$. To aid the comprehension of numerical results, we have put the smallest error for each value of N in a box.

We can see below that the characteristics of the error in estimating If with $I_N f$ depends on n, α, the range of p, and the mapping function w. So we will investigate these tables separately, pointing out interesting features as follows:

Tables 1.1, 1.2, and 1.3 ($\alpha = 0.5$, $n = 0, 4, 16$)

Considering these tables together, we can see that as p increases, the range of N for which the EOC stabilises at αp reduces.

For $p = 2(1)9$ [except $p = 6$], initially as N increases from $N = 2$, the EOC fluctuates and then it stabilises at αp. It is observed that the EOC fluctuates again when the error reaches about 10^{-8}. This 10^{-8} level is consistent with the prediction of (1.51). Using (1.48) for large values of N when (1.47) is undefined does not offer any improvement. We have no explanation as to why the results for $p = 6$ are much better in terms of faster than anticipated convergence rate and seemingly less effect of rounding errors, at least initially for $N \leq 256$. For $p = 6$ [$\alpha p = 3$], similarly, as N increases from $N = 2$, the EOC fluctuates and it stabilises at $\alpha p + 1$. Then it fluctuates again when the error reaches about 10^{-10}.

For $p = 10(5)25$, as N increases from $N = 2$, the EOC increases significantly and drops again when the error level 10^{-8} is approached. An asymptotic 10^{-8} error level as $N \to \infty$ is also observed for these values of p. However, an EOC of αp is never discernible:

we guess that rounding error effects intervene before this asymptotic convergence rate is achieved.

In Table 1.3 ($n = 16$), the errors are larger when N is smaller, reflecting the increased complexity of the integrand.

Tables 1.4, 1.5, and 1.6 ($\alpha = 1.5$, $n = 0, 4, 16$)

As predicted by (1.45), since $\alpha = 3/2 > 1$, there is no problem with rounding errors in this case. It is seen that results close to machine precision are obtained for all p.

For $p = 2$ [$\alpha p = 3$], again a larger than expected EOC of $\alpha p + 1$ is obtained.

For $p = 3(1)5$, stabilisation for a while at an EOC of αp is observed. As p increases, the range of N for which the EOC stabilises at αp reduces.

For $p = 6(1)10, 15(5)25$, an EOC of αp is never discernible, again, we imagine, because of the intervention of rounding error effects.

Tables 1.7 and 1.8 ($\alpha = 0.5, 1.5$, $n = 4$, w given by (1.31) and (1.32))

The calculations in these tables are identical with those in Tables 1.2 and 1.5 except that the function w is different, given by the simpler formulae (1.31) and (1.32). The more sophisticated function w of equations (1.31) and (1.33), proposed by Kress [33], achieves an approximately constant density of integration points around $x = 0$ as p increases. By contrast, (1.31) and (1.32) give a decreasing density of points around $x = 0$ as p increases, the points being redistributed towards ± 1. On the whole, the results in Tables 1.2 and 1.5 are better, at least for smaller values of N. In particular, in Tables 1.2 and 1.5, for $N = 2, 4, 8, 16, 32$, the minimum error achieved over all values of p is much better than in Tables 1.7 and 1.8, respectively, and for large values of N there is not much to choose between these tables.

Tables 1.9 and 1.10 ($\alpha = 0.5, 1.5$, $n = 4$, w given by (1.31) and (1.34))

We note that w given by equations (1.31) and (1.34) does not satisfy Assumption 1.1 since $w^{(p)}(\pm 1) = 0$ for all $p \in \mathbb{N}$. So Theorem 1.3 does not apply in this case, though, since $w^{(p)}(\pm 1) = 0$ for all $p \in \mathbb{N}$, we would expect that $|If - I_N f| = O(N^{-r})$ as $N \to \infty$ for all $r \in \mathbb{N}$. However, for $\alpha = 0.5$, we can see that the quadrature rule (1.26) with w given by (1.31) and (1.34) will encounter effects of rounding errors even for N not too large (from Table 1.11, for $N \geq 37$), suggesting that the quadrature rule (1.26) is overgraded, i.e., that its abscissae are too close to ± 1. Comparing Tables 1.9 and 1.10 with Tables 1.2 and 1.5, in which identical calculations are carried out except that w given by (1.31) and (1.33) is used, we see that w given by (1.31) and (1.34), which has all derivatives vanishing at ± 1, leads to much less accurate results than w given by (1.31) and (1.33) with $p = 6$, which has only derivatives up to order 5 vanishing at ± 1.

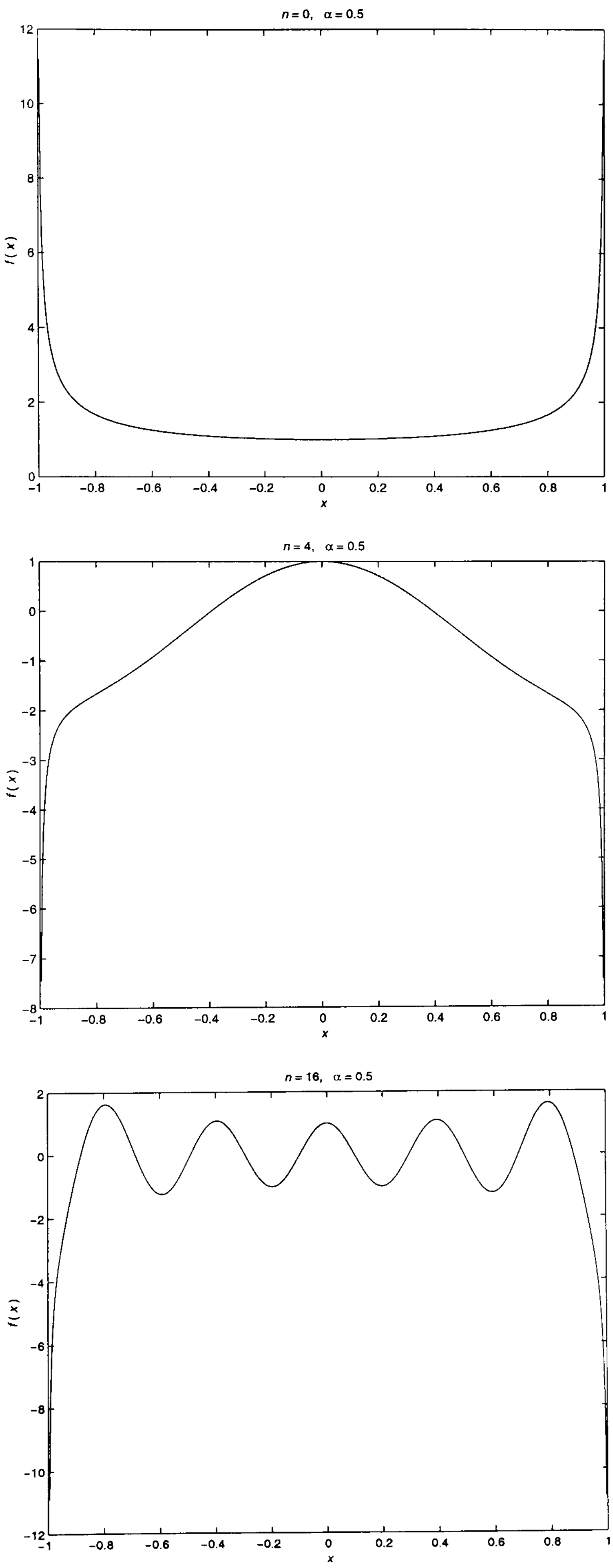


Figure 1.4: $f(x)$ vs. x, with f given by equation (1.42) for $n = 0, 4, 16$ and $\alpha = 0.5$.

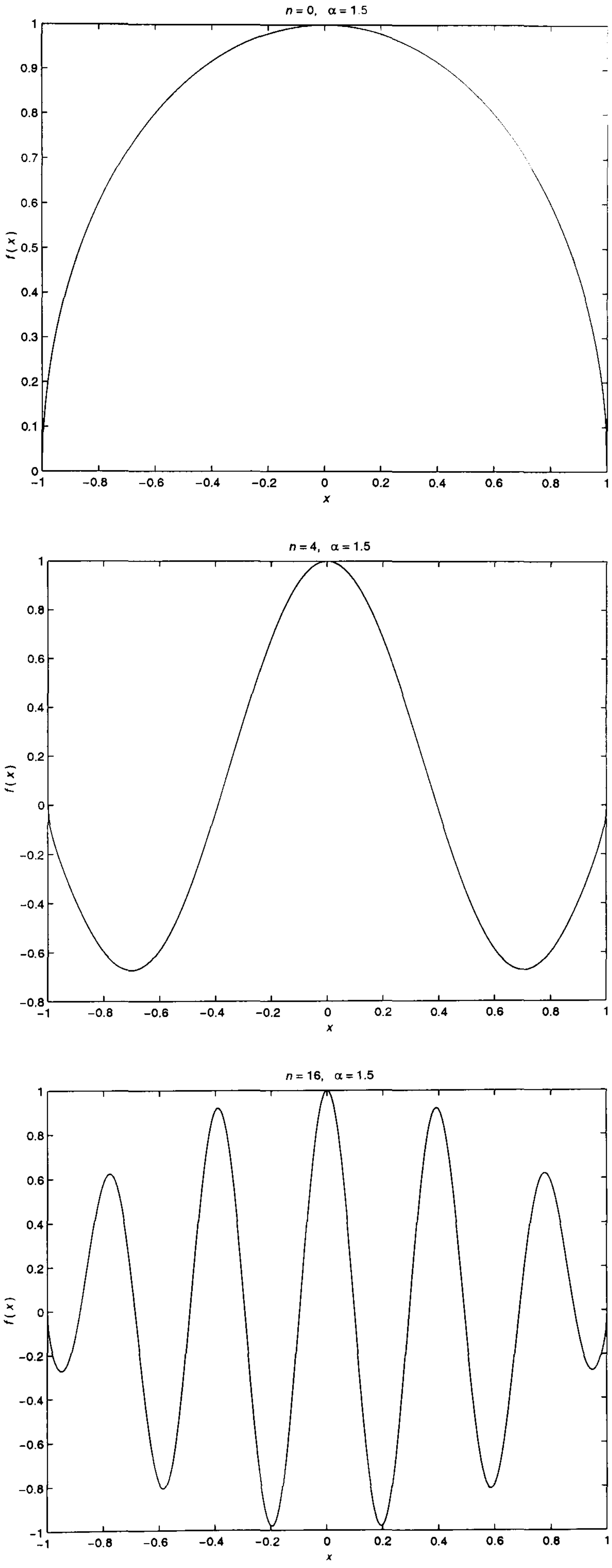


Figure 1.5: $f(x)$ vs. x, with f given by equation (1.42) for $n = 0, 4, 16$ and $\alpha = 1.5$.

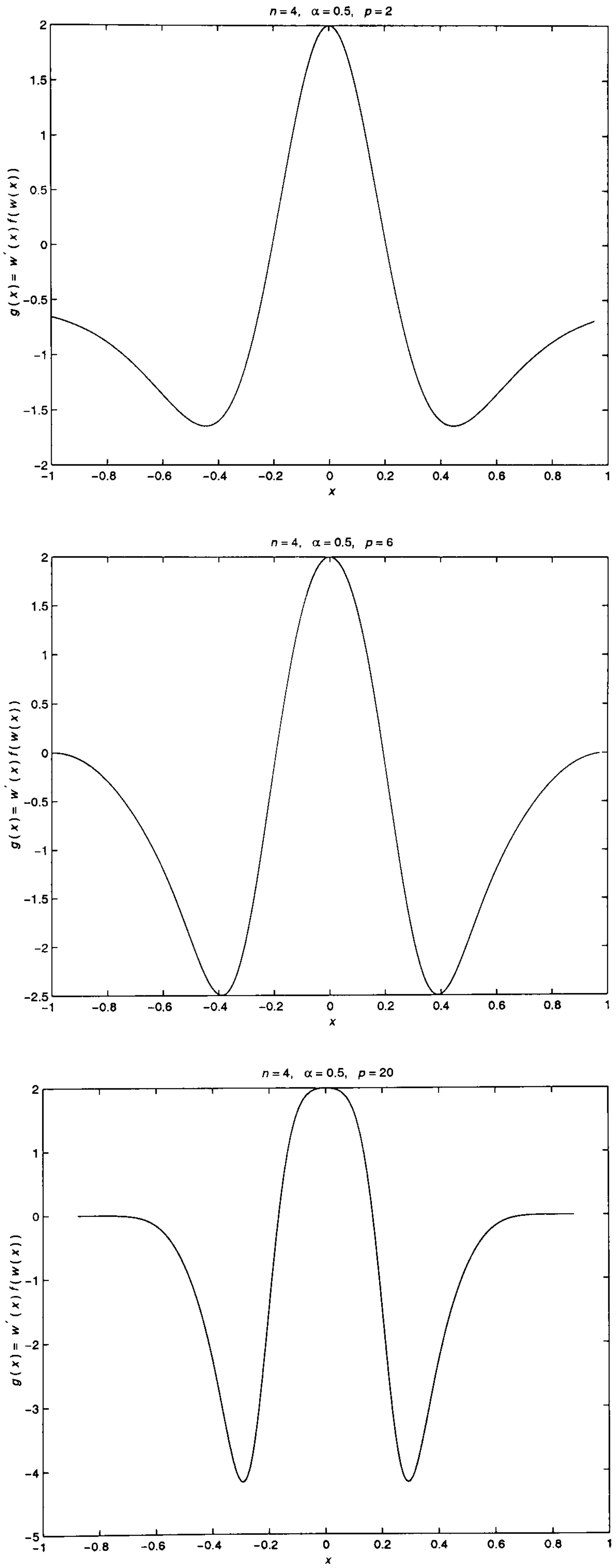


Figure 1.6: $g(x)$ vs. x, with f given by equation (1.42) for $n = 4$ and $\alpha = 0.5$.

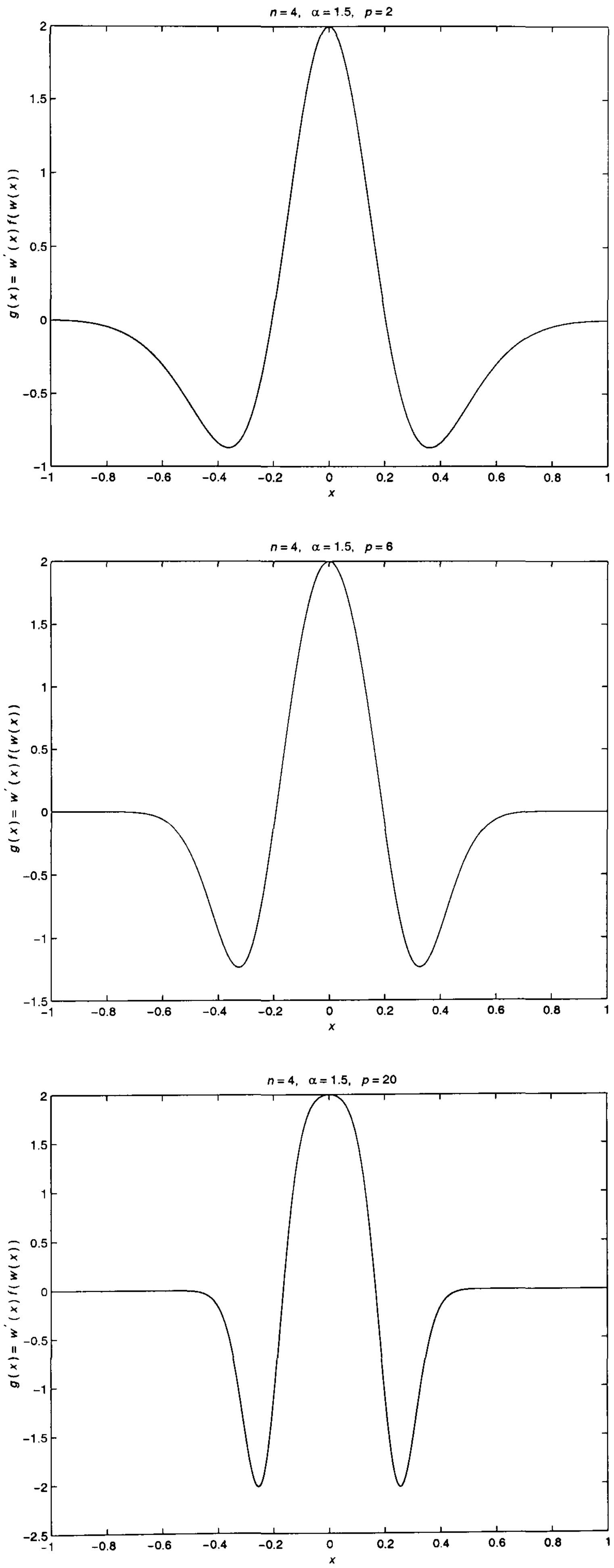


Figure 1.7: $g(x)$ vs. x, with f given by equation (1.42) for $n = 4$ and $\alpha = 1.5$.

Table 1.1: $n = 0$, $\alpha = 0.5$, $If = \pi$

	$p=2, \quad \alpha p=1.0$		$p=3, \quad \alpha p=1.5$		$p=4, \quad \alpha p=2.0$	
N	$\lvert If - I_N f\rvert$	EOC	$\lvert If - I_N f\rvert$	EOC	$\lvert If - I_N f\rvert$	EOC
2	5.4159E−01		3.4867E−01		1.6212E−01	
		1.0564		1.5286		1.9525
4	2.6042E−01		1.2086E−01		4.1886E−02	
		1.0291		1.5139		2.0056
8	1.2760E−01		4.2319E−02		1.0431E−02	
		1.0148		1.5067		2.0015
16	6.3151E−02		1.4893E−02		2.6051E−03	
		1.0075		1.5033		2.0004
32	3.1413E−02		5.2536E−03		6.5110E−04	
		1.0037		1.5016		2.0001
64	1.5666E−02		1.8553E−03		1.6276E−04	
		1.0019		1.5008		2.0000
128	7.8227E−03		6.5559E−04		4.0690E−05	
		1.0009		1.5004		2.0000
256	3.9088E−03		2.3172E−04		1.0173E−05	
		1.0005		1.5002		2.0000
512	1.9538E−03		8.1915E−05		2.5431E−06	
		1.0002		1.5001		2.0000
1024	9.7672E−04		2.8959E−05		6.3578E−07	
		1.0001		1.5000		2.0043
2048	4.8832E−04		1.0238E−05		1.5847E−07	

	$p=5, \quad \alpha p=2.5$		$p=6, \quad \alpha p=3.0$		$p=7, \quad \alpha p=3.5$	
N	$\lvert If - I_N f\rvert$	EOC	$\lvert If - I_N f\rvert$	EOC	$\lvert If - I_N f\rvert$	EOC
2	2.5374E−02		5.9704E−02		9.8951E−02	
		1.4419		6.1604		5.5761
4	9.3395E−03		8.3469E−04		2.0741E−03	
		2.4429		4.0888		3.5271
8	1.7177E−03		4.9054E−05		1.7992E−04	
		2.4722		4.0236		3.5757
16	3.0956E−04		3.0162E−06		1.5089E−05	
		2.4857		4.0058		3.5362
32	5.5269E−05		1.8775E−07		1.3007E−06	
		2.4927		3.9947		3.5252
64	9.8197E−06		1.1778E−08		1.1297E−07	
		2.4963		3.9701		3.0661
128	1.7403E−06		7.5154E−10		1.3490E−08	
		2.4987		−1.4235		
256	3.0793E−07		2.0159E−09		(1.0119E−07)	
		2.4941		−3.2021		(0.7316)
512	5.4658E−08		1.8552E−08		(6.0940E−08)	
		2.2821				(0.6098)
1024	1.1237E−08		(8.8040E−09)		(3.9932E−08)	
				(−1.6897)		(0.3394)
2048	(6.9460E−08)		(2.8401E−08)		(3.1562E−08)	

N	$p = 8, \quad \alpha p = 4.0$ $\lvert If - I_N f \rvert$	EOC	$p = 9, \quad \alpha p = 4.5$ $\lvert If - I_N f \rvert$	EOC	$p = 10, \quad \alpha p = 5.0$ $\lvert If - I_N f \rvert$	EOC
2	9.9871E−02		6.9896E−02		1.5783E−02	
4	5.5146E−04	7.5007	1.3449E−03	5.6997	2.9422E−03	2.4234
8	8.0160E−05	2.7823	1.7244E−05	6.2852	2.3903E−06	10.2655
16	4.9782E−06	4.0092	8.3994E−07	4.3597	4.0450E−08	5.8849
32	3.1080E−07	4.0016	3.9703E−08	4.4029	5.5812E−09	2.8575
64	2.3015E−08	3.7553	7.3444E−09	2.4345	(7.3843E−08)	
128	1.5627E−08	0.5586	(2.2580E−08)		(4.2402E−08)	(0.8003)
256	(1.8995E−08)		(5.1661E−08)	(−1.1940)	(3.5151E−08)	(0.2706)
512	(2.4354E−08)	(−0.3586)	(3.0075E−08)	(0.7805)	(3.7188E−08)	(−0.0813)
1024	(3.0648E−08)	(−0.3316)	(2.8339E−08)	(0.0858)	(3.1962E−08)	(0.2185)
2048	(3.3471E−08)	(−0.1271)	(3.2429E−08)	(−0.1945)	(3.5008E−08)	(−0.1313)

N	$p = 15, \quad \alpha p = 7.5$ $\lvert If - I_N f \rvert$	EOC	$p = 20, \quad \alpha p = 10.0$ $\lvert If - I_N f \rvert$	EOC	$p = 25, \quad \alpha p = 12.5$ $\lvert If - I_N f \rvert$	EOC
2	4.4122E−01		9.4406E−01		1.3486E+00	
4	7.9163E−03	5.8005	3.5939E−03	8.0372	2.3873E−02	5.8199
8	2.1257E−06	11.8626	4.5405E−05	6.3065	(7.6575E−05)	
16	7.7765E−08	4.7727	(4.3376E−09)		(1.2800E−08)	(12.5465)
32	(3.9542E−08)		(2.7525E−08)	(−2.6658)	(1.4489E−09)	(3.1431)
64	(3.1448E−08)	(0.3304)	(1.7446E−08)	(0.6579)	(1.8242E−08)	(−3.6542)
128	(3.3021E−08)	(−0.0704)	(3.0985E−08)	(−0.8287)	(3.6937E−08)	(−1.0178)
256	(4.1652E−08)	(−0.3350)	(3.5651E−08)	(−0.2024)	(3.8754E−08)	(−0.0693)
512	(4.2590E−08)	(−0.0321)	(3.4489E−08)	(0.0478)	(3.6389E−08)	(0.0909)
1024	(4.0766E−08)	(0.0632)	(2.9958E−08)	(0.2032)	(3.6575E−08)	(−0.0074)
2048	(4.2353E−08)	(−0.0551)	(3.1533E−08)	(−0.0739)	(3.4585E−08)	(0.0807)

Table 1.2: $n = 4$, $\alpha = 0.5$, $If = \pi \mathrm{J}_0(4) \approx -1.2477$

	$p = 2$, $\alpha p = 1.0$		$p = 3$, $\alpha p = 1.5$		$p = 4$, $\alpha p = 2.0$	
N	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC
2	6.5041E−01		4.8109E−01		3.5563E−01	
		1.9326		2.6100		3.6622
4	1.7038E−01		7.8801E−02		2.8092E−02	
		1.0307		1.5106		2.0426
8	8.3395E−02		2.7656E−02		6.8188E−03	
		1.0146		1.5064		2.0016
16	4.1278E−02		9.7345E−03		1.7028E−03	
		1.0074		1.5032		2.0004
32	2.0533E−02		3.4340E−03		4.2559E−04	
		1.0037		1.5016		2.0001
64	1.0240E−02		1.2127E−03		1.0639E−04	
		1.0019		1.5008		2.0000
128	5.1132E−03		4.2852E−04		2.6597E−05	
		1.0009		1.5004		2.0000
256	2.5550E−03		1.5146E−04		6.6492E−06	
		1.0005		1.5002		2.0000
512	1.2771E−03		5.3543E−05		1.6623E−06	
		1.0002		1.5001		2.0000
1024	6.3843E−04		1.8929E−05		4.1557E−07	
		1.0001		1.5000		2.0043
2048	3.1919E−04		6.6922E−06		1.0358E−07	

	$p = 5$, $\alpha p = 2.5$		$p = 6$, $\alpha p = 3.0$		$p = 7$, $\alpha p = 3.5$	
N	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC
2	3.0644E−01		3.1776E−01		3.6947E−01	
		4.9003		5.1495		4.9575
4	1.0262E−02		8.9527E−03		1.1891E−02	
		3.1923		8.1384		6.7344
8	1.1226E−03		3.1773E−05		1.1168E−04	
		2.4720		4.0104		3.5012
16	2.0234E−04		1.9715E−06		9.8630E−06	
		2.4857		4.0058		3.5362
32	3.6126E−05		1.2272E−07		8.5019E−07	
		2.4927		3.9947		3.5252
64	6.4186E−06		7.6985E−09		7.3845E−08	
		2.4963		3.9701		3.0661
128	1.1375E−06		4.9124E−10		8.8175E−09	
		2.4987		−1.4235		
256	2.0127E−07		1.3177E−09		(6.6143E−08)	
		2.4941		−3.2021		(0.7316)
512	3.5727E−08		1.2127E−08		(3.9833E−08)	
		2.2821				(0.6098)
1024	7.3452E−09		(5.7546E−09)		(2.6102E−08)	
				(−1.6897)		(0.3394)
2048	(4.5402E−08)		(1.8564E−08)		(2.0630E−08)	

N	$p=8,\quad \alpha p=4.0$		$p=9,\quad \alpha p=4.5$		$p=10,\quad \alpha p=5.0$	
	$\lvert If-I_Nf\rvert$	EOC	$\lvert If-I_Nf\rvert$	EOC	$\lvert If-I_Nf\rvert$	EOC
2	4.4534E−01		5.3413E−01		6.2866E−01	
		5.2613		6.8911		5.8995
4	1.1611E−02		4.5001E−03		1.0532E−02	
		8.9632		5.9360		5.8616
8	2.3264E−05		7.3505E−05		1.8113E−04	
		2.8378		7.0648		12.7461
16	3.2540E−06		5.4902E−07		2.6365E−08	
		4.0016		4.4029		2.8534
32	2.0315E−07		2.5952E−08		3.6481E−09	
		3.7553		2.4345		
64	1.5044E−08		4.8006E−09		(4.8267E−08)	
		0.5586				(0.8003)
128	1.0215E−08		(1.4760E−08)		(2.7716E−08)	
				(−1.1940)		(0.2706)
256	(1.2416E−08)		(3.3768E−08)		(2.2977E−08)	
		(−0.3586)		(0.7805)		(−0.0813)
512	(1.5919E−08)		(1.9658E−08)		(2.4308E−08)	
		(−0.3316)		(0.0858)		(0.2185)
1024	(2.0033E−08)		(1.8524E−08)		(2.0892E−08)	
		(−0.1271)		(−0.1945)		(−0.1313)
2048	(2.1878E−08)		(2.1197E−08)		(2.2883E−08)	

N	$p=15,\quad \alpha p=7.5$		$p=20,\quad \alpha p=10.0$		$p=25,\quad \alpha p=12.5$	
	$\lvert If-I_Nf\rvert$	EOC	$\lvert If-I_Nf\rvert$	EOC	$\lvert If-I_Nf\rvert$	EOC
2	1.0862E+00		1.4547E+00		1.7274E+00	
		2.6073		1.8239		1.4366
4	1.7826E−01		4.1090E−01		6.3816E−01	
		9.8468		6.3414		
8	1.9358E−04		5.0674E−03		(1.6034E−02)	
		11.5683				(13.0059)
16	6.3747E−08		(5.4460E−08)		(1.9493E−06)	
				(1.5979)		(11.0072)
32	(2.5847E−08)		(1.7992E−08)		(9.4709E−10)	
		(0.3304)		(0.6579)		(−3.6542)
64	(2.0556E−08)		(1.1403E−08)		(1.1924E−08)	
		(−0.0704)		(−0.8287)		(−1.0178)
128	(2.1584E−08)		(2.0253E−08)		(2.4143E−08)	
		(−0.3350)		(−0.2024)		(−0.0693)
256	(2.7226E−08)		(2.3303E−08)		(2.5331E−08)	
		(−0.0321)		(0.0478)		(0.0909)
512	(2.7839E−08)		(2.2543E−08)		(2.3785E−08)	
		(0.0632)		(0.2032)		(−0.0074)
1024	(2.6646E−08)		(1.9582E−08)		(2.3907E−08)	
		(−0.0551)		(−0.0739)		(0.0807)
2048	(2.7684E−08)		(2.0611E−08)		(2.2606E−08)	

Table 1.3: $n = 16$, $\alpha = 0.5$, $If = \pi J_0(16) \approx -5.4946 \times 10^{-1}$

	$p=2, \quad \alpha p = 1.0$		$p=3, \quad \alpha p = 1.5$		$p=4, \quad \alpha p = 2.0$	
N	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC
2	3.1060E+00		2.9364E+00		2.2792E+00	
		1.0251		1.1683		1.3394
4	1.5262E+00		1.3065E+00		9.0066E−01	
		3.5972		4.9882		6.9320
8	1.2611E−01		4.1165E−02		7.3763E−03	
		1.0602		1.5292		1.5640
16	6.0476E−02		1.4262E−02		2.4948E−03	
		1.0074		1.5032		2.0004
32	3.0083E−02		5.0311E−03		6.2353E−04	
		1.0037		1.5016		2.0001
64	1.5002E−02		1.7768E−03		1.5587E−04	
		1.0019		1.5008		2.0000
128	7.4915E−03		6.2783E−04		3.8967E−05	
		1.0009		1.5004		2.0000
256	3.7433E−03		2.2191E−04		9.7418E−06	
		1.0005		1.5002		2.0000
512	1.8710E−03		7.8446E−05		2.4354E−06	
		1.0002		1.5001		2.0000
1024	9.3537E−04		2.7733E−05		6.0886E−07	
		1.0001		1.5000		2.0043
2048	4.6765E−04		9.8048E−06		1.5176E−07	

	$p=5, \quad \alpha p = 2.5$		$p=6, \quad \alpha p = 3.0$		$p=7, \quad \alpha p = 3.5$	
N	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC
2	1.4073E+00		6.1903E−01		4.5558E−02	
		1.8931		2.2375		−3.6235
4	3.7888E−01		1.3127E−01		5.6152E−01	
		6.9528		3.4441		3.8647
8	3.0584E−03		1.2061E−02		3.8546E−02	
		3.3669		12.0297		11.3980
16	2.9645E−04		2.8845E−06		1.4284E−05	
		2.4857		4.0038		3.5195
32	5.2929E−05		1.7980E−07		1.2456E−06	
		2.4927		3.9947		3.5252
64	9.4039E−06		1.1279E−08		1.0819E−07	
		2.4963		3.9701		3.0660
128	1.6666E−06		7.1972E−10		1.2919E−08	
		2.4987		−1.4235		
256	2.9489E−07		1.9306E−09		(9.6907E−08)	
		2.4941		−3.2021		(0.7316)
512	5.2344E−08		1.7767E−08		(5.8360E−08)	
		2.2821				(0.6098)
1024	1.0761E−08		(8.4312E−09)		(3.8242E−08)	
				(−1.6897)		(0.3394)
2048	(6.6519E−08)		(2.7198E−08)		(3.0226E−08)	

N	$p=8,\quad \alpha p=4.0$ $\lvert If-I_Nf\rvert$	EOC	$p=9,\quad \alpha p=4.5$ $\lvert If-I_Nf\rvert$	EOC	$p=10,\quad \alpha p=5.0$ $\lvert If-I_Nf\rvert$	EOC
2	3.0680E−01		4.8377E−01		5.3900E−01	
		−1.5507		−1.2540		−1.3150
4	8.9878E−01		1.1538E+00		1.3410E+00	
		3.2148		2.5892		2.0754
8	9.6807E−02		1.9173E−01		3.1819E−01	
		14.8644		15.1164		14.5810
16	3.2455E−06		5.3975E−06		1.2982E−05	
		3.4468		7.1493		11.2461
32	2.9764E−07		3.8022E−08		5.3449E−09	
		3.7553		2.4345		(−3.7258)
64	2.2041E−08		7.0335E−09		(7.0716E−08)	
		0.5586				(0.8003)
128	1.4965E−08		(2.1624E−08)		(4.0607E−08)	
				(−1.1940)		(0.2706)
256	(1.8190E−08)		(4.9473E−08)		(3.3663E−08)	
		(−0.3586)		(0.7805)		(−0.0813)
512	(2.3323E−08)		(2.8802E−08)		(3.5614E−08)	
		(−0.3316)		(0.0858)		(0.2185)
1024	(2.9351E−08)		(2.7139E−08)		(3.0608E−08)	
		(−0.1271)		(−0.1945)		(−0.1313)
2048	(3.2054E−08)		(3.1056E−08)		(3.3525E−08)	

N	$p=15,\quad \alpha p=7.5$ $\lvert If-I_Nf\rvert$	EOC	$p=20,\quad \alpha p=10.0$ $\lvert If-I_Nf\rvert$	EOC	$p=25,\quad \alpha p=12.5$ $\lvert If-I_Nf\rvert$	EOC
2	1.3571E−01		3.8819E−01		7.8713E−01	
		−3.4723		−0.5684		−0.3301
4	1.5061E+00		5.7563E−01		9.8951E−01	
		0.6461		−0.5842		
8	9.6240E−01		8.6299E−01		(1.0224E−01)	
		10.1813				(2.4613)
16	8.2884E−04		(1.5721E−04)		(1.8566E−02)	
				(12.5519)		(21.0464)
32	(3.7870E−08)		(2.6181E−08)		(8.5729E−09)	
		(0.3305)		(0.6480)		(−1.0270)
64	(3.0116E−08)		(1.6707E−08)		(1.7469E−08)	
		(−0.0704)		(−0.8287)		(−1.0178)
128	(3.1623E−08)		(2.9673E−08)		(3.5373E−08)	
		(−0.3350)		(−0.2024)		(−0.0693)
256	(3.9889E−08)		(3.4142E−08)		(3.7113E−08)	
		(−0.0321)		(0.0478)		(0.0909)
512	(4.0787E−08)		(3.3028E−08)		(3.4848E−08)	
		(0.0632)		(0.2032)		(−0.0074)
1024	(3.9040E−08)		(2.8689E−08)		(3.5026E−08)	
		(−0.0551)		(−0.0739)		(0.0807)
2048	(4.0560E−08)		(3.0198E−08)		(3.3120E−08)	

Table 1.4: $n = 0$, $\alpha = 1.5$, $If = \pi/2$

N	$p=2,\ \alpha p=3.0$: $\lvert If - I_N f\rvert$	EOC	$p=3,\ \alpha p=4.5$: $\lvert If - I_N f\rvert$	EOC	$p=4,\ \alpha p=6.0$: $\lvert If - I_N f\rvert$	EOC
2	5.2037E−03		7.9525E−03		5.5261E−02	
		5.3283		6.8776		9.0321
4	1.2952E−04		6.7629E−05		1.0556E−04	
		3.9939		4.2374		7.7530
8	8.1295E−06		3.5856E−06		4.8932E−07	
		3.9988		4.4075		6.0103
16	5.0850E−07		1.6895E−07		7.5911E−09	
		3.9997		4.4576		6.0031
32	3.1787E−08		7.6895E−09		1.1835E−10	
		3.9999		4.4794		6.0008
64	1.9868E−09		3.4472E−10		1.8483E−12	
		4.0000		4.4898		6.0007
128	1.2418E−10		1.5343E−11		2.8866E−14	
		3.9999		4.4956		4.4374
256	7.7616E−12		6.8012E−13		1.3323E−15	
		4.0031		4.5584		1.0000
512	4.8406E−13		2.8866E−14		6.6613E−16	
		3.8807		5.0224		−0.7370
1024	3.2863E−14		8.8818E−16		1.1102E−15	
		4.6245		−2.0000		−0.8480
2048	1.3323E−15		3.5527E−15		1.9984E−15	
N	$p=5,\ \alpha p=7.5$: $\lvert If - I_N f\rvert$	EOC	$p=6,\ \alpha p=9.0$: $\lvert If - I_N f\rvert$	EOC	$p=7,\ \alpha p=10.5$: $\lvert If - I_N f\rvert$	EOC
2	1.2246E−01		1.9579E−01		2.6628E−01	
		7.8849		7.3457		8.0077
4	5.1811E−04		1.2037E−03		1.0346E−03	
		13.2541		15.0568		11.8127
8	5.3034E−08		3.5316E−08		2.8761E−07	
		7.7402		13.0131		19.6115
16	2.4803E−10		4.2719E−12		3.5905E−13	
		7.6211		10.0618		8.6591
32	1.2599E−12		3.9968E−15		8.8818E−16	
		7.4702		3.1699		–
64	7.1054E−15		4.4409E−16		0	
		–		−2.1699		–
128	0		1.9984E−15		2.2204E−16	
		–				−3.0000
256	4.4409E−16		0		1.7764E−15	
		−0.5850				0.6781
512	6.6613E−16		1.7764E−15		1.1102E−15	
		−1.8745		1.0000		−0.8480
1024	2.4425E−15		8.8818E−16		1.9984E−15	
		−0.4475		−0.8074		−1.3536
2048	3.3307E−15		1.5543E−015		5.1070E−15	

N	$p = 8,\quad \alpha p = 12.0$ $\lvert If - I_N f\rvert$	EOC	$p = 9,\quad \alpha p = 13.5$ $\lvert If - I_N f\rvert$	EOC	$p = 10,\quad \alpha p = 15.0$ $\lvert If - I_N f\rvert$	EOC
2	3.2915E−01		3.8250E−01		4.2621E−01	
		8.2749		6.1026		5.1039
4	1.0627E−03		5.5664E−03		1.2393E−02	
		10.8531		13.3272		11.0877
8	5.7450E−07		5.4160E−07		5.6945E−06	
		22.9559		24.3011		24.4526
16	7.0610E−14		2.6201E−14		2.4802E−13	
		8.3129		5.8826		9.1254
32	2.2204E−16		4.4409E−16		4.4409E−16	
		0		1.0000		–
64	2.2204E−16		2.2204E−16		0	
		–		–		–
128	0		2.2204E−16		0	
		–		–		–
256	6.6613E−16		0		6.6613E−16	
		−0.7370		2.5850		–
512	1.1102E−15		2.2204E−16		0	
		–		−3.0000		–
1024	0		1.7764E−15		4.4409E−16	
		–		−0.9069		−3.0000
2048	1.3323E−15		3.3307E−15		3.5527E−15	

N	$p = 15,\quad \alpha p = 22.5$ $\lvert If - I_N f\rvert$	EOC	$p = 20,\quad \alpha p = 30.0$ $\lvert If - I_N f\rvert$	EOC	$p = 25,\quad \alpha p = 37.5$ $\lvert If - I_N f\rvert$	EOC
2	5.3734E−01		5.6402E−01		5.6951E−02	
		3.0920		2.5065		2.5216
4	6.3016E−02		9.9261E−02		9.9183E−04	
		9.8921		7.7463		5.8172
8	6.6316E−05		4.6228E−04		1.7591E−07	
		18.5824		16.9398		16.9778
16	1.6895E−10		3.6772E−09		1.3629E−09	
		19.5373		22.9812		–
32	2.2204E−16		4.4409E−16		0	
		−1.0000		1.0000		–
64	4.4409E−16		2.2204E−16		2.2204E−16	
		−0.5850		−1.0000		−1.5850
128	6.6613E−16		4.4409E−16		6.6613E−16	
		0.5850		−0.5850		–
256	4.4409E−16		6.6613E−16		0	
		−1.8074		0.5850		–
512	1.5543E−15		4.4409E−16		2.2204E−16	
		0.8074		−2.1699		−2.5850
1024	8.8818E−16		1.9984E−15		1.3323E−15	
		−2.3923		−0.2895		0.5850
2048	4.6629E−15		2.4425E−15		8.8818E−16	

Table 1.5: $n = 4$, $\alpha = 1.5$, $If = \frac{\pi}{4}\mathrm{J}_1(4) \approx -5.1870 \times 10^{-2}$

	$p = 2, \quad \alpha p = 3.0$		$p = 3, \quad \alpha p = 4.5$		$p = 4, \quad \alpha p = 6.0$	
N	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC
2	4.7685E−01		4.9729E−01		5.5910E−01	
		8.5017		10.2763		7.9099
4	1.3156E−03		4.0100E−04		2.3247E−03	
		7.9897		7.4051		12.7413
8	5.1761E−06		2.3658E−06		3.3950E−07	
		3.9703		4.4197		6.0960
16	3.3023E−07		1.1054E−07		4.9632E−09	
		3.9927		4.4588		6.0035
32	2.0744E−08		5.0268E−09		7.7362E−11	
		3.9982		4.4796		6.0010
64	1.2981E−09		2.2533E−10		1.2079E−12	
		3.9995		4.4898		5.9842
128	8.1159E−11		1.0029E−11		1.9082E−14	
		3.9999		4.4949		11.4252
256	5.0729E−12		4.4478E−13		6.9389E−18	
		3.9989		4.4657		−2.5850
512	3.1730E−13		2.0130E−14		4.1633E−17	
		3.9859		4.6320		−2.3219
1024	2.0026E−14		8.1185E−16		2.0817E−16	
		3.9024		1.1424		−0.9511
2048	1.3392E−15		3.6776E−16		4.0246E−16	

	$p = 5, \quad \alpha p = 7.5$		$p = 6, \quad \alpha p = 9.0$		$p = 7, \quad \alpha p = 10.5$	
N	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC
2	6.4061E−01		7.2310E−01		7.9660E−01	
		6.6882		5.5982		4.7156
4	6.2120E−03		1.4926E−02		3.0318E−02	
		13.3336		11.1520		9.9873
8	6.0174E−07		6.5595E−06		2.9871E−05	
		11.8578		21.1480		25.1863
16	1.6213E−10		2.8229E−12		7.8236E−13	
		7.6210		10.1342		12.4608
32	8.2362E−13		2.5119E−15		1.3878E−16	
		7.5350		6.4998		0.7370
64	4.4409E−15		2.7756E−17		8.3267E−17	
		4.7370		−0.5850		−1.4150
128	1.6653E−16		4.1633E−17		2.2204E−16	
		0.1926		−1.1155		0.6781
256	1.4572E−16		9.0206E−17		1.3878E−16	
		−0.8171		−1.6919		0.2345
512	2.5674E−16		2.9143E−16		1.1796E−16	
		3.6245		−0.4406		−0.9125
1024	2.0817E−17		3.9552E−16		2.2204E−16	
		−3.7370		1.8329		−0.7004
2048	2.7756E−16		1.1102E−16		3.6082E−16	

N	$p = 8, \quad \alpha p = 12.0$		$p = 9, \quad \alpha p = 13.5$		$p = 10, \quad \alpha p = 15.0$	
	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC
2	8.5757E−01		9.0597E−01		9.4336E−01	
		4.0262		3.4834		3.0481
4	5.2635E−02		8.1005E−02		1.1405E−01	
		9.3849		9.2201		9.5821
8	7.8727E−05		1.3583E−04		1.4880E−04	
		24.1591		20.7433		18.7256
16	4.2025E−12		7.7382E−11		3.4328E−10	
		15.4008		18.7103		21.1007
32	9.7145E−17		1.8041E−16		1.5266E−16	
		−1.6521		−0.6215		−0.9329
64	3.0531E−16		2.7756E−16		2.9143E−16	
		1.8745		0.8625		3.3923
128	8.3267E−17		1.5266E−16		2.7756E−17	
		−1.5443		−1.5178		−2.4594
256	2.4286E−16		4.3715E−16		1.5266E−16	
		−0.6781		1.4537		−0.1844
512	3.8858E−16		1.5959E−16		1.7347E−16	
		0.5594		1.0641		3.0589
1024	2.6368E−16		7.6328E−17		2.0817E−17	
		−0.3959		−2.0000		−3.8745
2048	3.4694E−16		3.0531E−16		3.0531E−16	

N	$p = 15, \quad \alpha p = 22.5$		$p = 20, \quad \alpha p = 30.0$		$p = 25, \quad \alpha p = 37.5$	
	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC
2	1.0290E+00		1.0474E+00		1.0510E+00	
		1.7632		1.1910		0.9499
4	3.0313E−01		4.5876E−01		5.4410E−01	
		6.7295		5.4159		5.2848
8	2.8566E−03		1.0746E−02		1.3957E−02	
		15.7100		13.8778		11.8507
16	5.3291E−08		7.1383E−07		3.7791E−06	
		28.5165		32.5821		27.4195
32	1.3878E−16		1.1102E−16		2.1053E−14	
		−0.1375		−0.5850		3.9971
64	1.5266E−16		1.6653E−16		1.3184E−15	
		0.6521		0.2630		4.2479
128	9.7145E−17		1.3878E−16		6.9389E−17	
		3.8074		0.6215		−0.4854
256	6.9389E−18		9.0206E−17		9.7145E−17	
		−5.6724		−0.8845		−1.3219
512	3.5388E−16		1.6653E−16		2.4286E−16	
		2.6724		0.6781		2.5443
1024	5.5511E−17		1.0408E−16		4.1633E−17	
		−1.3923		−1.3785		−3.3458
2048	1.4572E−16		2.7062E−16		4.2327E−16	

Table 1.6: $n = 16$, $\alpha = 1.5$, $If = \frac{\pi}{16} J_1(16) \approx 1.7749 \times 10^{-2}$

N	$p=2$, $\alpha p = 3.0$ $\|If - I_N f\|$	EOC	$p=3$, $\alpha p = 4.5$ $\|If - I_N f\|$	EOC	$p=4$, $\alpha p = 6.0$ $\|If - I_N f\|$	EOC
2	1.5426E+00		1.4176E+00		1.1723E+00	
		0.7010		0.7789		0.9795
4	9.4893E−01		8.2622E−01		5.9452E−01	
		7.1107		8.6674		6.8160
8	6.8660E−03		2.0321E−03		5.2764E−03	
		13.7937		13.6150		19.4680
16	4.8349E−07		1.6197E−07		7.2758E−09	
		3.9918		4.4589		6.0043
32	3.0389E−08		7.3648E−09		1.1334E−10	
		3.9981		4.4796		6.0007
64	1.9019E−09		3.3013E−10		1.7702E−12	
		3.9995		4.4899		5.9818
128	1.1891E−10		1.4693E−11		2.8009E−14	
		3.9999		4.4954		5.1085
256	7.4320E−12		6.5140E−13		8.1185E−16	
		4.0006		4.5148		0.8931
512	4.6432E−13		2.8495E−14		4.3715E−16	
		4.0183		4.8489		0.9773
1024	2.8654E−14		9.8879E−16		2.2204E−16	
		4.2109		2.1325		−0.7549
2048	1.5474E−15		2.2551E−16		3.7470E−16	

N	$p=5$, $\alpha p = 7.5$ $\|If - I_N f\|$	EOC	$p=6$, $\alpha p = 9.0$ $\|If - I_N f\|$	EOC	$p=7$, $\alpha p = 10.5$ $\|If - I_N f\|$	EOC
2	9.5213E−01		8.2375E−01		7.7785E−01	
		1.4709		2.7512		3.6545
4	3.4349E−01		1.2235E−01		6.1771E−02	
		4.3161		1.5423		−0.5023
8	1.7245E−02		4.2007E−02		8.7496E−02	
		24.8646		20.2882		17.7249
16	5.6451E−10		3.2807E−08		4.0389E−07	
		8.8705		22.8509		30.3010
32	1.2064E−12		4.3368E−15		3.0531E−16	
		7.6242		3.6012		0.0332
64	6.1132E−15		3.5735E−16		2.9837E−16	
		4.7386		0.0718		1.2563
128	2.2898E−16		3.4001E−16		1.2490E−16	
		−0.2035		0.4053		−1.8524
256	2.6368E−16		2.5674E−16		4.5103E−16	
		0.4406		−0.2168		0.1895
512	1.9429E−16		2.9837E−16		3.9552E−16	
		−0.5850		0.1783		−0.5334
1024	2.9143E−16		2.6368E−16		5.7246E−16	
		0.5097		−0.3067		1.4594
2048	2.0470E−16		3.2613E−16		2.0817E−16	

N	$p = 8, \quad \alpha p = 12.0$		$p = 9, \quad \alpha p = 13.5$		$p = 10, \quad \alpha p = 15.0$	
	$\|If - I_N f\|$	EOC	$\|If - I_N f\|$	EOC	$\|If - I_N f\|$	EOC
2	7.8213E−01		8.0913E−01		8.4228E−01	
		1.8577		1.2264		0.8927
4	2.1581E−01		3.4581E−01		4.5367E−01	
		0.4770		0.5345		0.4657
8	1.5505E−01		2.3874E−01		3.2851E−01	
		16.3200		16.2276		15.6164
16	1.8953E−06		3.1113E−06		6.5395E−06	
		32.0367		36.1210		31.8292
32	4.3021E−16		4.1633E−17		1.7139E−15	
		0.3692		−1.7726		5.3634
64	3.3307E−16		1.4225E−16		4.1633E−17	
		−0.2730		0.2701		−1.7004
128	4.0246E−16		1.1796E−16		1.3531E−16	
		0.2141		−0.9125		−1.0896
256	3.4694E−16		2.2204E−16		2.8796E−16	
		0.1203		0.1420		−0.5076
512	3.1919E−16		2.0123E−16		4.0939E−16	
		−0.3833		−0.8969		0.9284
1024	4.1633E−16		3.7470E−16		2.1511E−16	
		0.7984		−0.1640		−1.0902
2048	2.3939E−16		4.1980E−16		4.5797E−16	

N	$p = 15, \quad \alpha p = 22.5$		$p = 20, \quad \alpha p = 30.0$		$p = 25, \quad \alpha p = 37.5$	
	$\|If - I_N f\|$	EOC	$\|If - I_N f\|$	EOC	$\|If - I_N f\|$	EOC
2	9.4909E−01		9.7568E−01		9.8102E−01	
		0.6442		3.0475		0.5998
4	6.0729E−01		1.1801E−01		6.4734E−01	
		0.0800		−1.4126		1.9097
8	5.7454E−01		3.1415E−01		1.7229E−01	
		9.6879		6.1974		3.2244
16	6.9658E−04		4.2808E−03		1.8434E−02	
		29.8489		24.1337		25.8454
32	7.2040E−13		2.3257E−10		3.0576E−10	
		11.2043		20.7130		17.4158
64	3.0531E−16		1.3531E−16		1.7486E−15	
		0.6521		−1.6919		0.9112
128	1.9429E−16		4.3715E−16		9.2981E−16	
		−0.1468		0.1699		1.1592
256	2.1511E−16		3.8858E−16		4.1633E−16	
		−0.7600		0.4854		−0.0818
512	3.6429E−16		2.7756E−16		4.4062E−16	
		0.1907		−0.4854		0.3305
1024	3.1919E−16		3.8858E−16		3.5041E−16	
		−0.5317		0.0525		1.3007
2048	4.6144E−16		3.7470E−16		1.4225E−16	

Table 1.7: $n = 4$, $\alpha = 0.5$, $If = \pi J_0(4) \approx -1.2477$. The mapping function w is given by (1.31) and (1.32).

	$p=2, \quad \alpha p = 1.0$		$p=3, \quad \alpha p = 1.5$		$p=4, \quad \alpha p = 2.0$	
N	$\lvert If - I_N f\rvert$	EOC	$\lvert If - I_N f\rvert$	EOC	$\lvert If - I_N f\rvert$	EOC
2	6.5041E−01		1.4999E+00		2.3998E+00	
		1.9326		4.0340		2.8025
4	1.7038E−01		9.1563E−02		3.4398E−01	
		1.0307		2.8184		7.0010
8	8.3395E−02		1.2980E−02		2.6854E−03	
		1.0146		1.5136		2.6586
16	4.1278E−02		4.5463E−03		4.2530E−04	
		1.0074		1.5067		1.9994
32	2.0533E−02		1.5999E−03		1.0637E−04	
		1.0037		1.5034		1.9998
64	1.0240E−02		5.6433E−04		2.6596E−05	
		1.0019		1.5017		2.0000
128	5.1132E−03		1.9929E−04		6.6491E−06	
		1.0009		1.5009		2.0000
256	2.5550E−03		7.0416E−05		1.6623E−06	
		1.0005		1.5004		2.0001
512	1.2771E−03		2.4888E−05		4.1555E−07	
		1.0002		1.5002		2.0001
1024	6.3843E−04		8.7981E−06		1.0388E−07	
		1.0001		1.5001		2.0095
2048	3.1919E−04		3.1104E−06		2.5800E−08	

	$p=5, \quad \alpha p = 2.5$		$p=6, \quad \alpha p = 3.0$		$p=7, \quad \alpha p = 3.5$	
N	$\lvert If - I_N f\rvert$	EOC	$\lvert If - I_N f\rvert$	EOC	$\lvert If - I_N f\rvert$	EOC
2	3.1701E+00		3.8560E+00		4.4858E+00	
		1.9412		1.4953		1.2540
4	8.2550E−01		1.3677E+00		1.8809E+00	
		5.9613		4.4621		3.4568
8	1.3249E−02		6.2057E−02		1.7130E−01	
		8.8892		12.2091		9.8653
16	2.7943E−05		1.3107E−05		1.8365E−04	
		2.4857		9.7168		12.2142
32	4.9891E−06		1.5575E−08		3.8652E−08	
		2.4863		3.7755		4.0890
64	8.9040E−07		1.1374E−09		2.2713E−09	
		2.4929		−0.4653		
128	1.5818E−07		1.5702E−09		(3.4613E−08)	
		2.4976				(0.9781)
256	2.8010E−08		(5.9244E−08)		(1.7571E−08)	
		2.6633		(0.6447)		(0.1139)
512	4.4215E−09		(3.7893E−08)		(1.6238E−08)	
				(0.4360)		(−0.0875)
1024	(3.5464E−08)		(2.8009E−08)		(1.7252E−08)	
		(0.6084)		(0.3270)		(−0.2348)
2048	(2.3262E−08)		(2.2330E−08)		(2.0302E−08)	

N	$p = 8, \quad \alpha p = 4.0$		$p = 9, \quad \alpha p = 4.5$		$p = 10, \quad \alpha p = 5.0$	
	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC
2	5.0753E+00		5.6358E+00		6.1759E+00	
4	2.3433E+00	1.1149	2.7604E+00	1.0297	3.1427E+00	0.9747
8	3.4478E−01	2.7648	5.6921E−01	2.2778	8.2480E−01	1.9299
16	1.1994E−03	8.1673	4.8361E−03	6.8790	1.4092E−02	5.8711
32	2.2267E−09	19.0389	(1.2274E−07)		(3.7922E−07)	
64	(4.1176E−08)		(5.0295E−08)	(1.2870)	(4.3144E−08)	(3.1358)
128	(2.3156E−08)	(0.8304)	(3.7074E−08)	(0.4400)	(2.8754E−08)	(0.5854)
256	(1.8448E−08)	(0.3279)	(2.4115E−08)	(0.6205)	(2.5478E−08)	(0.1745)
512	(2.2009E−08)	(−0.2546)	(2.1882E−08)	(0.1402)	(2.4055E−08)	(0.0830)
1024	(2.1640E−08)	(0.0244)	(2.1605E−08)	(0.0184)	(2.4801E−08)	(−0.0441)
2048	(2.1173E−08)	(0.0315)	(2.0634E−08)	(0.0663)	(2.4702E−08)	(0.0057)

N	$p = 15, \quad \alpha p = 7.5$		$p = 20, \quad \alpha p = 10.0$		$p = 25, \quad \alpha p = 12.5$	
	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC	$\lvert If - I_N f \rvert$	EOC
2	8.7408E+00		1.1247E+01		1.3748E+01	
4	4.7666E+00	0.8748	(6.1630E+00)		(7.4683E+00)	
8	(2.1109E+00)		(3.1365E+00)	(0.9745)	(3.9933E+00)	(0.9032)
16	(2.5265E−01)	(3.0626)	(8.2480E−01)	(1.9270)	(1.4927E+00)	(1.4196)
32	(5.3693E−04)	(8.8782)	(1.4342E−02)	(5.8457)	(8.5760E−02)	(4.1215)
64	(3.7467E−08)	(13.8068)	(4.1809E−07)	(15.0661)	(3.2940E−05)	(11.3463)
128	(3.0282E−08)	(0.3071)	(2.3133E−08)	(4.1758)	(2.1313E−08)	(10.5939)
256	(2.7627E−08)	(0.1324)	(2.0969E−08)	(0.1417)	(2.2794E−08)	(−0.0970)
512	(2.7154E−08)	(0.0249)	(2.1776E−08)	(−0.0545)	(2.1479E−08)	(0.0858)
1024	(2.7564E−08)	(−0.0216)	(2.1156E−08)	(0.0417)	(2.2566E−08)	(−0.0712)
2048	(2.6893E−08)	(0.0355)	(2.1139E−08)	(0.0012)	(2.2629E−08)	(−0.0041)

Table 1.8: $n = 4$, $\alpha = 1.5$, $If = \frac{\pi}{4}\mathrm{J}_1(4) \approx -5.1870 \times 10^{-2}$. The mapping function w is given by (1.31) and (1.32).

N	$p=2,\quad \alpha p = 3.0$ $\lvert If - I_N f\rvert$	EOC	$p=3,\quad \alpha p = 4.5$ $\lvert If - I_N f\rvert$	EOC	$p=4,\quad \alpha p = 6.0$ $\lvert If - I_N f\rvert$	EOC
2	4.7685E−01		1.3800E+00		2.0110E+00	
		8.5017		3.6679		2.0675
4	1.3156E−03		1.0858E−01		4.7978E−01	
		7.9897		11.8064		7.3518
8	5.1761E−06		3.0314E−05		2.9372E−03	
		3.9703		11.5331		19.7548
16	3.3023E−07		1.0229E−08		3.3200E−09	
		3.9927		4.3934		11.4352
32	2.0744E−08		4.8672E−10		1.1990E−12	
		3.9982		4.4519		6.0042
64	1.2981E−09		2.2239E−11		1.8680E−14	
		3.9995		4.4771		6.8095
128	8.1159E−11		9.9855E−13		1.6653E−16	
		3.9999		4.4860		2.5850
256	5.0729E−12		4.4562E−14		2.7756E−17	
		3.9989		4.6658		−3.5236
512	3.1730E−13		1.7555E−15		3.1919E−16	
		3.9859		4.1756		−0.6262
1024	2.0026E−14		9.7145E−17		4.9266E−16	
		3.9024		−3.0255		2.4493
2048	1.3392E−15		7.9103E−16		9.0206E−17	

N	$p=5,\quad \alpha p = 7.5$ $\lvert If - I_N f\rvert$	EOC	$p=6,\quad \alpha p = 9.0$ $\lvert If - I_N f\rvert$	EOC	$p=7,\quad \alpha p = 10.5$ $\lvert If - I_N f\rvert$	EOC
2	2.5424E+00		3.0497E+00		3.5514E+00	
		1.4322		1.1720		1.0642
4	9.4215E−01		1.3535E+00		1.6984E+00	
		4.9725		3.5411		2.6381
8	3.0008E−02		1.1628E−01		2.7283E−01	
		14.4825		11.1307		8.8232
16	1.3109E−06		5.1858E−05		6.0235E−04	
		29.0411		27.6954		22.7533
32	2.3731E−15		2.3860E−13		8.5200E−11	
		4.2479		10.6101		22.5496
64	1.2490E−16		1.5266E−16		1.3878E−17	
		−0.9175		0		−3.8074
128	2.3592E−16		1.5266E−16		1.9429E−16	
		−0.2345		0.4594		−0.3626
256	2.7756E−16		1.1102E−16		2.4980E−16	
		1.8625		−0.3219		1.8480
512	7.6328E−17		1.3878E−16		6.9389E−17	
		−1.7105		0.2345		−0.2630
1024	2.4980E−16		1.1796E−16		8.3267E−17	
		1.1699		−1.3049		3.5850
2048	1.1102E−16		2.9143E−16		6.9389E−18	

N	$p = 8,\quad \alpha p = 12.0$		$p = 9,\quad \alpha p = 13.5$		$p = 10,\quad \alpha p = 15.0$	
	$\lvert If - I_N f\rvert$	EOC	$\lvert If - I_N f\rvert$	EOC	$\lvert If - I_N f\rvert$	EOC
2	4.0518E+00		4.5518E+00		5.0519E+00	
		1.0193		1.0006		0.9930
4	1.9990E+00		2.2750E+00		2.5383E+00	
		2.0577		1.6821		1.4386
8	4.8014E−01		7.0894E−01		9.3647E−01	
		7.1444		5.8770		4.8964
16	3.3939E−03		1.2063E−02		3.1444E−02	
		19.1328		16.3678		14.1890
32	5.9040E−09		1.4264E−07		1.6835E−06	
		24.7575		31.6739		33.6500
64	2.0817E−16		4.1633E−17		1.2490E−16	
		−0.0931		1.5850		−1.0780
128	2.2204E−16		1.3878E−17		2.6368E−16	
		0.4150		−3.7004		1.0780
256	1.6653E−16		1.8041E−16		1.2490E−16	
		0.7776		0.1155		1.1699
512	9.7145E−17		1.6653E−16		5.5511E−17	
		−0.8365		−0.3692		−3.0444
1024	1.7347E−16		2.1511E−16		4.5797E−16	
		−1.1375		0.7843		3.4594
2048	3.8164E−16		1.2490E−16		4.1633E−17	

N	$p = 15,\quad \alpha p = 22.5$		$p = 20,\quad \alpha p = 30.0$		$p = 25,\quad \alpha p = 37.5$	
	$\lvert If - I_N f\rvert$	EOC	$\lvert If - I_N f\rvert$	EOC	$\lvert If - I_N f\rvert$	EOC
2	7.5519E+00		1.0052E+01		1.2552E+01	
		0.9903		0.9926		0.9941
4	3.8014E+00		5.0519E+00		6.3019E+00	
		1.0398		0.9936		0.9894
8	1.8490E+00		2.5372E+00		3.1742E+00	
		2.3109		1.4401		1.1423
16	3.7263E−01		9.3509E−01		1.4380E+00	
		7.8581		4.8780		3.2480
32	1.6061E−03		3.1801E−02		1.5136E−01	
		20.6202		14.1183		10.3170
64	9.9644E−10		1.7882E−06		1.1866E−04	
		26.0975		33.0000		25.8503
128	1.3878E−17		2.0817E−16		1.9614E−12	
		−3.3219		3.9069		13.2019
256	1.3878E−16		1.3878E−17		2.0817E−16	
		−1.3219		−2.5850		–
512	3.4694E−16		8.3267E−17		0	
		3.0589		−1.3219		–
1024	4.1633E−17		2.0817E−16		6.9389E−17	
		−0.7370		−0.3410		−0.6781
2048	6.9389E−17		2.6368E−16		1.1102E−16	

Table 1.9: $n = 4$, $\alpha = 0.5$, $If = \pi \mathrm{J}_0(4) \approx -1.2477$. The mapping function w is given by (1.31) and (1.34).

N	$\lvert If - I_N f \rvert$	EOC
2	5.0316E−01	
4	2.7910E−04	10.8160
8	2.0245E−02	−6.1806
16	1.3897E−03	3.8647
32	8.7604E−06	7.3095
64	(6.0798E−08)	
128	(1.2829E−08)	(2.2446)
256	(7.9516E−09)	(0.6901)
512	(1.4126E−08)	(−0.8291)
1024	(2.4405E−08)	(−0.7888)
2048	(2.4659E−08)	(−0.0150)

Table 1.10: $n = 4$, $\alpha = 1.5$, $If = \frac{\pi}{4} \mathrm{J}_1(4) \approx -5.1870 \times 10^{-2}$. The mapping function w is given by (1.31) and (1.34).

N	$\lvert If - I_N f \rvert$	EOC
2	2.6997E−01	
4	2.2999E−02	3.5531
8	1.5805E−04	7.1850
16	8.3198E−07	7.5697
32	1.4578E−09	9.1566
64	1.0700E−13	13.7339
128	3.2613E−16	8.3579
256	1.0408E−16	1.6477
512	4.1633E−16	−2.0000
1024	1.8735E−16	1.1520
2048	4.0246E−16	−1.1031

Table 1.11: N_0 computed from (1.52), (1.53), and (1.54)

p	N_0 (1.52)	N_0 (1.53)	N_0 (1.54)
			37
2	33554432	33554432	
3	82570	137617	
4	4096	8192	
5	676	1486	
6	203	474	
7	86	209	
8	45	113	
9	28	70	
10	19	48	
15	6	15	
20	4	9	
25	3	6	

Chapter 2

Numerical Quadrature Methods for Integrals on the Real Line of Steepest Descent Type

In this chapter, we consider the problem of evaluating numerically the integral

$$\int_{-\infty}^{+\infty} e^{-\rho s^2} \Phi(s)\, ds, \tag{2.1}$$

for $\rho \geq 0$ in the case when Φ is a smooth function on the real line. We may write (2.1) as

$$Jf := \int_{-\infty}^{+\infty} e^{-\rho s^2} f(s^2)\, ds, \tag{2.2}$$

where $f : [0, \infty) \to \mathbb{C}$ is defined by

$$f(s) = \frac{1}{2}\big(\Phi(\sqrt{s}\,) + \Phi(-\sqrt{s}\,)\big).$$

It is clear that different numerical quadrature methods may be appropriate for evaluating (2.1) or (2.2) depending on the magnitude of ρ. We implement and discuss three different numerical quadrature methods aimed at different ranges of ρ. For ρ not too small, Gaussian quadrature for weight function $e^{-\rho s^2}$ (Gauss–Hermite quadrature) is an appropriate and standard method and this is discussed in Section 2.1. Clearly this Gauss quadrature method is not appropriate if $\rho = 0$. In Sections 2.2 and 2.3 we propose and analyse quadrature methods which the theoretical analysis suggests are suitable for small and intermediate ranges of ρ, respectively. Another method very suitable for the evaluation of (2.1) when ρ is not too small is the trapezium rule with an equal mesh size over $(-\infty, +\infty)$, as first noted by Goodwin [20] and see Hunter [24] for an important application close to that of Chapter 3. This method can be modified to retain high accuracy in the presence of poles of Φ on or near the path of integration: see Hunter [25, 26].

2.1 Gaussian Quadrature

To evaluate (2.1) using Gaussian quadrature with weight function e^{-x^2}, we substitute $\sqrt{\rho}\, s = x$ for $\rho > 0$, and then apply Gauss–Hermite quadrature to get

$$\int_{-\infty}^{+\infty} e^{-\rho s^2}\Phi(s)\, ds = \frac{1}{\sqrt{\rho}}\int_{-\infty}^{+\infty} e^{-x^2}\Phi\left(\frac{x}{\sqrt{\rho}}\right) dx \approx \frac{1}{\sqrt{\rho}}\sum_{j=1}^{N} w_j\,\Phi\left(\frac{x_j}{\sqrt{\rho}}\right),$$

where the abscissa x_j is the jth zero of the Hermite polynomial of degree N (Andrews [2]),

$$H_N(x) = \sum_{k=0}^{[N/2]} \frac{(-1)^k N!}{k!\,(N-2k)!}(2x)^{N-2k}, \tag{2.3}$$

and the weight is (Abramowitz and Stegun [1])

$$w_j = \frac{2^{N-1}N!\,\sqrt{\pi}}{N^2\,[H_{N-1}(x_j)]^2}\,. \tag{2.4}$$

From (2.3) and (2.4) it can be seen that the abscissae $x_1 < x_2 < \cdots < x_N$ and weights w_j have the symmetry properties that

$$x_j = -x_{N+1-j}, \qquad w_j = w_{N+1-j}, \qquad j = 1, 2, \ldots, N. \tag{2.5}$$

Equivalently, we can substitute $\sqrt{\rho}\, s = x$ in (2.2) and apply Gauss–Hermite quadrature to Jf to get

$$Jf \approx J_N^{GH} f := \frac{1}{\sqrt{\rho}}\sum_{j=1}^{N} w_j\, f\left(\frac{x_j^2}{\rho}\right) = \frac{1}{\sqrt{\rho}}\sum_{j=1}^{N} w_j\,\Phi\left(\frac{x_j}{\sqrt{\rho}}\right).$$

Note that, in view of (2.5),

$$J_{2N}^{GH} f = \frac{2}{\sqrt{\rho}}\sum_{j=1}^{N} w_j\, f\left(\frac{x_j^2}{\rho}\right),$$

where x_j and w_j are here the abscissae and weights for the Gauss–Hermite quadrature rule of degree $2N$.

A further alternative is first to substitute $\rho s^2 = t$ in (2.2) and then apply generalised Gauss–Laguerre quadrature with weight function $t^{-1/2}e^{-t}$ to get

$$Jf = \frac{1}{\sqrt{\rho}}\int_0^{\infty} t^{-1/2}e^{-t} f\left(\frac{t}{\rho}\right) dt \approx J_N^{GL} f := \frac{1}{\sqrt{\rho}}\sum_{j=1}^{N} \widetilde{w}_j\, f\left(\frac{t_j}{\rho}\right), \tag{2.6}$$

where the weights $\widetilde{w}_j$ and abscissae t_j are tabulated for $N = 1, 2, \ldots, 15$ in Concus *et al.* [15], or can be calculated by using standard subroutine libraries [37]. It can be shown that

$$J_N^{GL} f = J_{2N}^{GH} f.$$

A modified Gauss–Laguerre quadrature method has been employed in [12], neglecting the smaller weights in the quadrature rule. It also has been suggested in [12] that this modified quadrature can be cheaper than, but almost as accurate as, the standard Gauss–Laguerre quadrature. In the following theorems, we present a preliminary bound on the derivatives of an analytic function f and the error estimates for Gauss–Laguerre quadrature method used in [12].

Theorem 2.1 *For $\eta > 0$, let $\mathcal{D}_\eta := \{z \in \mathbb{C} : |z| < \eta$ or $\operatorname{Re} z > 0$ and $|\operatorname{Im} z| < \eta\}$ denote that part of the complex plane lying within distance η of the positive real axis. If, for some $C > 0$, $g(z)$ is analytic and $|g(z)| \leq C$ in $\mathcal{D}_\eta$, then, for all non-negative integers n and $t \geq 0$,*

$$|g^{(n)}(t)| \leq \frac{n!C}{\eta^n}.$$

The following notations are introduced and will be used in Theorem 2.2:

$$\widetilde{J}g := \int_0^\infty t^{-1/2} e^{-t} g(t)\, dt,$$

$$\widetilde{J}_{n,m}\, g := \sum_{j=1}^{m} \widetilde{w}_{j,n}\, g(t_{j,n}), \qquad m = 1, 2, \ldots, n, \qquad n = 1, 2, \ldots,$$

where $\widetilde{w}_{1,n}, \widetilde{w}_{2,n}, \ldots, \widetilde{w}_{n,n}$ and $0 < t_{1,n} < t_{2,n} < \cdots < t_{n,n}$ are the weights and abscissae of the n-point Gauss–Laguerre quadrature method for weight function $t^{-1/2}e^{-t}$, and the error in $\widetilde{J}_{n,m}\, g$ is

$$E_{n,m}\, g := \widetilde{J}g - \widetilde{J}_{n,m}\, g\,.$$

Theorem 2.2 [12] *If, for some $C > 0$, $g(z)$ is analytic and $|g(z)| \leq C$ in $\mathcal{D}_\eta$ for $\eta > 0$, then*

(i) $|E_{n,n}\, g| \leq e_n C$, *where e_n is independent of g and $e_n \to 0$ as $n \to \infty$;*

(ii) $$|E_{n,n}\, g| \leq \frac{(2n)!\sqrt{2\pi}}{(2\eta)^{2n}} C;$$

(iii) $$|E_{n,m}\, g| \leq |E_{n,n} g| + C \sum_{j=m+1}^{n} w_{j,n}.$$

Theorem 2.3 *If, for some $C > 0$, $f(z)$ is analytic and $|f(z)| \leq C$ in $\mathcal{D}_\eta$ for $\eta > 0$, then the error in the Gauss–Laguerre quadrature can be bounded by*

$$\left|Jf - J_N^{GL} f\right| \leq \frac{C(2N)!\sqrt{2\pi}}{(2\eta)^{2N}} \rho^{-(2N+1/2)}.$$

Proof. From (2.6), Theorem 2.2 (*ii*), and the fact that $t/\rho \in \mathcal{D}_\eta$ iff $t \in \mathcal{D}_{\rho\eta}$, we have that, where $g(t) := f(t/\rho)$,

$$\begin{aligned} \left|Jf - J_N^{GL} f\right| &= \left| \frac{1}{\sqrt{\rho}} \int_0^\infty t^{-1/2} e^{-t} g(t) dt - \frac{1}{\sqrt{\rho}} \sum_{j=1}^N \widetilde{w}_j \, g(t_j) \right| \\ &= E_{N,N} g \\ &\leq \frac{C(2N)!\sqrt{2\pi}}{(2\rho\eta)^{2N}} \rho^{-1/2} \\ &= \frac{C(2N)!\sqrt{2\pi}}{(2\eta)^{2N}} \rho^{-(2N+1/2)}. \end{aligned}$$

■

Clearly this quadrature method will be very accurate when ρ is large even for fairly small values of N.

2.2 A Quadrature Method Suitable for ρ Small

We apply the quadrature method and error analysis, developed in Sections 1.1 and 1.2, to numerically evaluate Jf, for ρ small. For the purpose of the later error analysis, we require that f satisfies the following assumption.

Assumption 2.1 *For some $q \in \mathbb{N}$, $f \in C^q[0,\infty)$ and there exists $c > 0$ and $r > 1/2$ such that, for $n = 0, 1, \ldots, q$, it holds that*

$$|f^{(n)}(t)| \leq c(1+t)^{-r-n}, \qquad t \geq 0.$$

Note that if Φ is analytic in a neighbourhood of the real axis then f is analytic in a neighbourhood of the positive real axis, so that certainly $f \in C^\infty[0,\infty)$. In the examples we study later, f will be analytic in a sector of the complex plane containing the positive real axis, and Assumption 2.1 will follow from the following assumption on f.

Assumption 2.1′ *For some $\varepsilon > 0$ and $\theta \in (0, \pi/2]$, the function f is analytic on $\mathcal{D}_{\varepsilon,\theta}$, where (see Figure 2.1)*

$$\mathcal{D}_{\varepsilon,\theta} := \Big\{ z \in \mathbb{C} : |\arg(z+\varepsilon)| < \theta \Big\}.$$

Further, for some $\widetilde{c} > 0$ and $r > 1/2$,

$$|f(z)| \le \widetilde{c}\,(1+|z|)^{-r}, \qquad z \in \mathcal{D}_{\varepsilon,\theta}.$$

Lemma 2.1 *Let f satisfy Assumption 2.1′. Then, where $\bar{\varepsilon} = \min\{\varepsilon, 1\}$,*

$$|f^{(n)}(t)| \le \widetilde{C}_n (1+t)^{-r-n},$$

for $t \ge 0$ and $n = 0, 1, \ldots$, where

$$\widetilde{C}_n := \frac{n!\,\widetilde{c}\,2^{n+r}}{(\bar{\varepsilon}\sin\theta)^n}.$$

Proof. From Cauchy's integral formula with circular contour $C_\eta(t)$, the circle of radius η centred at t, and with $\eta = \frac{1}{2}(\bar{\varepsilon}+t)\sin\theta$ (see Figure 2.2),

$$\begin{aligned} |f^{(n)}(t)| &= \left| \frac{n!}{2\pi i} \int_{C_\eta(t)} \frac{f(z)}{(z-t)^{n+1}}\, dz \right| \\ &\le \frac{n!}{\eta^n} \max_{z \in C_\eta(t)} |f(z)| \\ &\le \frac{n!\,\widetilde{c}}{\eta^n} \max_{z \in C_\eta(t)} (1+|z|)^{-r}. \end{aligned}$$

Now $\eta \le \frac{1}{2}(1+t)$ so that (see Figure 2.2), for $z \in C_\eta(t)$, $1+|z| \ge 1+t-\eta \ge \frac{1}{2}(1+t)$. Thus

$$\begin{aligned} |f^{(n)}(t)| &\le \frac{n!\,\widetilde{c}}{\left(\frac{1}{2}(\bar{\varepsilon}+t)\sin\theta\right)^n} \left(\frac{1+t}{2}\right)^{-r} \\ &\le \frac{n!\,\widetilde{c}\,2^{n+r}}{(\bar{\varepsilon}\sin\theta)^n}(1+t)^{-r-n}. \end{aligned}$$

■

Throughout this section we let $C_m > 0$ denote a generic constant whose value depends at most on $m \in \mathbb{N}$, and we let $C > 0$ denote a generic constant whose value depends at most on the values of q, r in Assumption 2.1.

To apply the results and methods from Chapter 1, we substitute $s = u/\sqrt{1-u^2}$ in (2.2) and see that

$$Jf = \int_{-1}^{+1} F(u)\, du = IF, \tag{2.7}$$

where

$$F(u) := \frac{f(P(u))e^{-\rho P(u)}}{(1-u^2)^{3/2}}, \qquad -1 < u < 1,$$

$$P(u) := \frac{u^2}{1-u^2} \geq 0, \qquad -1 < u < 1.$$

For $\rho = 0$ the function F may be weakly singular at ± 1. For $\rho > 0$, because the function $e^{-\rho P(u)}$ is infinitely differentiable and all its derivatives vanish at ± 1, the function F inherits these properties if $f \in C^\infty[0, \infty)$. From Theorem 1.1 it follows that the trapezium rule is superalgebraically convergent when applied to evaluating $\int_{-1}^{+1} F(u)du$ for $\rho > 0$. However, $e^{-\rho P(u)} \leq 1$ and $e^{-\rho P(u)} \to 1$ as $\rho \to 0$ for $-1 < u < 1$. Thus the error in the trapezium rule for ρ small must be approximately the error for $\rho = 0$. But for $\rho = 0$ the trapezium rule applied to $\int_{-1}^{+1} F(u)du$ will converge only slowly. Thus the trapezium rule will not be satisfactory for ρ small. Instead we consider the application of the method of Chapter 1 which involves first substituting $u = w(x)$ for some function w satisfying Assumption 1.1 and then applying the trapezium rule.

To apply the error analysis of Section 1.2, we have to show that $F \in S^{q,\alpha}[-1, 1]$ for some $q \in \mathbb{N}$ and $\alpha > 0$, or in other words that, for $j = 0, 1, \ldots, q$ and some $C > 0$ which is an upper bound for $\|F\|_{q,\alpha}$,

$$|F^{(j)}(u)| \leq C(1-u^2)^{\alpha-1-j}, \qquad -1 < u < 1.$$

By Leibnitz's rule, the jth derivative of $F(u)$, for $-1 < u < 1$, is

$$F^{(j)}(u) = \sum_{k=0}^{j} \left\{ \binom{j}{k} F_1^{(j-k)}(u) \left[\sum_{n=0}^{k} \binom{k}{n} F_2^{(k-n)}(u) F_3^{(n)}(u) \right] \right\}, \tag{2.8}$$

where

$$F_1(u) := (1-u^2)^{-3/2}, \qquad F_2(u) := e^{-\rho P(u)}, \qquad F_3(u) := f(P(u)).$$

For F_1 and its derivatives, it can easily be shown that, for $m = 0, 1, \ldots,$

$$|F_1^{(m)}(u)| \leq C_m (1-u^2)^{-3/2-m}, \qquad -1 < u < 1. \tag{2.9}$$

To obtain bounds on F_2, F_3 and their derivatives, we need the following lemmas.

Lemma 2.2 *For $m = 0, 1, \ldots$, $P^{(m)}(u)$ has poles of order not more than $m+1$ at ± 1, so that*

$$|P^{(m)}(u)| \leq C_m(1-u^2)^{-m-1}, \qquad -1 < u < 1.$$

Proof. From the Laurent expansions of P centred on ± 1, the validity of this lemma is obvious. ■

The next few results are concerned with obtaining bounds for the derivatives of $G(u) := g(P(u))$. For expressions for these derivatives we need the following.

For $m = 0, 1, \ldots$, and $j = 0, 1, \ldots, m$, let U_j^m be defined recursively by

$$U_0^0(u) = 1,$$

$$U_j^{m+1}(u) = \begin{cases} \dfrac{dU_0^m(u)}{du}, & \text{if } j = 0, \\ \dfrac{dU_j^m(u)}{du} + U_{j-1}^m(u)P'(u), & \text{if } j = 1, 2, \ldots, m, \\ U_m^m(u)P'(u), & \text{if } j = m+1. \end{cases}$$

Note that this definition implies that $U_0^m(u) = 0$ if $m \in \mathbb{N}$. Since $P(u)$ is a meromorphic function with poles only at ± 1, it is easy to see that $U_j^m(u)$ is also a meromorphic function with poles only at ± 1.

Lemma 2.3 *For $m = 0, 1, \ldots$, and $j = 0, 1, \ldots, m$, $U_j^m(u)$ has poles of order not more than $m + j$ at ± 1, so that*

$$|U_j^m(u)| \leq C_m(1-u^2)^{-m-j}, \qquad -1 < u < 1.$$

Proof. Clearly, the lemma is true for $m = 0$. If $m \in \{0, 1, \ldots\}$ and U_j^m has a pole of order not more than $m + j$, for $j = 0, 1, \ldots m$, then

$$U_0^{m+1}(u) = \frac{dU_0^m(u)}{du}$$

has a pole of order not more than $m + 1$ and, for $j = 1, 2, \ldots, m$, using Lemma 2.2

$$U_j^{m+1}(u) = \frac{dU_j^m(u)}{du} + U_{j-1}^m(u)P'(u)$$

has a pole of order not more than $m + 1 + j$. Further,

$$U_{m+1}^{m+1}(u) = U_m^m(u)P'(u)$$

has a pole of order not more than $m + m + 2 = (m+1) + (m+1)$. Thus, the lemma follows by induction. ■

Lemma 2.4 *If $g \in \mathcal{C}^\infty(-1,1)$ and $G(u) := g(P(u))$ then, for $m = 0, 1, \ldots$,*

$$G^{(m)}(u) = \sum_{j=0}^{m} U_j^m(u) g^{(j)}(P(u)), \qquad -1 < u < 1.$$

Proof. We use a proof by induction. For $m = 0$,

$$G^{(m)}(u) = G(u) := g(P(u)) = U_0^0(u) g(P(u)).$$

If $m \in \{0, 1, \ldots\}$ and

$$G^{(m)}(u) = \sum_{j=0}^{m} U_j^m(u) g^{(j)}(P(u)), \qquad -1 < u < 1,$$

then

$$\begin{aligned} G^{(m+1)}(u) &= \sum_{j=0}^{m} \left[\frac{dU_j^m(u)}{du} g^{(j)}(P(u)) + U_j^m(u) P'(u) g^{(j+1)}(P(u)) \right] \\ &= \frac{dU_0^m(u)}{du} g(P(u)) + \sum_{j=1}^{m} \left[\frac{dU_j^m(u)}{du} + U_{j-1}^m(u) P'(u) \right] g^{(j)}(P(u)) \\ &\quad + U_m^m(u) P'(u) g^{(m+1)}(P(u)) \\ &= \sum_{j=0}^{m+1} U_j^{m+1}(u) g^{(j)}(P(u)). \end{aligned}$$

■

Now we bound the derivatives of F_2 and F_3. Using Lemma 2.4 and Lemma 2.3, since $F_2(u) = e^{-\rho P(u)}$ for $-1 < u < 1$ and $P(u) \geq 0$, then, for $m = 0, 1, \ldots$,

$$\begin{aligned} \left| F_2^{(m)}(u) \right| &\leq \sum_{j=0}^{m} \left| U_j^m(u) \right| \rho^j e^{-\rho P(u)} \\ &\leq C_m (1-u^2)^{-m} \sum_{j=0}^{m} \rho^j (1-u^2)^{-j} e^{-\rho P(u)} \\ &= C_m (1-u^2)^{-m} \sum_{j=0}^{m} s^j e^{-s} u^{-2j}, \end{aligned}$$

where $s := \rho P(u) = \rho u^2/(1-u^2)$. Let $\mu_j := \max_{s\geq 0} s^j e^{-s}$. Then

$$\left|F_2^{(m)}(u)\right| \leq \begin{cases} C_m(1-u^2)^{-m}\sum_{j=0}^{m} 2^j\rho^j, & \text{if } u^2 \leq 1/2, \\ C_m(1-u^2)^{-m}\sum_{j=0}^{m} 2^j\mu_j, & \text{if } u^2 \geq 1/2, \end{cases}$$

so that

$$\left|F_2^{(m)}(u)\right| \leq \begin{cases} C_m\,(1+\rho^m)\,(1-u^2)^{-m}, & \text{if } u^2 \leq 1/2, \\ C_m(1-u^2)^{-m}, & \text{if } u^2 \geq 1/2, \end{cases}$$

and

$$\left|F_2^{(m)}(u)\right| \leq C_m\,(1+\rho^m)\,(1-u^2)^{-m}, \qquad -1 < u < 1. \tag{2.10}$$

Similarly, using Lemma 2.4 and Lemma 2.3, since $F_3(u) = f(P(u))$ for $-1 < u < 1$ and $P(u) \geq 0$, $1 + P(u) = 1/(1-u^2)$, and Assumption 2.1 holds, then, for $m = 0, 1, \ldots$,

$$\begin{aligned} \left|F_3^{(m)}(u)\right| &\leq \sum_{j=0}^{m} \left|U_j^m(u) f^{(j)}(P(u))\right| \\ &\leq C_m \sum_{j=0}^{m} (1-u^2)^{-m-j} |f^{(j)}(P(u))| \\ &\leq c\,C_m \sum_{j=0}^{m} (1-u^2)^{-m-j}(1-u^2)^{r+j} \\ &\leq c\,C_m (1-u^2)^{r-m}. \end{aligned} \tag{2.11}$$

Theorem 2.4 *If Assumption 2.1 holds then, for $j = 0, 1, \ldots, q$,*

$$|F^{(j)}(u)| \leq c\,C(1+\rho^q)(1-u^2)^{r-3/2-j}, \qquad -1 < u < 1,$$

where the constant $C > 0$ depends only on q and r.

Proof. Using (2.8) to (2.11), we find that

$$\begin{aligned} |F^{(j)}(u)| &\leq c\,C(1+\rho^q)\sum_{k=0}^{j}\left\{(1-u^2)^{-3/2-j+k}\sum_{n=0}^{k}(1-u^2)^{r-k}\right\} \\ &\leq c\,C(1+\rho^q)\sum_{k=0}^{j}(1-u^2)^{r-3/2-j} \\ &\leq c\,C(1+\rho^q)(1-u^2)^{r-3/2-j}. \end{aligned}$$

■

Note that we have shown that if Assumption 2.1 holds then $F \in \mathcal{S}^{q,\alpha}[-1,1]$ with $\alpha = r - 1/2$, and

$$\|F\|_{q,\alpha} \le c\, C(1+\rho^q), \tag{2.12}$$

where the value of the constant $C > 0$ depends only on q and r.

Choosing $w \in \mathcal{C}^\infty[-1,1]$ which satisfies Assumption 1.1 and applying the quadrature rule (1.26) to (2.7), we get that (note that F is an even function)

$$Jf \approx J_N f := a_0 F(0) + 2\sum_{k=1}^{N-1} a_k F(x_k), \tag{2.13}$$

where, for $k = 1, \ldots, N-1$,

$$a_k := \frac{1}{N} w'\left(\frac{k}{N}\right), \qquad x_k := w\left(\frac{k}{N}\right),$$

and

$$F(u) := \frac{f(P(u))e^{-\rho P(u)}}{(1-u^2)^{3/2}}, \qquad P(u) := \frac{u^2}{1-u^2} \ge 0, \qquad -1 < u < 1.$$

In view of the bound (2.12) and applying Theorem 1.3, we get the following error estimate.

Theorem 2.5 *Suppose that w satisfies Assumption 1.1, f satisfies Assumption 2.1, and $1 < s < q$, where $s := (r - 1/2)p$. Then, for $s \notin \mathbb{N}$, the error in the quadrature (2.13) can be bounded by*

$$|Jf - J_N f| \le c\, C(1+\rho^q) N^{-s},$$

where the constant C depends only on q, r, and on the choice of the function w.

Combining Theorem 2.5 with Lemma 2.1, we obtain the following corollary.

Corollary 2.1 *Suppose that w satisfies Assumption 1.1, f satisfies Assumption 2.1′, and $1 < s < q$, where $s := (r - 1/2)p$. Then, for $s \notin \mathbb{N}$, the error in the quadrature (2.13) can be bounded by*

$$|Jf - J_N f| \le \frac{\tilde{c}\, C(1+\rho^q)}{(\bar{\varepsilon}\sin\theta)^q} N^{-s},$$

where $\bar{\varepsilon} = \min\{\varepsilon, 1\}$ and the constant C depends only on q, r, and on the choice of the function w.

Remark 2.1 *Note that Theorem 2.5 and Corollary 2.1 apparently do not apply if* s *is an integer. However, note that if Assumption 2.1 or 2.1′ hold with a particular value of* $r > 1/2$, *then they also hold with* r *replaced by* r' *for* $1/2 < r' < r$. *Thus, if* $s = (r - 1/2)p$ *is an integer, Theorem 2.5 and Corollary 2.1 can be applied with* $s' := (r' - 1/2)p$ *for all* $1/2 < r' < r$, *for which* s' *is not an integer. Thus, for all* $\delta > 0$,

$$|Jf - J_N f| = O(N^{\delta - s}) \quad \text{as} \quad N \to \infty.$$

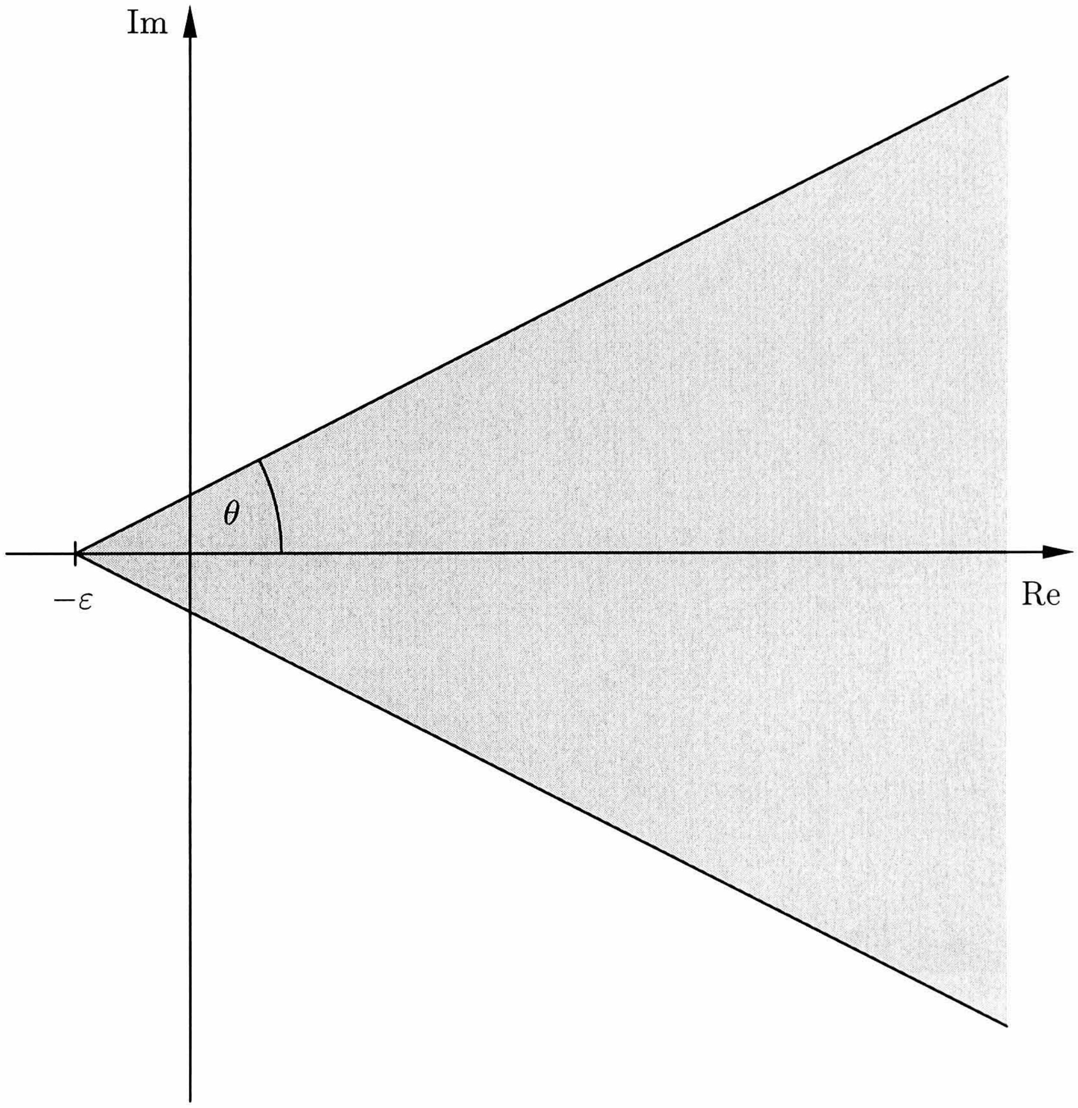


Figure 2.1: $\mathcal{D}_{\varepsilon,\theta}$ in Assumption 2.1′.

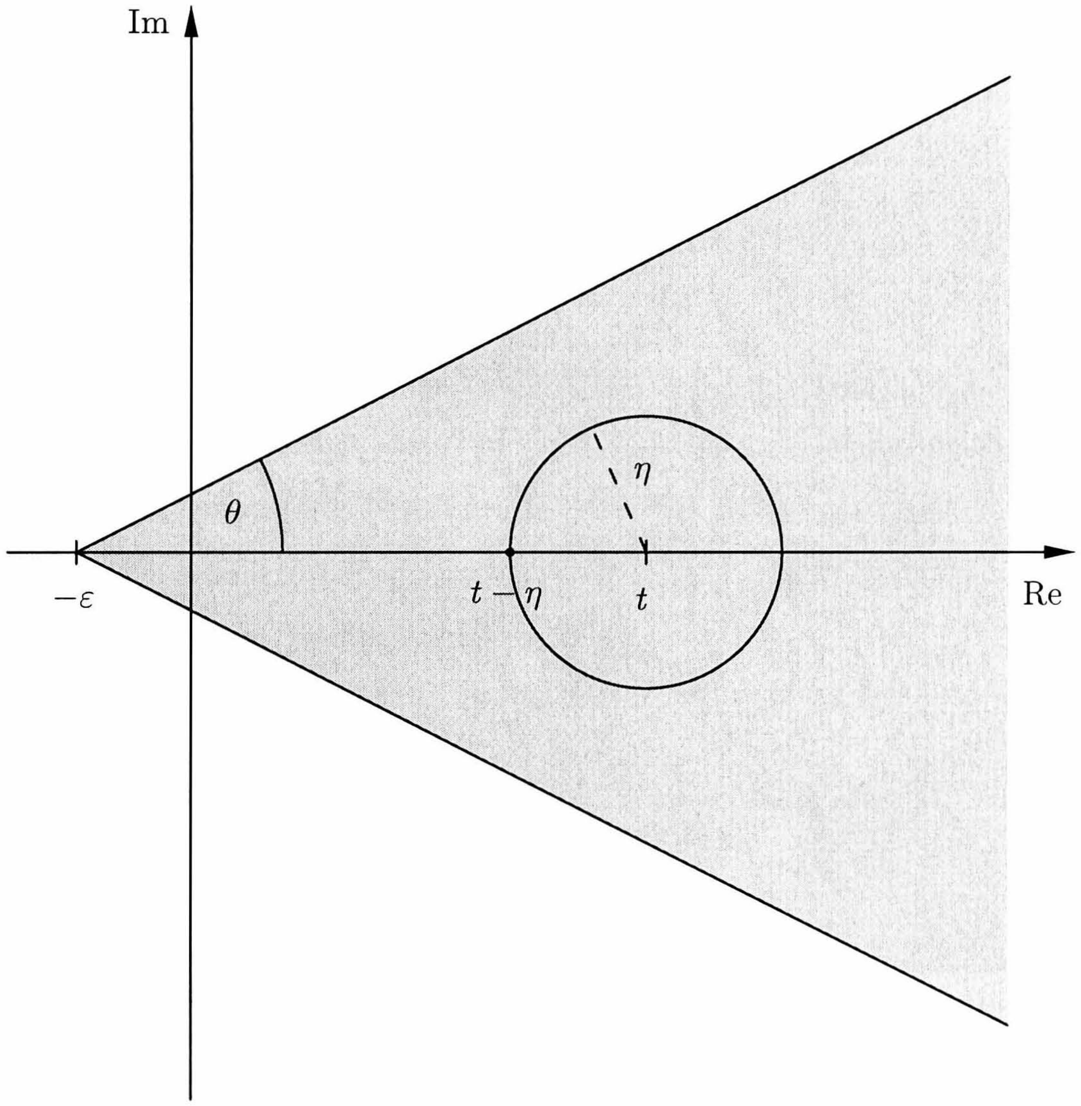


Figure 2.2: $\mathcal{D}_{\varepsilon,\theta}$ and the circular contour $C_\eta(t)$ used in the proof of Lemma 2.1.

2.3 A Quadrature Method for Intermediate Values of ρ

In this section, the starting point is similar to the procedure used in Section 2.2 to get (2.7), except that we first substitute $s = \sqrt{\kappa}\,t$ where $\kappa := \rho_0/\rho$ and $\rho_0 > 0$ is a parameter at our disposal. We then substitute $t = u/\sqrt{1-u^2}$ in (2.2) to get

$$Jf = \int_{-1}^{+1} G(u)\,du = IG, \tag{2.14}$$

where

$$G(u) := \frac{\sqrt{\kappa}\, f(\kappa P(u)) e^{-\rho_0 P(u)}}{(1-u^2)^{3/2}}, \qquad -1 < u < 1,$$

$$P(u) = \frac{u^2}{1-u^2} \geq 0, \qquad -1 < u < 1.$$

Without the substitution $s = \sqrt{\kappa}\,t$, or in other words if we choose $\rho_0 = \rho$, we obtain the expression (2.7) for Jf, in other words $G = F$. The effect of including the substitution $s = \sqrt{\kappa}\,t$ is thus to replace $e^{-\rho P(u)}$ with $e^{-\rho_0 P(u)}$. The idea is to choose a fixed value for ρ_0 so that $e^{-\rho_0 P(u)}$, which is infinitely differentiable and has all derivatives vanishing at ± 1, is evaluated accurately by the trapezium rule.

The jth derivative of $G(u)$, for $-1 < u < 1$, is

$$G^{(j)}(u) = \sum_{k=0}^{j} \left\{ \binom{j}{k} G_1^{(j-k)}(u) \left[\sum_{n=0}^{k} \binom{k}{n} G_2^{(k-n)}(u) G_3^{(n)}(u) \right] \right\}, \tag{2.15}$$

where

$$G_1(u) := (1-u^2)^{-3/2}, \qquad G_2(u) := e^{-\rho_0 P(u)}, \qquad G_3(u) := \sqrt{\kappa}\, f(\kappa P(u)).$$

We argue for G_1 and G_3 in the same way as the results in Section 2.2. For G_1 and its derivatives, it can easily be shown that, for $m = 0, 1, \ldots$,

$$|G_1^{(m)}(u)| \leq C_m (1-u^2)^{-3/2-m}, \qquad -1 < u < 1. \tag{2.16}$$

For G_3, provided Assumption 2.1 holds, then, for $m = 0, 1, \ldots, q$, by Lemmas 2.4 and 2.3.

$$\begin{aligned}
\left|G_3^{(m)}(u)\right| &\le \sqrt{\kappa}\sum_{j=0}^{m}\left|U_j^m(u)\kappa^j f^{(j)}(\kappa P(u))\right| \\
&\le C_m\sqrt{\kappa}\sum_{j=0}^{m}(1-u^2)^{-m-j}\kappa^j\left|f^{(j)}(\kappa P(u))\right| \\
&\le c\,C_m\sqrt{\kappa}\sum_{j=0}^{m}(1-u^2)^{-m-j}\kappa^j\left(1+\frac{\kappa u^2}{1-u^2}\right)^{-r-j} \\
&= c\,C_m\sqrt{\kappa}\sum_{j=0}^{m}(1-u^2)^{-m-j}\kappa^j\left(\frac{1+(\kappa-1)u^2}{1-u^2}\right)^{-r-j}.
\end{aligned}$$

To bound this expression observe that for $0 < \kappa \le 1$, $-1 < u < 1$, $1 + (\kappa - 1)u^2 \ge \kappa$. Also observe that for $\kappa \ge 1$, $1 + (\kappa - 1)u^2 \ge 1$ and $(1 - u^2)^{-r-j} \le (1 - u^2)^{-r-m}$ for $j = 0, 1, \ldots, m$. Thus, for $-1 < u < 1$,

$$\left|G_3^{(m)}(u)\right| \le \begin{cases} c\,C_m\sqrt{\kappa}\displaystyle\sum_{j=0}^{m}\kappa^{-r}(1-u^2)^{r-m}, & \text{if } \; 0<\kappa\le 1, \\ c\,C_m\sqrt{\kappa}\displaystyle\sum_{j=0}^{m}\kappa^{j}(1-u^2)^{r-m}, & \text{if } \; \kappa\ge 1, \end{cases}$$

so that

$$\left|G_3^{(m)}(u)\right| \le \begin{cases} c\,C_m\kappa^{-r+1/2}(1-u^2)^{r-m}, & \text{if } \; 0<\kappa\le 1, \\ c\,C_m\kappa^{m+1/2}(1-u^2)^{r-m}, & \text{if } \; \kappa\ge 1, \end{cases}$$

and, for $\kappa > 0$,

$$\left|G_3^{(m)}(u)\right| \le c\,C_m(\kappa^{-r+1/2}+\kappa^{m+1/2})(1-u^2)^{r-m}, \qquad -1<u<1. \tag{2.17}$$

Let

$$\mathcal{C}_0^\infty[-1,1] := \left\{\phi \in \mathcal{C}^\infty[-1,1] : \phi^{(m)}(\pm 1) = 0,\ m = 0,1,\ldots\right\}. \tag{2.18}$$

Then $G_2 \in \mathcal{C}_0^\infty[-1,1]$, and arguing similarly to the proof of Lemma 1.2, we obtain that, for every $p \in \mathbb{N}$ and $m = 0, 1, \ldots,$

$$\left|G_2^{(m)}(u)\right| \le C(1-u^2)^{p-m}, \qquad -1<u<1, \tag{2.19}$$

where the constant $C > 0$ depends on ρ_0, p, and m.

Theorem 2.6 *If Assumption 2.1 holds then, for every $p \in \mathbb{N}$ and $j = 0, 1, \ldots, q$,*

$$|G^{(j)}(u)| \le c\,C(\rho^{r-1/2} + \rho^{-q-1/2})(1-u^2)^{p+r-3/2-j}, \qquad -1 < u < 1,$$

where the constant $C > 0$ depends only on q, r, p and ρ_0.

Proof. Using (2.15) to (2.19) and absorbing all the binomial coefficients into the constant C, we find that

$$\begin{aligned}|G^{(j)}(u)| &\le c\,C(\kappa^{-r+1/2} + \kappa^{m+1/2})\sum_{k=0}^{j}\left\{(1-u^2)^{-3/2-j+k}\sum_{n=0}^{k}(1-u^2)^{p+r-k}\right\}\\ &\le c\,C(\kappa^{-r+1/2} + \kappa^{m+1/2})\sum_{k=0}^{j}(1-u^2)^{p+r-3/2-j}\\ &\le c\,C(\kappa^{-r+1/2} + \kappa^{m+1/2})(1-u^2)^{p+r-3/2-j}\\ &\le c\,C(\rho^{r-1/2} + \rho^{-q-1/2})(1-u^2)^{p+r-3/2-j}.\end{aligned}$$

■

We have shown that if Assumption 2.1 holds then, for all $\alpha > 0$, $G \in \mathcal{S}^{q,\alpha}$ with

$$\|G\|_{q,\alpha} \le c\,C(\rho^{r-1/2} + \rho^{-q-1/2}), \tag{2.20}$$

where the constant $C > 0$ depends only on q, r, α, and ρ_0, so that G and its derivatives up to the qth order vanish at ± 1. Thus the trapezium rule approximates to IG will converge rapidly. Since G is even and vanishes at ± 1, this approximation is

$$T_N G := \frac{1}{N}\left[G(0) + 2\sum_{k=1}^{N-1} G\left(\frac{k}{N}\right)\right]. \tag{2.21}$$

In view of the bound (2.20) and applying Theorem 1.2, we get the following error estimate.

Theorem 2.7 *Suppose that f satisfies Assumption 2.1, $q \in \mathbb{N}$, $q \ge 2$, and $\alpha < q$. Then the error in the quadrature (2.21) can be bounded by*

$$|Jf - T_N G| = |IG - T_N G| \le c\,C(\rho^{r-1/2} + \rho^{-q-1/2})N^{-\alpha},$$

where the constant C depends only on q, r, α, and ρ_0.

Combining Theorem 2.7 with Lemma 2.1, we obtain the following corollary.

Corollary 2.2 *Suppose that f satisfies Assumption 2.1′, $q \in \mathbb{N}$, $q \geq 2$, and $\alpha < q$. Then the error in the quadrature (2.21) can be bounded by*

$$|Jf - T_N G| \leq \frac{\widetilde{c}\, C(\rho^{r-1/2} + \rho^{-q-1/2})}{(\bar{\varepsilon}\sin\theta)^q} N^{-\alpha},$$

where $\bar{\varepsilon} = \min\{\varepsilon, 1\}$ and the constant C depends only on q, r, α, and ρ_0.

2.4 Numerical Examples

Let

$$f(x) = \frac{1}{1+x}. \tag{2.22}$$

As an example to illustrate the use of the quadrature rule (1.26) applied to integrals on the real line of steepest descent type, we will consider the problem of finding the numerical value of

$$Jf = \int_{-\infty}^{+\infty} e^{-\rho s^2} f(s^2)\, ds, \tag{2.23}$$

for $\rho = 0, 0.00001, 0.0001, 0.001, 0.01, 0.1, 1$. Substituting $s = u/\sqrt{1-u^2}$ in (2.23) and then $u = w(x)$ using the Kress form of w given by

$$w(x) := \frac{V(x) - V(-x)}{V(x) + V(-x)}, \qquad -1 \le x \le 1, \tag{2.24}$$

$$V(x) := \left[\left(\frac{1}{2} - \frac{1}{p}\right)x^3 + \frac{1}{p}x + \frac{1}{2}\right]^p, \qquad -1 \le x \le 1, \tag{2.25}$$

for some $p \geq 2$, we see that

$$Jf = \int_{-1}^{+1} F(u)\, du = \int_{-1}^{+1} w'(x) F(w(x)) dx, \tag{2.26}$$

where

$$F(u) = \frac{f(P(u))e^{-\rho P(u)}}{(1-u^2)^{3/2}}, \qquad P(u) = \frac{u^2}{1-u^2}, \qquad -1 < u < 1.$$

To illustrate the use of the quadrature method (2.26), the graphs of the integrands $F(u)$ and $w'(x)F(w(x))$, for $\rho = 0, 0.001, 1$, are depicted in Figures 2.3–2.5, respectively. It can be observed qualitatively in these figures that the integrand $w'(x)F(w(x))$ is smoother than $F(u)$, for the same choice of ρ, in particular near the endpoints ± 1, where this smoothness increases as p increases.

In the following results, the integral Jf is estimated by $J_N f$, the quadrature rule approximation (2.13), with $2N - 1$ points. We note that, since F is even, and in view of the symmetry properties (1.28),

$$J_N f = a_0 F(0) + 2 \sum_{k=1}^{N-1} a_k F(x_k), \tag{2.27}$$

where, for $k = 1, \dots, N-1$,

$$a_k := \frac{1}{N} w'\left(\frac{k}{N}\right), \qquad x_k := w\left(\frac{k}{N}\right).$$

For f given by (2.22), the analytic value of the integral Jf can be evaluated by using equations (7.1.3) and (7.1.4) in [1] and that $\operatorname{erfc} z = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-t^2} dt$. Using these equations, we obtain that

$$Jf = \pi e^\rho \operatorname{erfc}(\sqrt{\rho}).$$

All numerical results in Tables 2.1–2.7 are evaluated using the mapping function w given by (2.24) and (2.25), suggested by Kress [33]. In our example $f(x) = 1/(1+x)$, the parameter r in Assumption 2.1 is 1. Recall that we compute the error in estimating Jf with $J_N f$ given by (2.27). So we calculate and tabulate the EOC given by (1.45) in these tables. We also show at the top of each column the value of $(r - 1/2)p$: note that it follows from Theorem 2.5 that, as $N \to \infty$, $|Jf - J_N f| = O(N^{-s})$ where $s = (r - 1/2)p$.

In Figure 2.6, we plot against ρ the error in estimating Jf, with f given by (2.22), by $J_{128} f$, the quadrature rule approximation (2.13). In Figure 2.7, we plot against ρ the error in estimating Jf, with f given by (2.22), by the approximation (2.21). Figure 2.6 suggests that the quadrature rule approximation (2.13) is an accurate quadrature method for $0 < \rho \leq 10$, though the accuracy deteriorates somewhat around 10^{-10}. Alternatively, the trapezium rule approximation (2.21) is a quadrature method that is accurate for $10^{-2} \leq \rho \leq 10$.

In Table 2.1, we can see that the predicted convergence rate $(r - 1/2)p = p/2$ is observed for $p = 2 - 9$ (except $p = 6$ for which the predicted convergence rate is $6/2 = 3$, and the observed rate is 4). We show this convergence rate graphically in Figure 2.8.

As discussed at the beginning of Section 2.2 (page 60), for $\rho > 0$ we expect that $|Jf - J_N f| = O(N^{-r})$ as $N \to \infty$ for every $r > 0$. However, since $|Jf - J_N f|$ depends continuously on ρ, if ρ is small this superalgebraic rate of convergence will not be discernible until N is large. This is observed in Table 2.2 which repeats the calculations of Table 2.1 but with $\rho = 0.00001$ rather than $\rho = 0$. Comparing Tables 2.1 and 2.2, we see that the corresponding errors differ, for the same values of N and p, by no more than ≈ 0.01. As a result, EOC values of $\approx p/2$ are observed for N small for $p = 2, 3$. Similarly, Tables 2.3–2.7 repeat the same calculations but with ρ increasing from one table to the next by a factor of 10, from 0.0001 to 1. The corresponding errors in Tables 2.1 and 2.3

differ by no more than ≈ 0.04 and an EOC of $\approx p/2$ is observed for N small for $p = 2$. As ρ increases, the superalgebraic rate of convergence becomes apparent for smaller values of N.

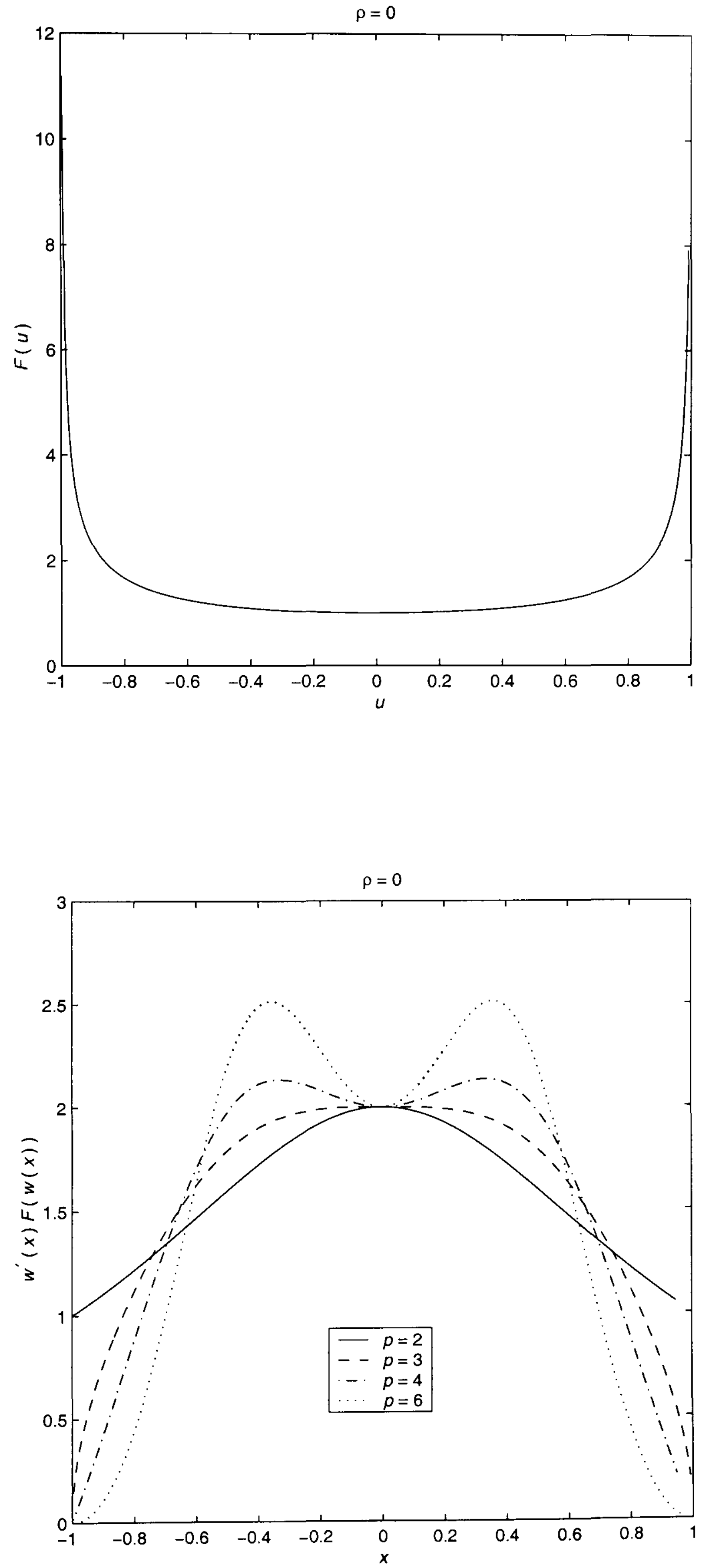


Figure 2.3: $F(u)$, $w'(x)F(w(x))$, with w given by equations (1.31) and (1.33) for $\rho = 0$.

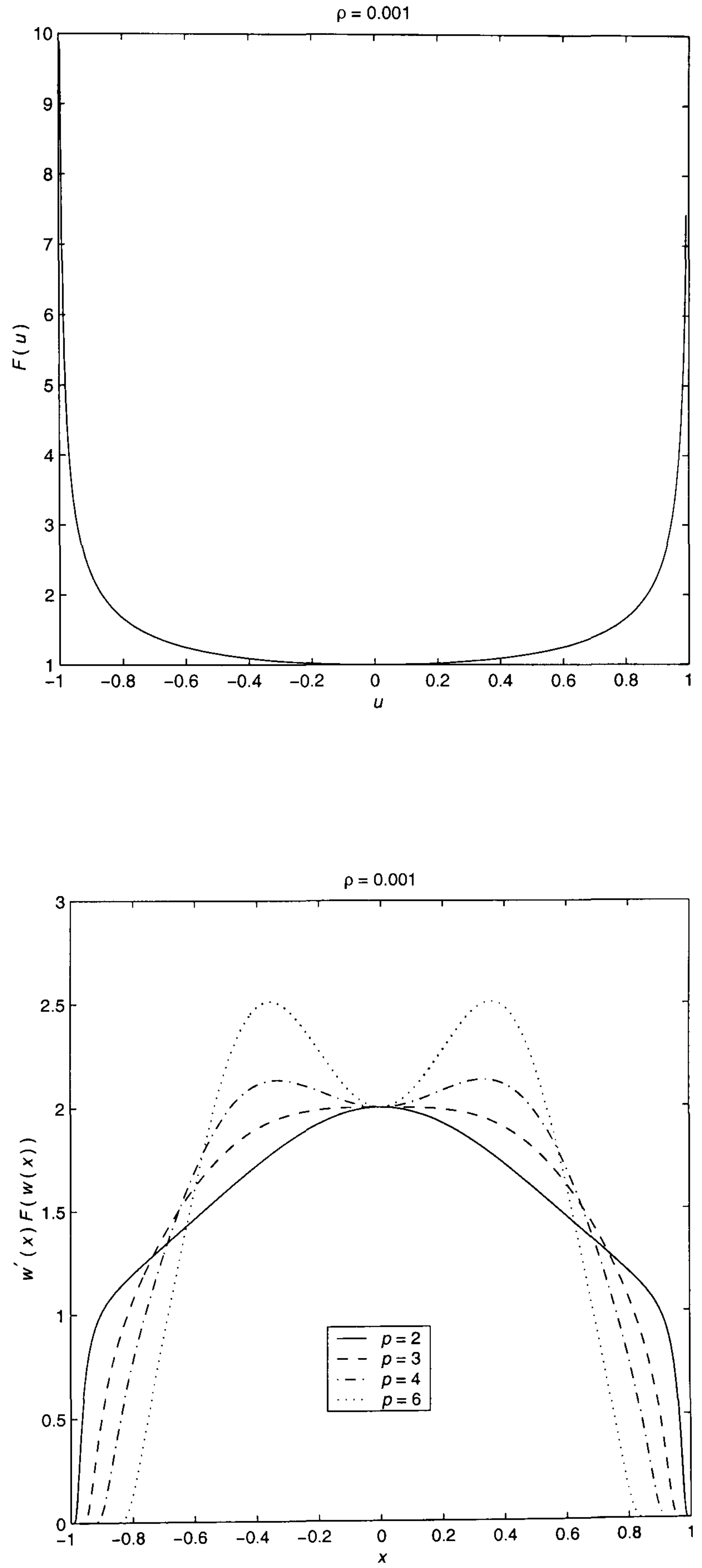


Figure 2.4: $F(u)$, $w'(x)F(w(x))$, with w given by equations (1.31) and (1.33) for $\rho = 0.001$.

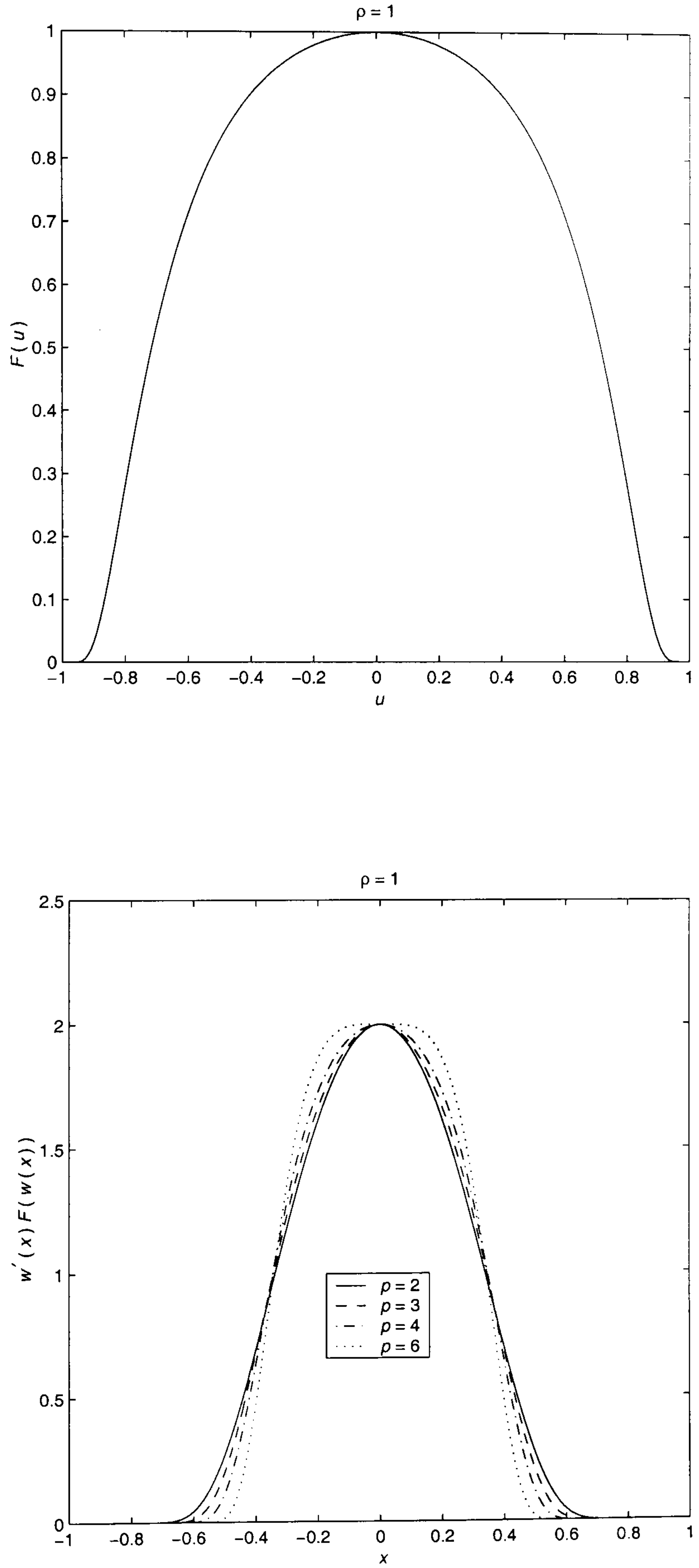


Figure 2.5: $F(u)$, $w'(x)F(w(x))$, with w given by equations (1.31) and (1.33) for $\rho = 1$.

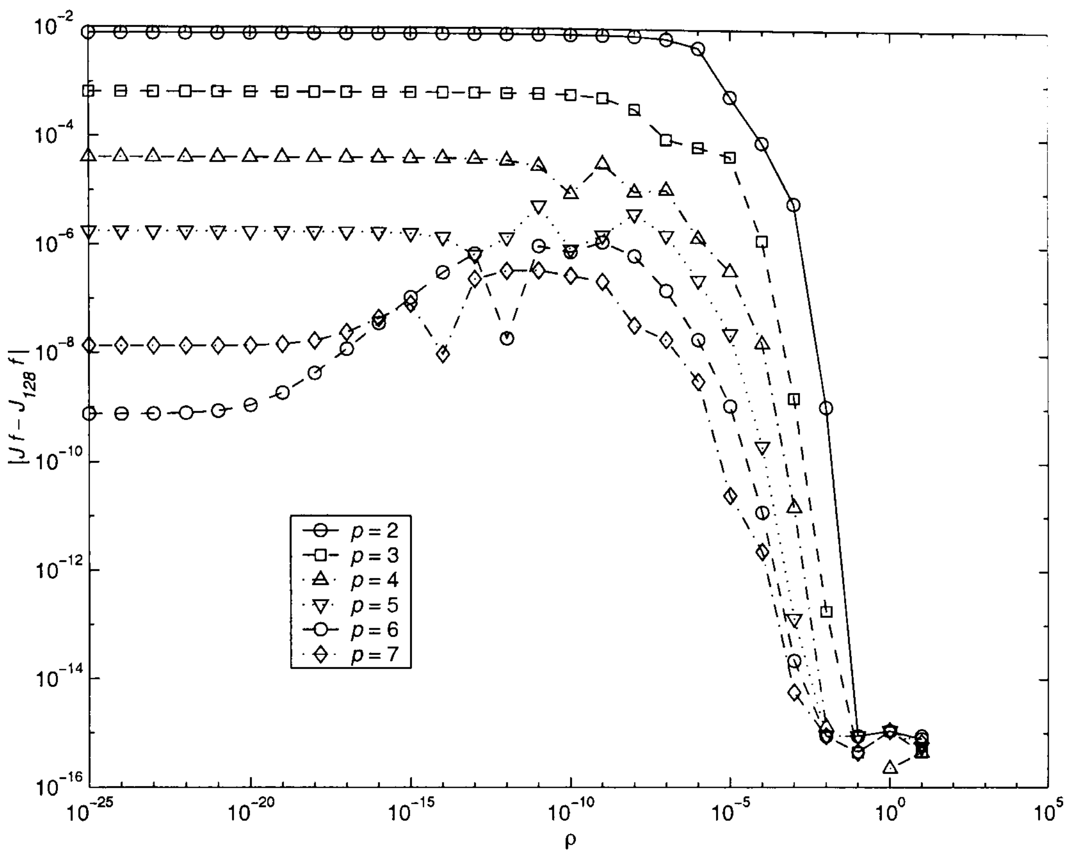


Figure 2.6: Error, $|Jf - J_{128}f|$, vs. ρ for $p = 2, \ldots, 7$.

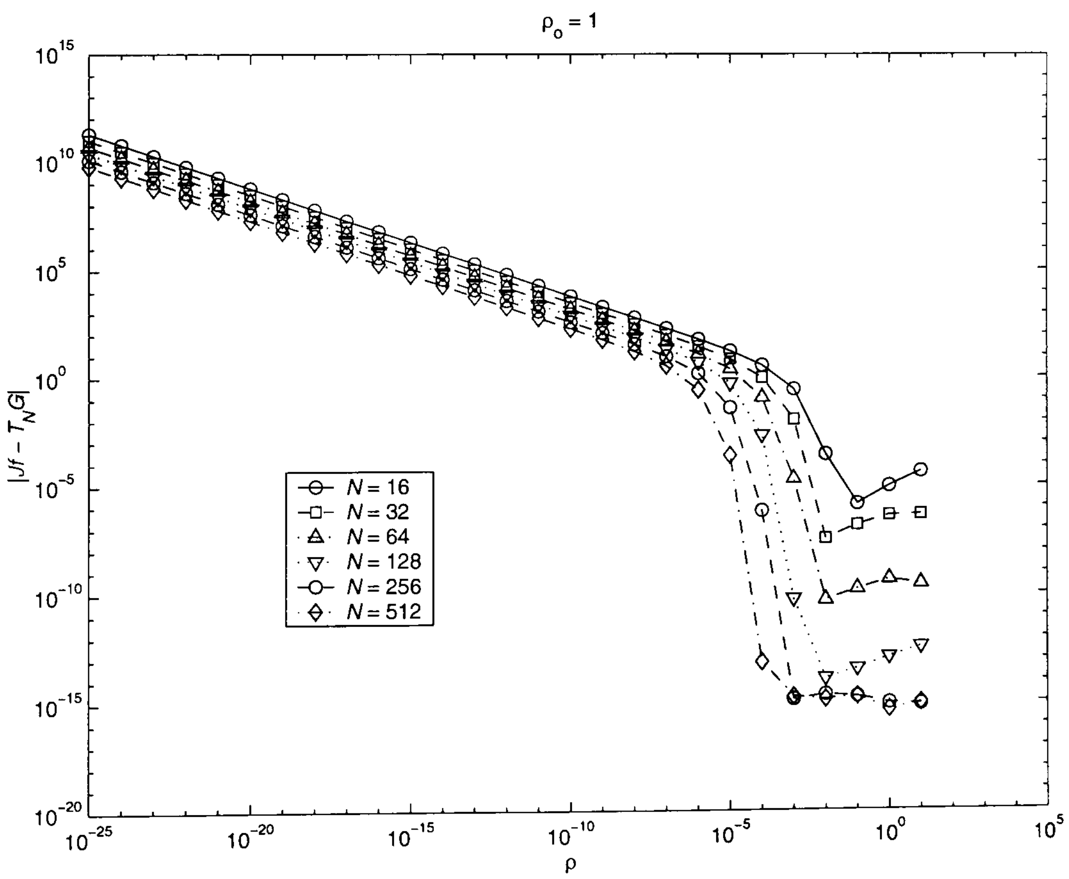


Figure 2.7: Error, $|Jf - T_N G|$, vs. ρ with $\rho_0 = 1$.

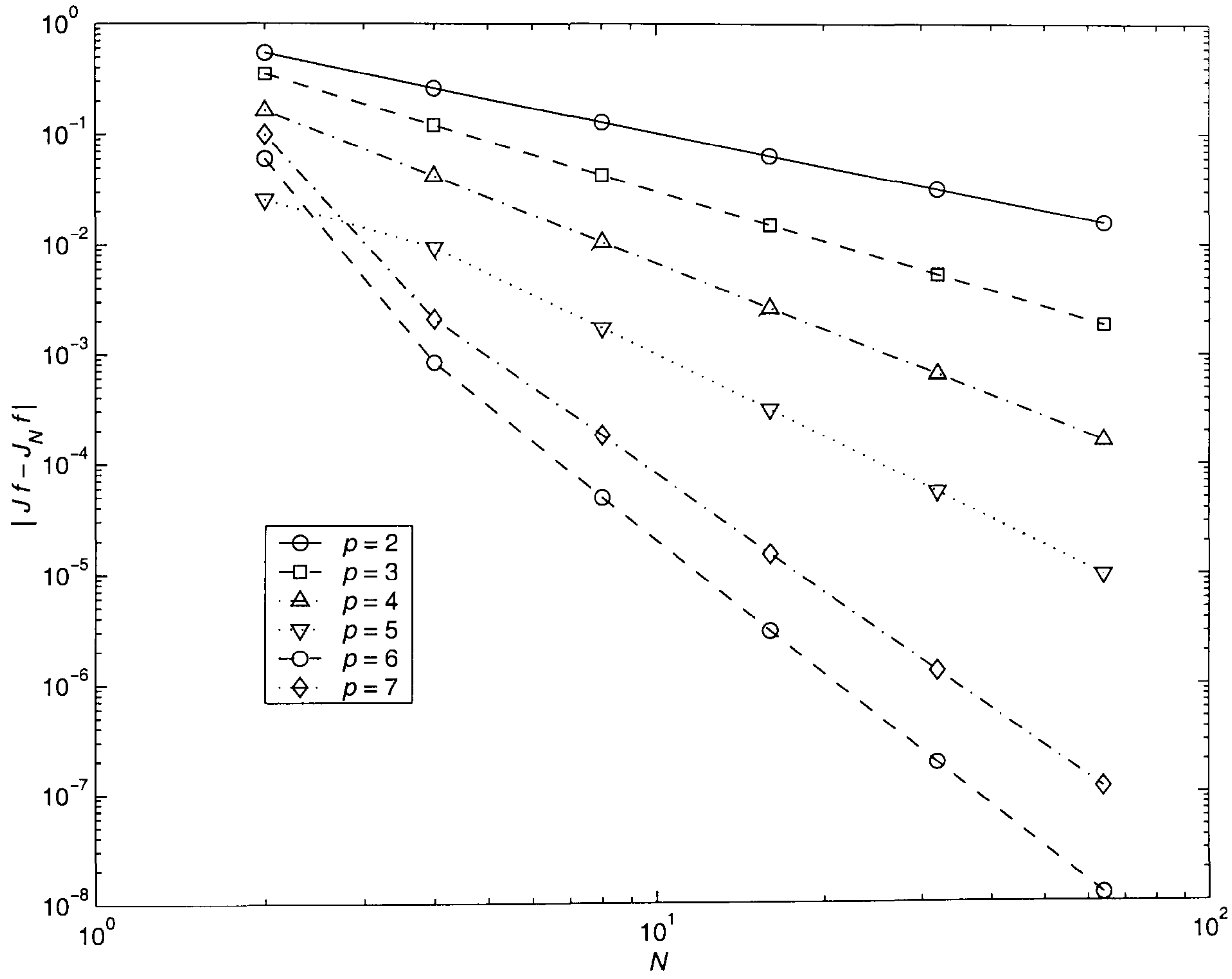


Figure 2.8: Error in estimating Jf with $J_N f$ for $\rho = 0$.

Table 2.1: $\rho = 0$

N	$p=2,\quad (r-1/2)p=1.0$ $\lvert Jf - J_N f\rvert$	EOC	$p=3,\quad (r-1/2)p=1.5$ $\lvert Jf - J_N f\rvert$	EOC	$p=4,\quad (r-1/2)p=2.0$ $\lvert Jf - J_N f\rvert$	EOC
2	5.4159E−01		3.4867E−01		1.6212E−01	
		1.0564		1.5286		1.9525
4	2.6042E−01		1.2086E−01		4.1886E−02	
		1.0291		1.5139		2.0056
8	1.2760E−01		4.2319E−02		1.0431E−02	
		1.0148		1.5067		2.0015
16	6.3151E−02		1.4893E−02		2.6051E−03	
		1.0075		1.5033		2.0004
32	3.1413E−02		5.2536E−03		6.5110E−04	
		1.0037		1.5016		2.0001
64	1.5666E−02		1.8553E−03		1.6276E−04	
		1.0019		1.5008		2.0000
128	7.8227E−03		6.5559E−04		4.0690E−05	
		1.0009		1.5004		2.0000
256	3.9088E−03		2.3172E−04		1.0173E−05	
		1.0005		1.5002		2.0000
512	1.9538E−03		8.1915E−05		2.5431E−06	
		1.0002		1.5001		2.0000
1024	9.7672E−04		2.8959E−05		6.3578E−07	
		1.0001		1.5000		2.0043
2048	4.8832E−04		1.0238E−05		1.5847E−07	
		1.0001		1.5000		2.0106
4096	2.4415E−04		3.6198E−06		3.9326E−08	

N	$p=5,\quad (r-1/2)p=2.5$ $\lvert Jf - J_N f\rvert$	EOC	$p=6,\quad (r-1/2)p=3.0$ $\lvert Jf - J_N f\rvert$	EOC	$p=7,\quad (r-1/2)p=3.5$ $\lvert Jf - J_N f\rvert$	EOC
2	2.5374E−02		5.9704E−02		9.8951E−02	
		1.4419		6.1604		5.5761
4	9.3395E−03		8.3469E−04		2.0741E−03	
		2.4429		4.0888		3.5271
8	1.7177E−03		4.9054E−05		1.7992E−04	
		2.4722		4.0236		3.5757
16	3.0956E−04		3.0162E−06		1.5089E−05	
		2.4857		4.0058		3.5362
32	5.5269E−05		1.8775E−07		1.3007E−06	
		2.4927		3.9947		3.5252
64	9.8197E−06		1.1778E−08		1.1297E−07	
		2.4963		3.9701		3.0661
128	1.7403E−06		7.5154E−10		1.3490E−08	
		2.4987		−1.4235		
256	3.0793E−07		2.0159E−09		(1.0119E−07)	
		2.4941		−3.2021		(0.7316)
512	5.4658E−08		1.8552E−08		(6.0940E−08)	
		2.2821				(0.6098)
1024	1.1237E−08		(8.8040E−09)		(3.9932E−08)	
				(−1.6897)		(0.3394)
2048	(6.9460E−08)		(2.8401E−08)		(3.1562E−08)	
		(0.6103)		(−0.0014)		(−0.0432)
4096	(4.5502E−08)		(2.8429E−08)		(3.2521E−08)	

N	$p=8,\quad (r-1/2)p=4.0$ $\lvert Jf-J_Nf\rvert$	EOC	$p=9,\quad (r-1/2)p=4.5$ $\lvert Jf-J_Nf\rvert$	EOC	$p=10,\quad (r-1/2)p=5.0$ $\lvert Jf-J_Nf\rvert$	EOC
2	9.9871E−02		6.9896E−02		1.5783E−02	
4	5.5146E−04	7.5007	1.3449E−03	5.6997	2.9422E−03	2.4234
8	8.0160E−05	2.7823	1.7244E−05	6.2852	2.3903E−06	10.2655
16	4.9782E−06	4.0092	8.3994E−07	4.3597	4.0450E−08	5.8849
32	3.1080E−07	4.0016	3.9703E−08	4.4029	5.5812E−09	2.8575
64	2.3015E−08	3.7553	7.3444E−09	2.4345	(7.3843E−08)	
128	1.5627E−08	0.5586	(2.2580E−08)		(4.2402E−08)	(0.8003)
256	(1.8995E−08)		(5.1661E−08)	(−1.1940)	(3.5151E−08)	(0.2706)
512	(2.4354E−08)	(−0.3586)	(3.0075E−08)	(0.7805)	(3.7188E−08)	(−0.0813)
1024	(3.0648E−08)	(−0.3316)	(2.8339E−08)	(0.0858)	(3.1962E−08)	(0.2185)
2048	(3.3471E−08)	(−0.1271)	(3.2429E−08)	(−0.1945)	(3.5008E−08)	(−0.1313)
4096	(2.9657E−08)	(0.1745)	(3.0797E−08)	(0.0745)	(3.6459E−08)	(−0.0586)

N	$p=15,\quad (r-1/2)p=7.5$ $\lvert Jf-J_Nf\rvert$	EOC	$p=20,\quad (r-1/2)p=10.0$ $\lvert Jf-J_Nf\rvert$	EOC	$p=25,\quad (r-1/2)p=12.5$ $\lvert Jf-J_Nf\rvert$	EOC
2	4.4122E−01		9.4406E−01		1.3486E+00	
4	7.9163E−03	5.8005	3.5939E−03	8.0372	2.3873E−02	5.8199
8	2.1257E−06	11.8626	4.5405E−05	6.3065	(7.6575E−05)	
16	7.7765E−08	4.7727	(4.3376E−09)		(1.2800E−08)	(12.5465)
32	(3.9542E−08)		(2.7525E−08)	(−2.6658)	(1.4489E−09)	(3.1431)
64	(3.1448E−08)	(0.3304)	(1.7446E−08)	(0.6579)	(1.8242E−08)	(−3.6542)
128	(3.3021E−08)	(−0.0704)	(3.0985E−08)	(−0.8287)	(3.6937E−08)	(−1.0178)
256	(4.1652E−08)	(−0.3350)	(3.5651E−08)	(−0.2024)	(3.8754E−08)	(−0.0693)
512	(4.2590E−08)	(−0.0321)	(3.4489E−08)	(0.0478)	(3.6389E−08)	(0.0909)
1024	(4.0766E−08)	(0.0632)	(2.9958E−08)	(0.2032)	(3.6575E−08)	(−0.0074)
2048	(4.2353E−08)	(−0.0551)	(3.1533E−08)	(−0.0739)	(3.4585E−08)	(0.0807)
4096	(4.2198E−08)	(0.0053)	(3.1814E−08)	(−0.0128)	(3.5196E−08)	(−0.0253)

Table 2.2: $\rho = 0.00001$

N	$p=2,\quad (r-1/2)p=1.0$ $\lvert Jf - J_N f\rvert$	EOC	$p=3,\quad (r-1/2)p=1.5$ $\lvert Jf - J_N f\rvert$	EOC	$p=4,\quad (r-1/2)p=2.0$ $\lvert Jf - J_N f\rvert$	EOC
2	5.3044E−01		3.3753E−01		1.5099E−01	
		1.0891		1.6195		2.2825
4	2.4933E−01		1.0985E−01		3.1035E−02	
		1.0959		1.7933		5.4812
8	1.1665E−01		3.1691E−02		6.9479E−04	
		1.1529		2.5687		−2.0853
16	5.2457E−02		5.3419E−03		2.9485E−03	
		1.3042		1.8882		2.1906
32	2.1242E−02		1.4431E−03		6.4587E−04	
		1.7032		7.2125		3.7783
64	6.5237E−03		9.7299E−06		4.7073E−05	
		3.4433		−2.2625		7.0701
128	5.9974E−04		4.6686E−05		3.5032E−07	
		0.6591		6.4893		8.7177
256	3.7980E−04		5.1964E−07		8.3213E−10	
		3.2302		9.2414		17.5156
512	4.0474E−05		8.5853E−10		4.4409E−15	
		4.4256		12.1045		−0.2630
1024	1.8834E−06		1.9496E−13		5.3291E−15	
		16.2373		3.9707		3.5850
2048	2.4380E−11		1.2434E−14		4.4409E−16	
		0.2611		2.4854		−3.4594
4096	2.0344E−11		2.2204E−15		4.8850E−15	

N	$p=5,\quad (r-1/2)p=2.5$ $\lvert Jf - J_N f\rvert$	EOC	$p=6,\quad (r-1/2)p=3.0$ $\lvert Jf - J_N f\rvert$	EOC	$p=7,\quad (r-1/2)p=3.5$ $\lvert Jf - J_N f\rvert$	EOC
2	1.4274E−02		7.0775E−02		1.0999E−01	
		3.5403		2.6993		3.2881
4	1.2269E−03		1.0897E−02		1.1260E−02	
		−2.2330		2.1481		1.4177
8	5.7679E−03		2.4586E−03		4.2145E−03	
		1.8137		1.5882		3.3710
16	1.6407E−03		8.1767E−04		4.0736E−04	
		3.8267		7.1026		3.5430
32	1.1563E−04		5.9495E−06		3.4948E−05	
		4.1803		3.2215		7.2839
64	6.3782E−06		6.3786E−07		2.2427E−07	
		8.0149		9.1352		13.1211
128	2.4659E−08		1.1344E−09		2.5172E−11	
		15.05347		17.2845		
256	7.2520E−13		7.1054E−15			
		6.6733		0.5406		
512	7.1054E−15		4.8850E−15			
		3.0000				
1024	8.8818E−16					
2048						
4096						

Table 2.3: $\rho = 0.0001$

N	$p=2,\quad (r-1/2)p = 1.0$		$p=3,\quad (r-1/2)p = 1.5$		$p=4,\quad (r-1/2)p = 2.0$	
	$\lvert Jf - J_N f\rvert$	EOC	$\lvert Jf - J_N f\rvert$	EOC	$\lvert Jf - J_N f\rvert$	EOC
2	5.0674E−01		3.1392E−01		1.2754E−01	
		1.1636		1.8444		3.6707
4	2.2620E−01		8.7420E−02		1.0015E−02	
		1.2563		2.7888		−0.1062
8	9.4690E−02		1.2650E−02		1.0780E−02	
		1.5283		1.3708		2.1607
16	3.2827E−02		4.8913E−03		2.4110E−03	
		2.4376		3.4048		5.4775
32	6.0598E−03		4.6181E−04		5.4115E−05	
		2.2249		2.2362		4.3730
64	1.2963E−03		9.8020E−05		2.6116E−06	
		3.9204		6.2175		7.3264
128	8.5614E−05		1.3173E−06		1.6272E−08	
		2.7740		7.9882		15.3164
256	1.2517E−05		5.1879E−09		3.9879E−13	
		6.3610		14.6801		6.4886
512	1.5229E−07		1.9762E−13		4.4409E−15	
		7.9209		5.9903		2.3219
1024	6.2837E−10		3.1086E−15		8.8818E−16	
		14.3879		−1.0000		−1.3219
2048	2.9310E−14		6.2172E−15		2.2204E−15	
		3.0444		1.4854		−1.2630
4096	3.5527E−15		2.2204E−15		5.3291E−15	

N	$p=5,\quad (r-1/2)p = 2.5$		$p=6,\quad (r-1/2)p = 3.0$		$p=7,\quad (r-1/2)p = 3.5$	
	$\lvert Jf - J_N f\rvert$	EOC	$\lvert Jf - J_N f\rvert$	EOC	$\lvert Jf - J_N f\rvert$	EOC
2	8.9761E−03		9.3769E−02		1.3266E−01	
		−1.1346		1.9098		2.8898
4	1.9708E−02		2.4956E−02		1.7899E−02	
		3.1384		1.5643		3.1307
8	2.2381E−03		8.4384E−03		2.0436E−03	
		0.7105		3.1423		1.5265
16	1.3677E−03		9.5572E−04		7.0935E−04	
		5.0151		5.1588		5.6413
32	4.2296E−05		2.6753E−05		1.4212E−05	
		8.4383		14.2180		8.4050
64	1.2193E−07		1.4038E−09		4.1927E−08	
		9.2026		6.8191		14.1437
128	2.0694E−10		1.2433E−11		2.3164E−12	
		18.8299		13.1880		
256	4.4409E−16		1.3323E−15		(3.5527E−15)	
		−1.0000		−1.0000		(−0.5850)
512	8.8818E−16		2.6645E−15		(5.3291E−15)	
		1.0000				
1024	4.4409E−16		(3.5527E−15)		(0)	
				(−0.4594)		
2048	(3.5527E−15)		(4.8850E−15)		(2.2204E−15)	
		(−0.5850)		(0.6521)		(−0.4854)
4096	(5.3291E−15)		(3.1086E−15)		(3.1086E−15)	

Table 2.4: $\rho = 0.001$

N	$p=2,\quad (r-1/2)p=1.0$ $\lvert Jf - J_N f\rvert$	EOC	$p=3,\quad (r-1/2)p=1.5$ $\lvert Jf - J_N f\rvert$	EOC	$p=4,\quad (r-1/2)p=2.0$ $\lvert Jf - J_N f\rvert$	EOC
2	4.3540E−01		2.4355E−01		5.8698E−02	
		1.4393		3.0860		0.7386
4	1.6055E−01		2.8681E−02		3.5179E−02	
		1.9911		0.8567		3.5885
8	4.0388E−02		1.5839E−02		2.9245E−03	
		5.1399		2.7158		1.3507
16	1.1455E−03		2.4109E−03		1.1467E−03	
		−0.9156		4.3347		4.6025
32	2.1608E−03		1.1948E−04		4.7204E−05	
		3.3696		4.6807		8.1830
64	2.0906E−04		4.6585E−06		1.6242E−07	
		5.0358		11.5104		13.3640
128	6.3730E−06		1.5969E−09		1.5406E−11	
		11.1396		13.0706		13.4973
256	2.8248E−09		1.8563E−13		1.3323E−15	
		8.8355				0
512	6.1835E−12		0		1.3323E−15	
		10.7653				−1.4150
1024	3.5527E−15		3.1086E−15		3.5527E−15	
		−0.9069		0		0.1926
2048	6.6613E−15		3.1086E−15		3.1086E−15	
		−0.1806		1.8074		−0.7776
4096	7.5495E−15		8.8818E−16		5.3291E−15	

N	$p=5,\quad (r-1/2)p=2.5$ $\lvert Jf - J_N f\rvert$	EOC	$p=6,\quad (r-1/2)p=3.0$ $\lvert Jf - J_N f\rvert$	EOC	$p=7,\quad (r-1/2)p=3.5$ $\lvert Jf - J_N f\rvert$	EOC
2	7.5799E−02		1.5804E−01		1.9378E−01	
		0.8556		3.6392		2.5622
4	4.1889E−02		1.2684E−02		3.2810E−02	
		3.1307		0.6561		8.4604
8	4.7826E−03		8.0496E−03		9.3146E−05	
		5.4722		4.0932		−2.4952
16	1.0774E−04		4.7162E−04		5.2515E−04	
		6.4514		5.7091		6.1952
32	1.2311E−06		9.0155E−06		7.1672E−06	
		6.7122		10.6196		12.3461
64	1.1742E−08		5.7302E−09		1.3766E−09	
		16.4274		17.9774		17.8633
128	1.3323E−13		2.2204E−14		5.7732E−15	
		7.2288		5.6439		
256	8.8818E−16		4.4409E−16		(0)	
		−1.3219		−1.0000		
512	2.2204E−15		8.8818E−16		(2.6645E−15)	
		1.3219				(−0.4150)
1024	8.8818E−16		(4.4409E−16)		(3.5527E−15)	
				(0)		(−0.1699)
2048	(5.7732E−15)		(4.4409E−16)		(3.9968E−15)	
		(0.5305)		(−4.5850)		(0.8480)
4096	(3.9968E−15)		(1.0658E−14)		(2.2204E−15)	

Table 2.5: $\rho = 0.01$

	$p=2, \quad (r-1/2)p = 1.0$		$p=3, \quad (r-1/2)p = 1.5$		$p=4, \quad (r-1/2)p = 2.0$	
N	$\lvert Jf - J_N f\rvert$	EOC	$\lvert Jf - J_N f\rvert$	EOC	$\lvert Jf - J_N f\rvert$	EOC
2	2.4450E−01		6.2135E−02		1.0775E−01	
		3.4180		0.3049		2.2331
4	2.2875E−02		5.0298E−02		2.2920E−02	
		0.6749		2.4919		1.8509
8	1.4328E−02		8.9414E−03		6.3537E−03	
		3.3129		6.6843		5.0750
16	1.4418E−03		8.6943E−05		1.8850E−04	
		4.0076		4.5002		7.1636
32	8.9640E−05		3.8419E−06		1.3147E−06	
		8.2577		8.4584		12.1228
64	2.9288E−07		1.0922E−08		2.9478E−10	
		8.0674		15.8865		17.7554
128	1.0918E−09		1.8030E−13		1.3323E−15	
		16.3225		8.6653		0.5850
256	1.3323E−14		4.4409E−16		8.8818E−16	
		2.9069		−2.3219		−0.5850
512	1.7764E−15		2.2204E−15		1.3323E−15	
		0.4150		−0.8480		−0.7370
1024	1.3323E−15		3.9968E−15		2.2204E−15	
		−1.8745		0		−1.1375
2048	4.8850E−15		3.9968E−15		4.8850E−15	
		1.1375		−1.0780		0
4096	2.2204E−15		8.4377E−15		4.8850E−15	

	$p=5, \quad (r-1/2)p = 2.5$		$p=6, \quad (r-1/2)p = 3.0$		$p=7, \quad (r-1/2)p = 3.5$	
N	$\lvert Jf - J_N f\rvert$	EOC	$\lvert Jf - J_N f\rvert$	EOC	$\lvert Jf - J_N f\rvert$	EOC
2	2.2263E−01		2.8036E−01		2.8623E−01	
		2.1593		2.1541		5.0806
4	4.9839E−02		6.2987E−02		8.4584E−03	
		4.6040		3.5561		0.2702
8	2.0494E−03		5.3550E−03		7.0138E−03	
		3.1081		4.5084		5.0742
16	2.3768E−04		2.3529E−04		2.0820E−04	
		8.6278		8.2714		9.7083
32	6.0082E−07		7.6147E−07		2.4888E−07	
		12.2058		13.5277		15.3859
64	1.2719E−10		6.4476E−11		5.8127E−12	
		18.1277		16.1476		12.6761
128	4.4409E−16		8.8818E−16		8.8818E−16	
		−1.0000		−0.5850		
256	8.8818E−16		1.3323E−15		(2.2204E−15)	
						(−0.2630)
512	0		0		(2.6645E−15)	
						(0.5850)
1024	8.8818E−16		(2.2204E−15)		(1.7764E−15)	
				(−0.6781)		(−1.0000)
2048	(1.3323E−15)		(3.5527E−15)		(3.5527E−15)	
		(−2.5850)		(−1.6439)		(−0.4594)
4096	(7.9936E−15)		(1.1102E−14)		(4.8850E−15)	

Table 2.6: $\rho = 0.1$

N	$p=2,\ (r-1/2)p=1.0$ $\lvert Jf - J_N f\rvert$	EOC	$p=3,\ (r-1/2)p=1.5$ $\lvert Jf - J_N f\rvert$	EOC	$p=4,\ (r-1/2)p=2.0$ $\lvert Jf - J_N f\rvert$	EOC
2	6.6217E−02		1.6776E−01		2.1695E−01	
		2.9051		2.4795		5.9936
4	8.8398E−03		3.0081E−02		3.4049E−03	
		4.8410		4.7354		1.3061
8	3.0843E−04		1.1293E−03		1.3769E−03	
		6.0792		6.4202		6.9261
16	4.5617E−06		1.3187E−05		1.1323E−05	
		10.6125		9.9232		12.4804
32	2.9138E−09		1.3582E−08		1.9814E−09	
		8.9254		15.7735		17.2818
64	5.9930E−12		2.4247E−13		1.2434E−14	
		12.1352		8.0928		
128	1.3323E−15		8.8818E−16		0	
		0		1.0000		
256	1.3323E−15		4.4409E−16		4.4409E−16	
		−0.4150		0		0
512	1.7764E−15		4.4409E−16		4.4409E−16	
		−0.5850		−1.5850		−2.0000
1024	2.6645E−15		1.3323E−15		1.7764E−15	
		0		0		−0.3219
2048	2.6645E−15		1.3323E−15		2.2204E−15	
		−2.3692		1.5850		0
4096	1.3767E−14		4.4409E−16		2.2204E−15	

N	$p=5,\ (r-1/2)p=2.5$ $\lvert Jf - J_N f\rvert$	EOC	$p=6,\ (r-1/2)p=3.0$ $\lvert Jf - J_N f\rvert$	EOC	$p=7,\ (r-1/2)p=3.5$ $\lvert Jf - J_N f\rvert$	EOC
2	1.8561E−01		7.9431E−02		8.6767E−02	
		2.1239		0.5550		1.3210
4	4.2584E−02		5.4065E−02		3.4729E−02	
		7.6012		3.7992		5.1565
8	2.1931E−04		3.8838E−03		9.7369E−04	
		3.0609		9.2030		7.2355
16	2.6281E−05		6.5897E−06		6.4615E−06	
		11.4393		8.3549		8.1229
32	9.4636E−09		2.0127E−08		2.3179E−08	
		18.1552		18.4565		18.2798
64	3.2419E−14		5.5955E−14		7.2831E−14	
		5.1898		5.9773		6.3576
128	8.8818E−16		8.8818E−16		8.8818E−16	
		1.0000		−0.5850		
256	4.4409E−16		1.3323E−15		(4.4409E−16)	
		−1.5850		0		
512	1.3323E−15		1.3323E−15		(0)	
		−0.4150				
1024	1.7764E−15		(3.5527E−15)		(1.7764E−15)	
				(2.0000)		
2048	(1.7764E−15)		(8.8818E−16)		(0)	
		(0.4150)		(1.0000)		
4096	(1.3323E−15)		(4.4409E−16)		(1.0658E−14)	

Table 2.7: $\rho = 1$

N	$p=2,\quad (r-1/2)p=1.0$		$p=3,\quad (r-1/2)p=1.5$		$p=4,\quad (r-1/2)p=2.0$	
	$\lvert Jf - J_N f\rvert$	EOC	$\lvert Jf - J_N f\rvert$	EOC	$\lvert Jf - J_N f\rvert$	EOC
2	7.2872E−02		1.4173E−01		2.2760E−01	
		9.6032		4.3773		3.9325
4	9.3695E−05		6.8197E−03		1.4907E−02	
		1.7595		6.1598		6.6580
8	2.7672E−05		9.5387E−05		1.4762E−04	
		10.7098		10.3620		8.9651
16	1.6523E−08		7.2477E−08		2.9537E−07	
		26.1490		16.6596		16.9967
32	2.2204E−16		7.0011E−13		2.2586E−12	
		−1.0000		10.6225		11.7274
64	4.4409E−16		4.4409E−16		6.6613E−16	
		−1.3219		−1.5850		−0.4150
128	1.1102E−15		1.3323E−15		8.8818E−16	
		1.3219		0.2630		−0.3219
256	4.4409E−16		1.1102E−15		1.1102E−15	
		0		−0.4854		2.3219
512	4.4409E−16		1.5543E−15		2.2204E−16	
		−1.0000		−1.0000		−1.0000
1024	8.8818E−16		3.1086E−15		4.4409E−16	
		−0.3219		0.4854		−2.7004
2048	1.1102E−15		2.2204E−15		2.8866E−15	
		−1.3785		−1.0704		0.1155
4096	2.8866E−15		4.6629E−15		2.6645E−15	

N	$p=5,\quad (r-1/2)p=2.5$		$p=6,\quad (r-1/2)p=3.0$		$p=7,\quad (r-1/2)p=3.5$	
	$\lvert Jf - J_N f\rvert$	EOC	$\lvert Jf - J_N f\rvert$	EOC	$\lvert Jf - J_N f\rvert$	EOC
2	2.9202E−01		3.2640E−01		3.3941E−01	
		4.5318		7.0559		3.7424
4	1.2624E−02		2.4531E−03		2.5360E−02	
		4.9943		2.2045		3.9877
8	3.9608E−04		5.3223E−04		1.5986E−03	
		8.9213		8.0254		8.3657
16	8.1695E−07		2.0427E−06		4.8465E−06	
		19.4170		15.5129		16.9311
32	1.1671E−12		4.3687E−11		3.8785E−11	
		12.3597		16.0010		15.8293
64	2.2204E−16		6.6613E−16		6.6613E−16	
		−2.3219		1.5850		−0.4150
128	1.1102E−15		2.2204E−16		8.8818E−16	
		−0.4854		−2.3219		
256	1.5543E−15		1.1102E−15		(2.2204E−16)	
		1.8074		0		(−1.5850)
512	4.4409E−16		1.1102E−15		(6.6613E−16)	
		−2.0000				
1024	1.7764E−15		(2.2204E−16)		(0)	
				(−4.0000)		
2048	(1.5543E−15)		(3.5527E−15)		(1.9984E−15)	
		(−0.5146)		(1.1926)		(0.8480)
4096	(2.2204E−15)		(1.5543E−15)		(1.1102E−15)	

Chapter 3

Efficient Evaluation of the Half-Plane Impedance Green's Function for the Helmholtz Equation

In this chapter, we consider the problem of efficient evaluation of the half-plane impedance Green's function for the Helmholtz equation. We develop methods based on applying the quadrature rule (2.13) and the main results in Chapter 2 to representations for the Green's function in terms of Laplace-type integrals of the form

$$\int_0^\infty t^{-1/2} e^{-\rho t} f(t)\, dt, \tag{3.1}$$

where $\rho \geq 0$, and $f(t)$ is an analytic function in a sector of the complex plane containing the positive real axis and satisfying Assumption 2.1′ in Section 2.2.

For ρ not too small, this type of integral can be effectively evaluated by Gauss–Laguerre quadrature as discussed in Section 2.1, and this method has been applied to evaluation of the half-plane impedance Green's function in Chandler-Wilde and Hothersall [11, 12]. For ρ large, asymptotic approximations, see e.g. Bender and Orszag [5] and Jones [29], based e.g. on Watson's lemma [5] are also accurate. Clearly, however, this Gauss–Laguerre quadrature method is not appropriate if $\rho = 0$, and is not accurate for ρ small. So the main objective of this chapter is to numerically evaluate the integral (3.1) for ρ small.

For completeness of this thesis and to see Laplace-type integrals of the form (3.1) in a real problem, we will start this chapter in Section 3.1 with a description (taken in quite large part from [11, 12]) of the problem of acoustic propagation from a monofrequency coherent line source above a plane of homogeneous surface impedance. A generalised asymptotic expansion for this Green's function in the far field using the modified steepest descent method of Ott [42] is presented in Chandler-Wilde and Hothersall [13].

3.1 Formulation of the Problem

We consider a model of outdoor sound propagation from a coherent line source (situated in a homogeneous and stationary fluid medium) parallel to a homogeneous impedance plane. This problem is effectively two-dimensional in the plane perpendicular to the line source (see Figure 3.1). Let $G_\beta(\mathbf{r}, \mathbf{r}_0)$ denote the acoustic pressure at the point $\mathbf{r}$ when a unit strength monopole source is located at $\mathbf{r}_0$ and the impedance plane has relative surface admittance β (with $\beta = 0$ for a rigid boundary and $\mathrm{Re}\,\beta > 0$ for an energy-absorbing boundary). Then $G_\beta(\mathbf{r}, \mathbf{r}_0)$ satisfies the inhomogeneous Helmholtz equation

$$(\Delta + k^2)G_\beta(\mathbf{r}, \mathbf{r}_0) = -\delta(\mathbf{r} - \mathbf{r}_0), \qquad \mathbf{r} \in U, \tag{3.2}$$

the impedance boundary condition

$$\frac{\partial}{\partial y} G_\beta(\mathbf{r}, \mathbf{r}_0) + ik\beta G_\beta(\mathbf{r}, \mathbf{r}_0) = 0, \qquad \mathbf{r} \in \partial U, \tag{3.3}$$

the Sommerfeld radiation and boundedness conditions,

$$\frac{\partial}{\partial r} G_\beta(\mathbf{r}, \mathbf{r}_0) - ikG_\beta(\mathbf{r}, \mathbf{r}_0) = o(r^{-1/2}), \qquad G_\beta(\mathbf{r}, \mathbf{r}_0) = O(r^{-1/2}), \tag{3.4}$$

uniformly in θ as $r \to \infty$ with $0 < \theta < \pi$, where (r, θ) are the plane polar coordinates of $\mathbf{r}$. We assume throughout that $\mathrm{Re}\,\beta \geq 0$, and express $G_\beta(\mathbf{r}, \mathbf{r}_0)$ as the sum of $G_0(\mathbf{r}, \mathbf{r}_0)$ and a correction $P_\beta(\mathbf{r}, \mathbf{r}_0)$, i.e.,

$$G_\beta(\mathbf{r}, \mathbf{r}_0) = G_0(\mathbf{r}, \mathbf{r}_0) + P_\beta(\mathbf{r}, \mathbf{r}_0), \tag{3.5}$$

where

$$G_0(\mathbf{r}, \mathbf{r}_0) = \frac{i}{4}\mathrm{H}_0^{(1)}(kR) + \frac{i}{4}\mathrm{H}_0^{(1)}(kR') \tag{3.6}$$

is the solution of equations (3.2) and (3.3) for $\beta = 0$, found by the method of images. Here $\mathrm{H}_0^{(1)}$ is the Hankel function of the first kind of order zero which has a representation as a Laplace-type integral as

$$\mathrm{H}_0^{(1)}(z) = -\frac{2i}{\pi}\int_0^\infty \frac{t^{-1/2}e^{(i-t)z}}{(t-2i)^{1/2}}\,dt, \qquad \mathrm{Re}\, z > 0, \tag{3.7}$$

or can be efficiently and accurately evaluated using e.g. equations (9.4.1) through (9.4.3) in [1]. To find P_β, we substitute (3.5) back into equations (3.2) to (3.4) and solve the boundary value problem for P_β by applying Fourier transform methods and the result (Erdelyi *et al.* [18]) that

$$\int_{-\infty}^{+\infty} \mathrm{H}_0^{(1)}\big(k(Y^2+X^2)^{1/2}\big)e^{iXt}\,dX = \frac{2}{(k^2-t^2)^{1/2}}e^{iY(k^2-t^2)^{1/2}}.$$

So we obtain an ordinary differential equation with boundary conditions which can be solved to obtain an expression for the Fourier transform of P_β. Taking the inverse Fourier transform and substituting $t = ks$, we get

$$P_\beta(\mathbf{r},\mathbf{r}_0) = -\frac{i\beta}{2\pi}\int_{-\infty}^{+\infty}\frac{\exp\big(ik\big[(y+y_0)(1-s^2)^{1/2}-(x-x_0)s\big]\big)}{(1-s^2)^{1/2}((1-s^2)^{1/2}+\beta)}\,ds, \tag{3.8}$$

with $\mathrm{Re}\,\{(1-s^2)^{1/2}\}, \mathrm{Im}\,\{(1-s^2)^{1/2}\} \geq 0$.

To make this representation for P_β suitable for numerical quadrature, the integrand is simplified and the branch point singularities at $s = \pm 1$ removed by making the substitution $s = \cos\theta$. Then the resulting integrand is deformed in the complex plane to the steepest descent path. As a result, the following representation for P_β is derived in [11, 12]:

$$P_\beta(\mathbf{r},\mathbf{r}_0) = -\frac{\beta e^{i\rho}}{\pi}\int_0^\infty t^{-1/2}e^{-\rho t}f(t)\,dt, \qquad \mathrm{Im}\,\beta \geq 0 \;\text{ or }\; \mathrm{Re}\, a_+ > 0, \tag{3.9}$$

where

$$f(t) = -\frac{\beta+\gamma(1+it)}{(t-2i)^{1/2}\,(t-ia_+)(t-ia_-)}, \tag{3.10}$$

$$\gamma = \cos\theta_0,$$

$$a_\pm = 1+\beta\gamma \mp (1-\beta^2)^{1/2}(1-\gamma^2)^{1/2}, \tag{3.11}$$

with $\mathrm{Re}\,\{(1-\beta^2)^{1/2}\}, \mathrm{Re}\,\{(t-2i)^{1/2}\} > 0$. Further, to remove the only singularity lying near the real axis $-\infty < t < \infty$, we regularize the integrand by removing the simple pole in $f(t)$ at ia_+ by defining $g(t)$ by

$$g(t) = f(t) - \frac{C}{t-ia_+}, \tag{3.12}$$

where C is the residue of $f(t)$ at $t = ia_+$. From the definition of $f(t)$ and the identity

$$(\beta + \gamma - \gamma a_\pm)^2 = -a_\pm(a_\pm - 2)(1 - \gamma^2),$$

we see that [11, 12]

$$C = -\frac{i(ia_+)^{1/2}}{2(1-\beta^2)^{1/2}}, \qquad -\frac{\pi}{4} < \arg\{(ia_+)^{1/2}\} < \frac{3\pi}{4}.$$

Thus, at least for $\operatorname{Im}\beta \geq 0$,

$$P_\beta(\mathbf{r}, \mathbf{r}_0) = -\frac{\beta e^{i\rho}}{\pi}\int_0^\infty t^{-1/2}e^{-\rho t}g(t)\,dt - \frac{\beta e^{i\rho}C}{\pi}\int_0^\infty \frac{t^{-1/2}e^{-\rho t}}{t - ia_+}\,dt. \tag{3.13}$$

Now, from equations (7.1.3) and (7.1.4) in [1], we have that

$$\frac{2iz}{\pi}\int_0^\infty \frac{e^{-t^2}}{z^2 - t^2}\,dt = e^{-z^2}\operatorname{erfc}(-iz), \qquad \operatorname{Im} z > 0. \tag{3.14}$$

Thus, by making the substitution $\rho t = s^2$ into the second integral on the right hand side in (3.13) and using equation (3.14), we see that, for $\operatorname{Im}\beta > 0$,

$$P_\beta(\mathbf{r}, \mathbf{r}_0) = -\frac{\beta e^{i\rho}}{\pi}\int_0^\infty t^{-1/2}e^{-\rho t}g(t)\,dt - \frac{\beta e^{i\rho(1-a_+)}}{2(1-\beta^2)^{1/2}}\operatorname{erfc}(e^{-i\pi/4}\sqrt{\rho}\sqrt{a_+}), \tag{3.15}$$

where

$$g(t) = f(t) - \frac{e^{-i\pi/4}\sqrt{a_+}}{2(1-\beta^2)^{1/2}(t - ia_+)},$$

with $\operatorname{Re}\sqrt{a_+}, \operatorname{Re}\{(1-\beta^2)^{1/2}\} > 0$. In fact, since (3.9) and (3.15) are equal for $\operatorname{Im}\beta > 0$ and are both analytic in $\operatorname{Re}\beta > 0$ with the cut $\beta \geq 1$ removed, by analytic continuation and continuity arguments [11, 12], they are equal for all β with $\operatorname{Re}\beta > 0$ except $\beta = 1$. Thus (3.15) holds for $\operatorname{Re}\beta > 0$, $\beta \neq 1$. The only singularities of $g(t)$ are a pole at $t = ia_-$ and a branch point singularity at $t = 2i$.

In order to obtain an integrand that decreases more rapidly when $t \to \infty$ (note that $g(t) = O(t^{-1})$ as $t \to \infty$ while $f(t) = O(t^{-3/2})$ as $t \to \infty$), we introduce $h(t)$ defined by

$$\begin{aligned} h(t) &= g(t) + \frac{C}{t - i\tilde{a}_+} \\ &= f(t) - \frac{C}{t - ia_+} + \frac{C}{t - i\tilde{a}_+} \\ &= f(t) + \frac{iC(1 - \operatorname{Re} a_+)}{(t - ia_+)(t - i\tilde{a}_+)}. \end{aligned} \tag{3.16}$$

where

$$\widetilde{a}_+ = 1 + i\mathrm{Im}\, a_+.$$

For $\mathrm{Re}\,\beta > 0$, $\beta \neq 1$, we write equation (3.15) in the form

$$\begin{aligned} P_\beta(\mathbf{r}, \mathbf{r}_0) \;=\; & -\frac{\beta e^{i\rho}}{\pi}\int_0^\infty t^{-1/2}e^{-\rho t}h(t)\,dt \;+\; \frac{\beta e^{i\rho}C}{\pi}\int_0^\infty \frac{t^{-1/2}e^{-\rho t}}{t - i\widetilde{a}_+}\,dt \\ & - \frac{\beta e^{i\rho(1-a_+)}}{2(1-\beta^2)^{1/2}}\,\mathrm{erfc}\,(e^{-i\pi/4}\sqrt{\rho}\sqrt{a_+}). \end{aligned} \tag{3.17}$$

Substituting $\rho t = s^2$ and using equation (3.14) again in the second part of the right hand side of (3.17), we have that, for $\mathrm{Re}\,\beta > 0$ and $\beta \neq 1$,

$$\begin{aligned} P_\beta(\mathbf{r}, \mathbf{r}_0) \;=\; & -\frac{\beta e^{i\rho}}{\pi}\int_0^\infty t^{-1/2}e^{-\rho t}h(t)\,dt \;+\; \frac{\beta e^{i\rho(1-\widetilde{a}_+)}\sqrt{a_+}}{2(1-\beta^2)^{1/2}\sqrt{\widetilde{a}_+}}\,\mathrm{erfc}\,(e^{-i\pi/4}\sqrt{\rho}\sqrt{\widetilde{a}_+}) \\ & - \frac{\beta e^{i\rho(1-a_+)}}{2(1-\beta^2)^{1/2}}\,\mathrm{erfc}\,(e^{-i\pi/4}\sqrt{\rho}\sqrt{a_+}), \end{aligned} \tag{3.18}$$

and

$$h(t) = f(t) + \frac{e^{i\pi/4}(1 - \mathrm{Re}\,a_+)\sqrt{a_+}}{2(1-\beta^2)^{1/2}(t - ia_+)(t - i\widetilde{a}_+)}, \tag{3.19}$$

with $\mathrm{Re}\,\sqrt{a_+}, \mathrm{Re}\left\{(1-\beta^2)^{1/2}\right\} > 0$. The only singularities of the analytic function $h(t)$ are poles at $t = ia_-$ and $t = i\widetilde{a}_+$, and a branch point at $t = 2i$, and $h(t) = O(t^{-3/2})$ as $t \to \infty$.

3.2 Evaluating $P_\beta(\mathbf{r}, \mathbf{r}_0)$

To apply the quadrature rule (2.13) to evaluate equation (3.9) and the first part of the right hand side in equation (3.18), we substitute $t = s^2$ into (3.9) and (3.18), and use the notation in Chapter 2 that

$$J\Psi := \int_{-\infty}^{+\infty} e^{-\rho s^2}\Psi(s^2)\,ds.$$

Thus, (3.9) and (3.18) become

$$P_\beta(\mathbf{r}, \mathbf{r}_0) = -\frac{\beta e^{i\rho}}{\pi}Jf, \qquad \mathrm{Im}\,\beta \geq 0 \;\text{ or }\; \mathrm{Re}\,a_+ > 0 \tag{3.20}$$

and, for $\mathrm{Re}\,\beta > 0$, $\beta \neq 1$,

$$P_\beta(\mathbf{r}, \mathbf{r}_0) = -\frac{\beta e^{i\rho}}{\pi} Jh + \frac{\beta e^{i\rho(1-\tilde{a}_+)}\sqrt{a_+}}{2(1-\beta^2)^{1/2}\sqrt{\tilde{a}_+}} \,\mathrm{erfc}\,(e^{-i\pi/4}\sqrt{\rho}\sqrt{\tilde{a}_+}) - \frac{\beta e^{i\rho(1-a_+)}}{2(1-\beta^2)^{1/2}} \,\mathrm{erfc}\,(e^{-i\pi/4}\sqrt{\rho}\sqrt{a_+}). \tag{3.21}$$

To apply the results in Section 2.2, we will show that f and h satisfy Assumption 2.1′ in the following theorems. As in [11, 12], we restrict attention to the case $|\beta| \leq 1$, which range of β includes most values of interest in outdoor sound propagation.

Theorem 3.1 *For $0 \leq \gamma \leq 1$, $|\beta| \leq 1$, $|1-\beta| \leq 0.1$, the function f, given by (3.10), satisfies Assumption 2.1′ with $\varepsilon = 1/4$, $\theta = \pi/6$, $r = 3/2$ and $\tilde{c} = 398$. If $\gamma = 0$, $|\beta| \leq 1$, $|1-\beta| \leq 0.1$, then Assumption 2.1′ is satisfied with $\varepsilon = 1/4$, $\theta = \pi/6$, $r = 5/2$ and $\tilde{c} = 199$.*

Proof. For $|\beta| \leq 1$, $|1-\beta| \leq 0.1$, $0 \leq \gamma \leq 1$, it can be seen that

$$|\mathrm{Im}\,\beta| \leq 0.1, \qquad \left|(1-\beta^2)^{1/2}\right| \leq \sqrt{0.2}\,, \qquad \left|\,\mathrm{Im}\left\{(1-\beta^2)^{1/2}\right\}\right| \leq \sqrt{0.1}\,,$$

(The third inequality is from $\left|\,\mathrm{Im}\left\{(1-\beta^2)^{1/2}\right\}\right| = \left[\,\frac{1}{2}\left(|1-\beta^2| - \mathrm{Re}\,(1-\beta^2)\right)\right]^{1/2}$, equation 3.7.27 in [1]) and hence that

$$\mathrm{Re}\,a_- \geq 1, \qquad \mathrm{Re}\,a_+ \geq 1 - \sqrt{0.2} > 0.552, \qquad |\mathrm{Im}\,a_\pm| \leq \sqrt{0.11} < 0.332, \qquad |a_\pm| < 2.1.$$

It follows that the function f is analytic on $\mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}$. For $t \in \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}$, we find that

$$|\beta + \gamma(1+it)| \leq \begin{cases} 2\,(1+|t|)\,, & \text{if} \quad 0 \leq \gamma \leq 1, \\ 1, & \text{if} \quad \gamma = 0, \end{cases} \tag{3.22}$$

and (see Figure 3.2),

$$|t - 2i| \geq d_1 := \frac{8\sqrt{3}-1}{8} > 1.6, \tag{3.23}$$

$$|t - ia_-| \geq d_2 := \frac{\sqrt{3}}{2}\left(1 - \frac{0.332}{\sqrt{3}} - \frac{1}{4\sqrt{3}}\right) > 0.57, \tag{3.24}$$

$$|t - ia_+| \geq d_3 := \frac{\sqrt{3}}{2}\left(0.552 - \frac{0.332}{\sqrt{3}} - \frac{1}{4\sqrt{3}}\right) > 0.18. \tag{3.25}$$

To see how to make use of these bounds, suppose that $A \in \mathbb{C}$,

$$|A| \leq K,$$

and that, for $t \in \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}$,

$$|t - iA| \geq B > 0.$$

Then, for $c > K$, we find that

$$|t - iA| \geq \begin{cases} \dfrac{B}{1+c}(1+|t|), & \text{if } \quad |t| \leq c, \\ \dfrac{c-K}{1+c}(1+|t|), & \text{if } \quad |t| \geq c, \end{cases}$$

so that

$$|t - iA| \geq C(1+|t|), \qquad t \in \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}, \tag{3.26}$$

where

$$C := \min\left\{ \frac{B}{1+c}, \frac{c-K}{1+c} \right\}.$$

We choose $c = B + K$ to maximise C, giving

$$C = \frac{B}{1+B+K}. \tag{3.27}$$

Applying these bounds with $A = 2$, $B = 1.6$ and $K = 2$, we see from (3.23) that, for $t \in \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}$,

$$\begin{aligned} |t - 2i| &\geq \frac{1.6}{1+1.6+2}(1+|t|) \\ &= \frac{8}{23}(1+|t|). \end{aligned} \tag{3.28}$$

Similarly, from (3.24), we see that

$$|t - ia_-| \geq \frac{57}{367}(1+|t|), \qquad t \in \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}, \tag{3.29}$$

and, from (3.25),

$$|t - ia_+| \geq \frac{9}{164}(1+|t|), \qquad t \in \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}. \tag{3.30}$$

Combining inequalities (3.22), (3.28) to (3.30), for $0 \leq \gamma \leq 1$,

$$\begin{aligned} |f(t)| &\leq 2\left(\frac{8}{23}\right)^{-1/2}\left(\frac{9}{164}\right)^{-1}\left(\frac{57}{367}\right)^{-1}(1+|t|)^{-3/2} \\ &< 398(1+|t|)^{-3/2}. \end{aligned}$$

Arguing in the same way for $\gamma = 0$, except that we use the fact that $|\beta + \gamma(1+it)| \leq 1$ in this case, we obtain

$$|f(t)| < 199(1+|t|)^{-5/2}.$$

■

Theorem 3.2 *For* $0 \leq \gamma \leq 1$, $\operatorname{Re}\beta \geq 0$, $|\beta| \leq 1$, $|1-\beta| \geq 0.1$, *the function* h, *given by (3.19), satisfies Assumption 2.1′ with* $\varepsilon = 1/4$, $\theta = \pi/6$, $r = 3/2$ *and* $\widetilde{c} = 845832$. *If* $\gamma = 0$, $|\beta| \leq 1$, $|1-\beta| \geq 0.1$, *then Assumption 2.1′ is satisfied with* $\varepsilon = 1/4$, $\theta = \pi/6$, $r = 2$ *and* $\widetilde{c} = 681158$.

Proof. For $|\beta| \leq 1$, $|1-\beta| \geq 0.1$, $0 \leq \gamma \leq 1$, it can be seen that

$$\operatorname{Re} a_- \geq 1, \qquad \operatorname{Re} a_+ \geq 2 - \operatorname{Re} a_-, \qquad |\operatorname{Im} a_\pm| \leq \sqrt{2},$$

and also that

$$\sqrt{2} \geq |(1-\beta^2)^{1/2}| \geq \sqrt{0.19}, \qquad |\sqrt{a_+}| \leq \left(1+\sqrt{3}\right)^{1/2}, \qquad |a_\pm| \leq 1 + \frac{1}{\sqrt{3}} + \frac{2}{\sqrt{3}} < 2.74.$$

Note that ia_+ may be outside or inside $\mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}$. Let

$$c_1 := \operatorname{dist}(2i, \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}), \qquad c_2 := \operatorname{dist}(ia_-, \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}), \qquad c_3 := \operatorname{dist}(i\widetilde{a}_+, \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}})$$

be the distances of the singularities of the function h from $\mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}$. To assist in bounding h on $\mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}$, we choose τ so that $0 < 2\tau < c_j$, for $j = 1,2,3$, and define $\widetilde{\mathcal{D}}_{\frac{1}{4},\frac{\pi}{6}} \supset \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}$ by

$$\widetilde{\mathcal{D}}_{\frac{1}{4},\frac{\pi}{6}} := \begin{cases} \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}, & \text{if } \operatorname{dist}(ia_+, \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}) \geq \tau, \\ \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}} \cup \left\{z \in \mathbb{C} : |z - ia_+| < \tau\right\}, & \text{if } \operatorname{dist}(ia_+, \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}) < \tau. \end{cases}$$

Then the function h is analytic on $\widetilde{\mathcal{D}}_{\frac{1}{4},\frac{\pi}{6}}$. We need to bound

$$M := \sup_{t \in \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}} |h(t)|(1+|t|)^{3/2}.$$

Since

$$1 + |t| \leq \frac{5}{3}|1+t|, \qquad \text{for } t \in \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}},$$

with equality when $t = -1/4$, we have that

$$M \le (5/3)^{3/2} \sup_{t \in \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}} \left|h(t)(1+t)^{3/2}\right|$$

$$\le (5/3)^{3/2} \sup_{t \in \widetilde{\mathcal{D}}_{\frac{1}{4},\frac{\pi}{6}}} \left|h(t)(1+t)^{3/2}\right|,$$

since $\mathcal{D}_{\frac{1}{4},\frac{\pi}{6}} \subset \widetilde{\mathcal{D}}_{\frac{1}{4},\frac{\pi}{6}}$. Now, by the maximum principle for analytic functions, it follows that

$$M \le (5/3)^{3/2} \sup_{t \in \partial\widetilde{\mathcal{D}}_{\frac{1}{4},\frac{\pi}{6}}} \left|h(t)(1+t)^{3/2}\right|. \tag{3.31}$$

For $t \in \partial\widetilde{\mathcal{D}}_{\frac{1}{4},\frac{\pi}{6}}$, we find that

$$|\beta + \gamma(1+it)| \le \begin{cases} 2(1+|t|), & \text{if} \quad 0 \le \gamma \le 1, \\ 1, & \text{if} \quad \gamma = 0, \end{cases} \tag{3.32}$$

and (see Figure 3.3)

$$|t - 2i| \ge c_1 - 2\tau, \tag{3.33}$$

$$|t - ia_-| \ge c_2 - 2\tau, \tag{3.34}$$

$$|t - i\widetilde{a}_+| \ge c_3 - 2\tau, \tag{3.35}$$

$$|t - ia_+| \ge \tau. \tag{3.36}$$

Lower bounds for c_1, c_2, and c_3 are

$$c_1 \ge e_1 := \frac{8\sqrt{3}-1}{8} > 1.6,$$

$$c_2 \ge e_2 := \frac{\sqrt{3}}{2}\left(1 - \frac{\sqrt{2}}{\sqrt{3}} - \frac{1}{4\sqrt{3}}\right) > 0.03,$$

$$c_3 \ge e_2 > 0.03.$$

Then we choose $\tau = 0.01$ so that $0 < 2\tau < c_j$, for $j = 1, 2, 3$. Hence, from inequalities (3.33) to (3.36), we obtain, for $t \in \partial\widetilde{\mathcal{D}}_{\frac{1}{4},\frac{\pi}{6}}$, that

$$|t - 2i| > 1.58, \tag{3.37}$$

$$|t - ia_-| > 0.01, \tag{3.38}$$

$$|t - i\widetilde{a}_+| > 0.01, \tag{3.39}$$

$$|t - ia_+| > 0.01. \tag{3.40}$$

To make use of these bounds, we use the argument leading to the inequality (3.26), with C given by (3.27). Applying these bounds with $A = 2$, $B = 1.58$ and $K = 2$, we see from (3.37) that, for $t \in \partial\widetilde{\mathcal{D}}_{\frac{1}{4},\frac{\pi}{6}}$,

$$\begin{aligned} |t - 2i| &\geq \frac{1.58}{1 + 1.58 + 2}(1 + |t|) \\ &= \frac{79}{229}(1 + |t|). \end{aligned} \tag{3.41}$$

Similarly, from (3.38), we see that

$$|t - ia_-| \geq \frac{1}{311}(1 + |t|), \qquad t \in \partial\widetilde{\mathcal{D}}_{\frac{1}{4},\frac{\pi}{6}}, \tag{3.42}$$

from (3.39),

$$|t - i\widetilde{a}_+| \geq \frac{5}{1171}(1 + |t|), \qquad t \in \partial\widetilde{\mathcal{D}}_{\frac{1}{4},\frac{\pi}{6}}, \tag{3.43}$$

and from (3.40),

$$|t - ia_+| \geq \frac{1}{311}(1 + |t|), \qquad t \in \partial\widetilde{\mathcal{D}}_{\frac{1}{4},\frac{\pi}{6}}. \tag{3.44}$$

Combining inequalities (3.32), (3.41) to (3.44), for $0 \leq \gamma \leq 1$,

$$\begin{aligned} |h(t)| &\leq 2\left(\frac{79}{229}\right)^{-1/2}\left(\frac{1}{311}\right)^{-1}\left(\frac{1}{311}\right)^{-1}(1 + |t|)^{-3/2} \\ &\quad + \left(\frac{187}{100}\right)\left(1 + \sqrt{3}\right)^{1/2}\left(\frac{19}{100}\right)^{-1/2}\left(\frac{1}{311}\right)^{-1}\left(\frac{5}{1171}\right)^{-1}(1 + |t|)^{-2} \\ &< 845832(1 + |t|)^{-3/2}. \end{aligned}$$

Arguing in the same way for $\gamma = 0$, except that we use the fact that $|\beta + \gamma(1+it)| \leq 1$ in this case, we obtain

$$|h(t)| < 681158(1 + |t|)^{-2}.$$

■

Combining Theorems 3.1 and 3.2 with Corollary 2.1, we obtain the following theorems.

Theorem 3.3 *Suppose that Assumption 1.1 on w holds and that $|\beta| \leq 1$, $|1-\beta| \leq 0.1$. Suppose also that $q \in \mathbb{N}$, $s \notin \mathbb{N}$, and $1 < s < q$. Then, where C is a constant whose value depends only on q, s, and on the choice of w and, in particular, on the value of p in Assumption 1.1, it holds that*

$$|Jf - J_N f| \leq C(1 + \rho^q)N^{-s},$$

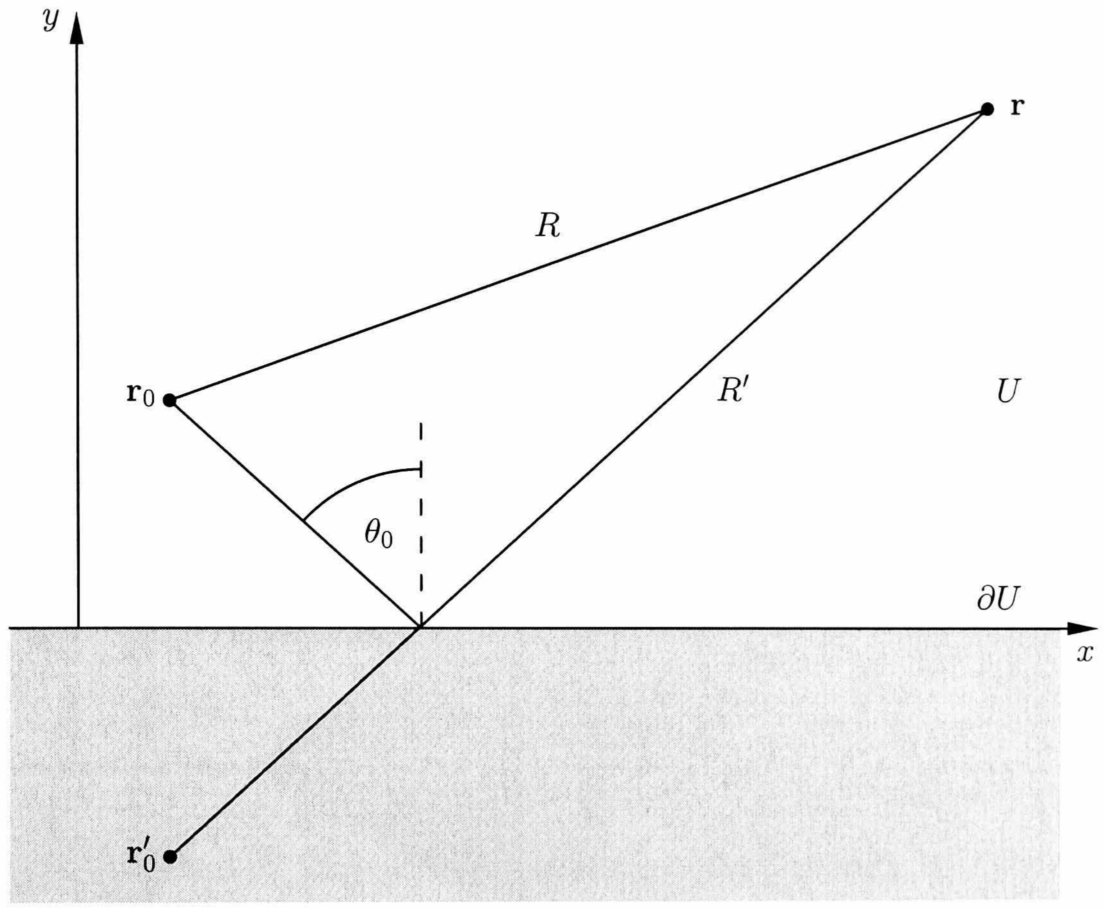
provided also $s < p$ if $0 \leq \gamma \leq 1$, $s < 2p$ if $\gamma = 0$.

Theorem 3.4 *Suppose that Assumption 1.1 on w holds and that $|\beta| \leq 1$, $|1-\beta| \geq 0.1$. Suppose also that $q \in \mathbb{N}$, $s \notin \mathbb{N}$, and $1 < s < q$. Then, where C is a constant whose value depends only on q, s, and on the choice of w and, in particular, on the value of p in Assumption 1.1, it holds that*

$$|Jh - J_N h| \leq C(1 + \rho^q)N^{-s},$$

provided also $s < p$ if $0 \leq \gamma \leq 1$, $s \leq 3p/2$ if $\gamma = 0$.

Note that both these theorems predict a faster convergence rate when $\gamma = \cos\theta_0 = 0$, i.e., when the angle of incidence $\theta_0 = \pi/2$ in Figure 3.1.



$\mathbf{r}_0 = (x_0, y_0)$	position of the source
$\mathbf{r}'_0 = (x_0, -y_0)$	position of the image of the source
$\mathbf{r} = (x, y)$	position of the receiver
$R = \lvert\mathbf{r} - \mathbf{r}_0\rvert$	distance from the source to the receiver
$R' = \lvert\mathbf{r} - \mathbf{r}'_0\rvert$	distance from the image to the receiver
θ_0	the angle of incidence
U	the region $y > 0$ above the impedance boundary
∂U	the boundary $y = 0$

Figure 3.1: The positions of the source $\mathbf{r}_0$ and the receiver $\mathbf{r}$ above the homogeneous impedance plane. The cross-section is in the plane perpendicular to the line source.

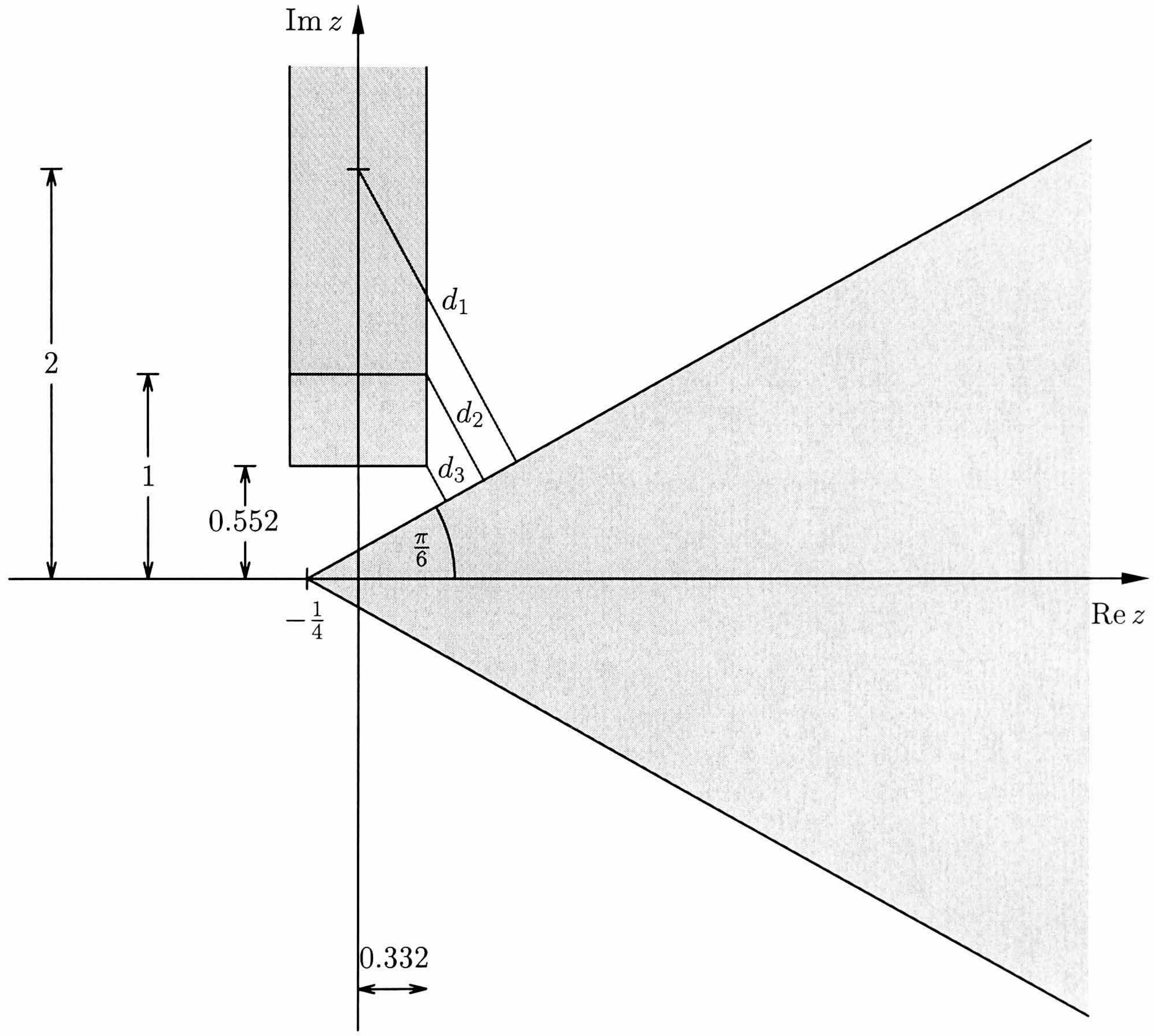


Figure 3.2: Regions of the complex plane referred to in the proof of Theorem 3.1. The shaded wedge-shaped region is $\mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}$. The other shaded area is the part of the complex plane in which ia_+ and ia_- lie, with ia_- additionally restricted to lie in $\operatorname{Im} ia_- \geq 1$.

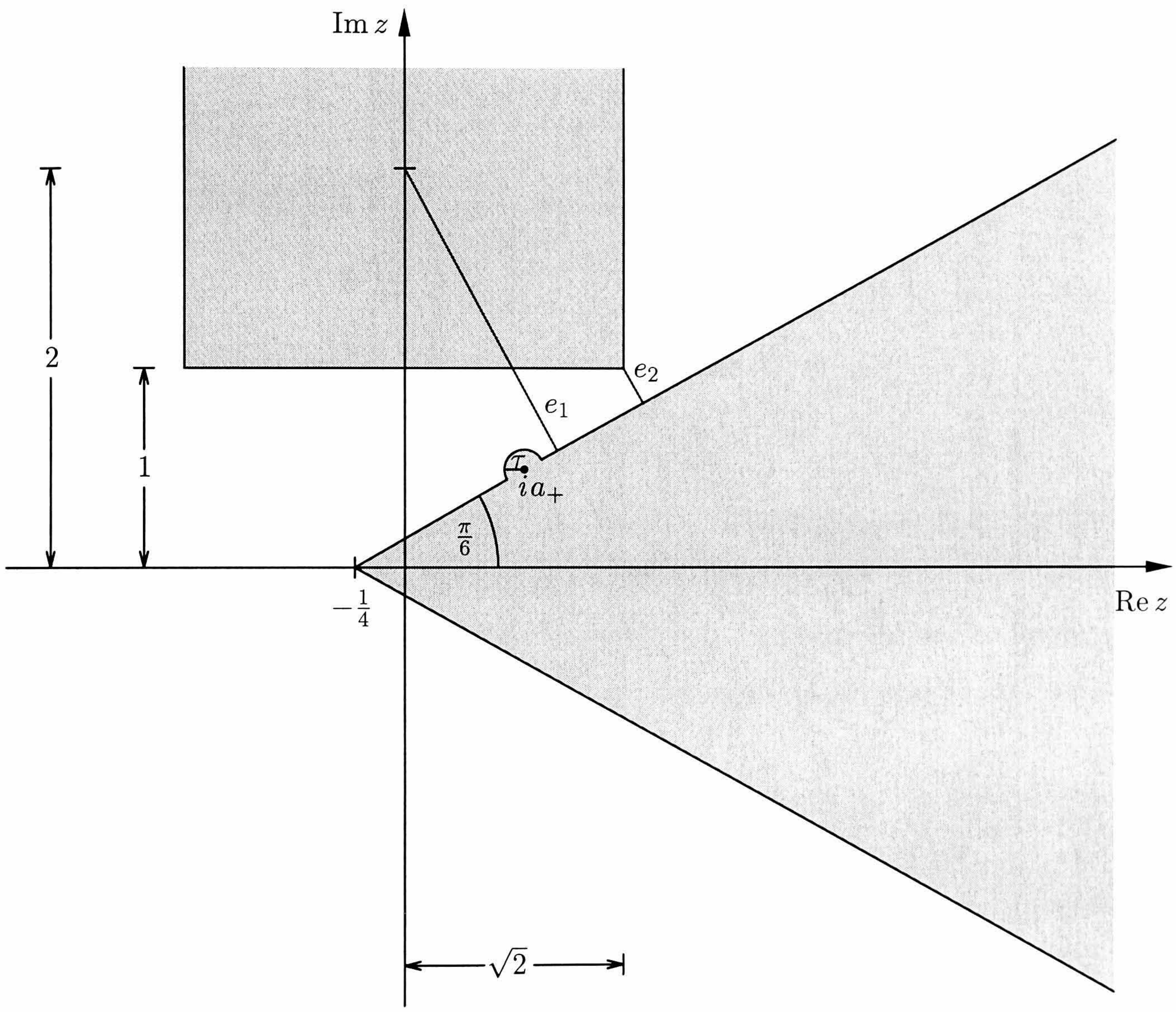


Figure 3.3: Regions of the complex plane referred to in the proof of Theorem 3.2. The shaded wedge-shaped region is $\widetilde{\mathcal{D}}_{\frac{1}{4},\frac{\pi}{6}}$. The other shaded area is the part of the complex plane in which ia_- lies.

3.3 Numerical Results

In the following results the expression for $P_\beta(\mathbf{r},\mathbf{r}_0)$ in (3.20), and the first part of the right hand side in (3.21) are estimated by $J_N f$ and $J_N h$, respectively, the quadrature rule approximation (2.13), with $2N-1$ points. We note that, since F is even, and in view of the symmetry properties (1.28),

$$J_N f = a_0 F(0) + 2\sum_{k=1}^{N-1} a_k F(x_k), \tag{3.45}$$

where, for $k = 1,\ldots,N-1$,

$$a_k := \frac{1}{N} w'\left(\frac{k}{N}\right), \qquad x_k := w\left(\frac{k}{N}\right),$$

and

$$F(u) := \frac{f(P(u))e^{-\rho P(u)}}{(1-u^2)^{3/2}}, \qquad P(u) := \frac{u^2}{1-u^2} \geq 0, \qquad -1 < u < 1.$$

The evaluation of the complementary error function, which occurs in (3.21), is discussed in Matta *et al.* [39], Chien *et al.* [14], and Chandler-Wilde [10].

As an example to illustrate the use of this quadrature rule applied to Laplace-type integrals of the form (3.1) with $f(t)$ given by equations (3.10) and (3.19), we choose $\beta = 0.99 - 0.01i, 0.1 - 0.2i$, $\gamma = 0, 1$, and $\rho = 0, 0.1, 1$.

For $\rho = 0$, the analytic value of $P_\beta(\mathbf{r},\mathbf{r}_0)$ is given, for $0 \leq \gamma \leq 1$, as (see [11, 12]),

$$P_\beta(\mathbf{r},\mathbf{r}_0) = \begin{cases} -1/\pi, & \text{if } \beta = 1, \\ -\dfrac{i\beta}{2\pi(1-\beta^2)^{1/2}} \ln\left(\dfrac{\beta - i(1-\beta^2)^{1/2}}{\beta + i(1-\beta^2)^{1/2}}\right), & \text{if } \beta \neq 1, \end{cases}$$

where $\mathrm{Re}\left\{(1-\beta^2)^{1/2}\right\} > 0$ and the principal value of the logarithm is taken. For $\rho = 0.1, 1$, we do not know the analytic values of $P_\beta(\mathbf{r},\mathbf{r}_0)$, so we will approximate the error in estimating $P_\beta(\mathbf{r},\mathbf{r}_0)$, for $\beta = 0.99 - 0.01i$, $\gamma = 0, 1$, $\rho = 0.1, 1$ by $|\beta||J_N f - J_{2N} f|/\pi$. Similarly, we will approximate the error in estimating $P_\beta(\mathbf{r},\mathbf{r}_0)$, for $\beta = 0.1 - 0.2i$, $\gamma = 0, 1$, $\rho = 0.1, 1$, by $|\beta||J_N h - J_{2N} h|/\pi$.

All numerical results in Tables 3.1–3.12 are evaluated using the mapping function w given by equations (1.31) and (1.33), suggested by Kress [33]. Recall that we compute the error in estimating JF with $J_N F$ given by (3.45), that it has been shown in Theorem 3.3 that, as $N \to \infty$, $|Jf - J_N f| = O(N^{-s})$ for $s < p$ if $0 \leq \gamma \leq 1$, $s < 2p$ if $\gamma = 0$, and that it has been shown in Theorem 3.4 that, as $N \to \infty$, $|Jh - J_N h| = O(N^{-s})$ for $s < p$ if $0 \le \gamma \le 1$, $s < 3p/2$ if $\gamma = 0$.

The error in estimating $P_\beta(\mathbf{r}, \mathbf{r}_0)$, for $\beta = 0.99 - 0.01i$, $\rho = 0, 0.1, 1$, is shown, for $\gamma = 0$ and 1, in Figures 3.4 and 3.5, respectively. From these figures, it is seen that numerical results close to machine precision level 10^{-16} are obtained for $p = 2 - 7$ for N large enough, and that the error in estimating $P_\beta(\mathbf{r}, \mathbf{r}_0)$ decreases significantly when ρ increases (these observations are also confirmed by the numerical values tabulated in Tables 3.1–3.6).

In Table 3.1, we can see that the predicted convergence rate $2p$ is observed for $p = 2, 3$. In Table 3.2, the predicted convergence rate p is observed for $p = 2, 4, 6$. In Table 3.2, a convergence rate $p + 1 = 4$, when the predicted rate is $p = 3$, is observed again, as in Chapter 1 and Chapter 2. For Tables 3.3–3.6, we can see that, for the same ρ, the behaviour of observed rate is similar to that of Chapter 2. So we refer to the discussion concerning the continuity of ρ in Section 2.4.

The error in estimating $P_\beta(\mathbf{r}, \mathbf{r}_0)$, for $\beta = 0.1 - 0.2i$, $\rho = 0, 0.1, 1$, is shown, for $\gamma = 0$ and 1, in Figures 3.6 and 3.7, respectively. From these figures, it is seen that the numerical results close to machine precision level 10^{-16} are obtained for $p = 2 - 7$ for N large enough, and that the error in estimating $P_\beta(\mathbf{r}, \mathbf{r}_0)$ decreases significantly when ρ increases (these observations are also confirmed by the numerical values tabulated in Tables 3.7–3.12).

In Table 3.7, we can see that the predicted convergence rate $3p/2$ is observed for $p = 3, 4$. In Table 3.8, the predicted convergence rate p is observed for $p = 2, 4, 6$. In Table 3.7, a convergence rate $3p/2 + 1 = 4$, when predicted rate is $3p/2 = 3$, is observed. In Table 3.8, convergence rates $p + 1 = 4$ and $p + 1 = 6$ are observed, when predicted rates are $p = 3$ and $p = 5$, respectively. Again for Tables 3.9–3.12, we can see that, for the same ρ, the behaviour of observed rate is similar to that of Chapter 2. So we refer to the discussion concerning the continuity of ρ in Section 2.4.

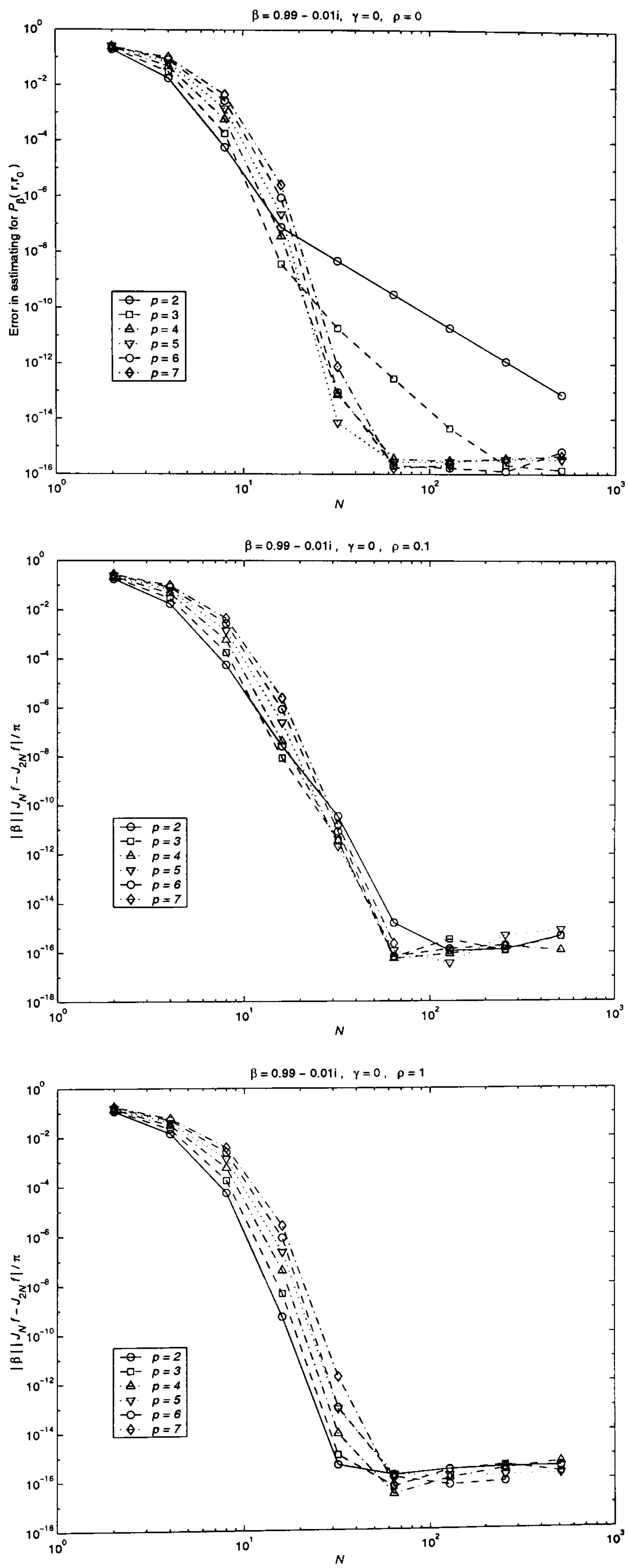


Figure 3.4: Error in estimating $P_\beta(\mathbf{r}, \mathbf{r}_0)$ vs. N, with f given by equation (3.10).

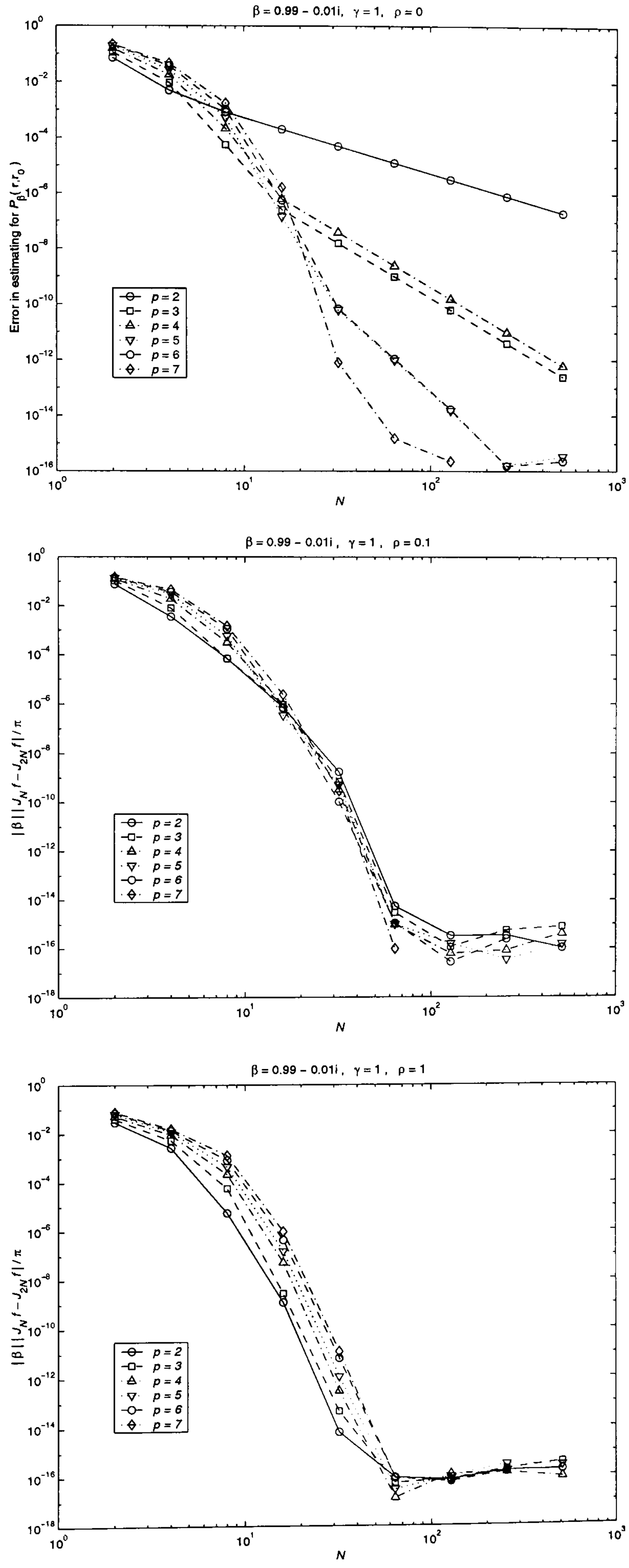


Figure 3.5: Error in estimating $P_\beta(\mathbf{r}, \mathbf{r}_0)$ vs. N, with f given by equation (3.10).

Table 3.1: $\beta = 0.99 - 0.01i$, $\gamma = 0$, $\rho = 0$

$$P_\beta(\mathbf{r}, \mathbf{r}_0) = -0.31618786918623 + 0.00213484680592i$$

NaN indicates that an implementation problem is encountered as described in Section 1.4 due to some x_k evaluating to ± 1 in (3.45).

	$p = 2, \quad 2p = 4.0$		$p = 3, \quad 2p = 6.0$		$p = 4, \quad 2p = 8.0$	
N	ERROR	EOC	ERROR	EOC	ERROR	EOC
2	1.9199E−01		2.2146E−01		2.4190E−01	
		3.4045		2.8611		2.3269
4	1.8131E−02		3.0481E−02		4.8214E−02	
		8.2707		7.3551		6.3241
8	5.8707E−05		1.8617E−04		6.0178E−04	
		9.5457		15.5896		13.9685
16	7.8550E−08		3.7754E−09		3.7541E−08	
		3.9889		7.6705		18.9190
32	4.9471E−09		1.8532E−11		7.5738E−14	
		3.9974		6.0003		8.8188
64	3.0976E−10		2.8949E−13		1.6772E−16	
		3.9993		5.9388		−0.4052
128	1.9369E−11		4.7194E−15		2.2211E−16	
		4.0000		5.1992		−0.5972
256	1.2106E−12		1.2846E−16		3.3599E−16	
		4.0018		−0.2473		−0.4896
512	7.5568E−14		1.5248E−16		4.7175E−16	

	$p = 5, \quad 2p = 10.0$		$p = 6, \quad 2p = 12.0$		$p = 7, \quad 2p = 14.0$	
N	ERROR	EOC	ERROR	EOC	ERROR	EOC
2	2.4926E−01		2.4874E−01		2.4488E−01	
		1.9069		1.5706		1.2946
4	6.6468E−02		8.3740E−02		9.9826E−02	
		5.5052		4.8884		4.4178
8	1.4635E−03		2.8274E−03		4.6704E−03	
		12.6225		11.6112		10.8040
16	2.3209E−07		9.0379E−07		2.6124E−06	
		24.9465		23.2407		21.6898
32	7.1781E−15		9.1183E−14		7.7225E−13	
		4.9605		8.6072		12.9983
64	2.3054E−16		2.3383E−16		9.4379E−17	
		−0.3078		0.6421		0.4165
128	2.8538E−16		1.4983E−16		7.0711E−17	
		−0.2865		−0.1069		
256	3.4806E−16		1.6136E−16		NaN	
		0.0005		−1.9276		
512	3.4793E−16		6.1385E−16		NaN	

Table 3.2: $\beta = 0.99 - 0.01i$, $\gamma = 1$, $\rho = 0$

$P_\beta(\mathbf{r}, \mathbf{r}_0) = -0.31618786918623 + 0.00213484680592i$

NaN indicates that an implementation problem is encountered as described in Section 1.4 due to some x_k evaluating to ± 1 in (3.45).

	$p = 2$, $1p = 2.0$		$p = 3$, $1p = 3.0$		$p = 4$, $1p = 4.0$	
N	ERROR	EOC	ERROR	EOC	ERROR	EOC
2	7.1743E−02		1.1260E−01		1.5773E−01	
		3.8624		3.5912		3.1449
4	4.9328E−03		9.3431E−03		1.7833E−02	
		2.5842		7.3906		6.3605
8	8.2259E−04		5.5680E−05		2.1703E−04	
		2.0048		7.7461		8.4083
16	2.0497E−04		2.5935E−07		6.3878E−07	
		1.9989		3.9992		3.9940
32	5.1280E−05		1.6218E−08		4.0090E−08	
		1.9997		3.9990		4.0005
64	1.2822E−05		1.0143E−09		2.5048E−09	
		1.9999		3.9998		4.0001
128	3.2057E−06		6.3407E−11		1.5654E−10	
		2.0000		3.9999		4.0000
256	8.0145E−07		3.9631E−12		9.7833E−12	
		2.0000		3.9996		4.0000
512	2.0036E−07		2.4777E−13		6.1147E−13	

	$p = 5$, $1p = 5.0$		$p = 6$, $1p = 6.0$		$p = 7$, $1p = 7.0$	
N	ERROR	EOC	ERROR	EOC	ERROR	EOC
2	1.9056E−01		2.0986E−01		2.1936E−01	
		2.8134		2.5165		2.2651
4	2.7109E−02		3.6676E−02		4.5633E−02	
		5.6839		5.1502		4.7278
8	5.2734E−04		1.0328E−03		1.7221E−03	
		11.8271		10.8182		10.0104
16	1.4514E−07		5.7202E−07		1.6697E−06	
		11.1554		12.9876		20.9721
32	6.3631E−11		7.0431E−11		8.1169E−13	
		6.0034		5.9985		9.2720
64	9.9192E−13		1.1016E−12		1.3129E−15	
		5.9952		5.9979		4.5465
128	1.5550E−14		1.7237E−14		5.6185E−17	
		5.5145		5.3968		
256	3.4019E−16		4.0913E−16		NaN	
		0.4172		1.2573		
512	2.5476E−16		1.7115E−16		NaN	

Table 3.3: $\beta = 0.99 - 0.01i$, $\gamma = 0$, $\rho = 0.1$

$P_\beta(\mathbf{r}, \mathbf{r}_0) \approx -0.31049907365896 - 0.04500700474089i$ (with $p = 4$, $N = 64$)

$P_\beta(\mathbf{r}, \mathbf{r}_0) \approx -0.30636827082809 - 0.07358297926066i$ (by Gauss–Laguerre quadrature)

NaN indicates that an implementation problem is encountered as described in Section 1.4 due to some x_k evaluating to ±1 in (3.45).

	$p = 2,\quad 2p = 4.0$		$p = 3,\quad 2p = 6.0$		$p = 4,\quad 2p = 8.0$	
N	$\lvert\beta\rvert \lvert J_N f - J_{2N} f\rvert/\pi$	EOC	$\lvert\beta\rvert \lvert J_N f - J_{2N} f\rvert/\pi$	EOC	$\lvert\beta\rvert \lvert J_N f - J_{2N} f\rvert/\pi$	EOC
2	1.7846E−01		2.0288E−01		2.2510E−01	
		3.3269		2.7634		2.2554
4	1.7785E−02		2.9880E−02		4.7145E−02	
		8.2632		7.3292		6.2977
8	5.7889E−05		1.8581E−04		5.9931E−04	
		11.0623		14.3552		13.7483
16	2.7072E−08		8.8659E−09		4.3550E−08	
		9.5612		11.1619		13.5738
32	3.5836E−11		3.8695E−12		3.5715E−12	
		14.4419		15.8712		15.9560
64	1.6102E−15		6.4559E−17		5.6185E−17	
		3.8091		−2.3921		−0.6550
128	1.1487E−16		3.3887E−16		8.8471E−17	
		−0.1887		1.5412		−1.0020
256	1.3092E−16		1.1643E−16		1.7719E−16	
		−1.8215		−1.9338		0.5870
512	4.6276E−16		4.4485E−16		1.1796E−16	

	$p = 5,\quad 2p = 10.0$		$p = 6,\quad 2p = 12.0$		$p = 7,\quad 2p = 14.0$	
N	$\lvert\beta\rvert \lvert J_N f - J_{2N} f\rvert/\pi$	EOC	$\lvert\beta\rvert \lvert J_N f - J_{2N} f\rvert/\pi$	EOC	$\lvert\beta\rvert \lvert J_N f - J_{2N} f\rvert/\pi$	EOC
2	2.4272E−01		2.5855E−01		2.7460E−01	
		1.8974		1.6524		1.4901
4	6.5153E−02		8.2247E−02		9.7753E−02	
		5.4878		4.8737		4.4071
8	1.4519E−03		2.8054E−03		4.6076E−03	
		12.4768		11.6201		10.8088
16	2.5472E−07		8.9121E−07		2.5686E−06	
		16.8759		16.6571		17.3790
32	2.1179E−12		8.6236E−12		1.5069E−11	
		14.1458		16.9232		15.9955
64	1.1685E−16		6.9389E−17		2.3066E−16	
		1.6814		−1.0000		
128	3.6429E−17		1.3878E−16		NaN	
		−3.7382		−0.4875		
256	4.8613E−16		1.9457E−16		NaN	
		−0.7162				
512	7.9861E−16		NaN		NaN	

Table 3.4: $\beta = 0.99 - 0.01i$, $\gamma = 1$, $\rho = 0.1$

$P_\beta(\mathbf{r}, \mathbf{r}_0) \approx -0.27196976811781 - 0.07688789372251i$ (with $p = 4$, $N = 64$)

$P_\beta(\mathbf{r}, \mathbf{r}_0) \approx -0.27170762031381 - 0.07601850661066i$ (by Gauss–Laguerre quadrature)

NaN indicates that an implementation problem is encountered as described in Section 1.4 due to some x_k evaluating to ± 1 in (3.45).

	$p = 2$, $1p = 2.0$		$p = 3$, $1p = 3.0$		$p = 4$, $1p = 4.0$	
N	$\lvert\beta\rvert\lvert J_N f - J_{2N} f\rvert/\pi$	EOC	$\lvert\beta\rvert\lvert J_N f - J_{2N} f\rvert/\pi$	EOC	$\lvert\beta\rvert\lvert J_N f - J_{2N} f\rvert/\pi$	EOC
2	7.5718E−02		1.0620E−01		1.2537E−01	
		4.4132		3.7192		2.7194
4	3.5538E−03		8.0632E−03		1.9036E−02	
		5.6909		6.8852		5.9387
8	6.8794E−05		6.8211E−05		3.1035E−04	
		6.5815		6.1560		8.3313
16	7.1834E−07		9.5659E−07		9.6357E−07	
		8.6838		10.4040		11.4900
32	1.7469E−09		7.0603E−10		3.3501E−10	
		18.2884		17.8500		18.4171
64	5.4565E−15		2.9883E−15		9.5709E−16	
		4.0291		4.6832		3.9468
128	3.3422E−16		1.1632E−16		6.2063E−17	
		−0.0199		−2.2619		−0.4290
256	3.3887E−16		5.5788E−16		8.3555E−17	
		1.7030		−0.4865		−2.2603
512	1.0408E−16		7.8160E−16		4.0030E−16	

	$p = 5$, $1p = 5.0$		$p = 6$, $1p = 6.0$		$p = 7$, $1p = 7.0$	
N	$\lvert\beta\rvert\lvert J_N f - J_{2N} f\rvert/\pi$	EOC	$\lvert\beta\rvert\lvert J_N f - J_{2N} f\rvert/\pi$	EOC	$\lvert\beta\rvert\lvert J_N f - J_{2N} f\rvert/\pi$	EOC
2	1.3547E−01		1.4206E−01		1.4781E−01	
		2.2228		1.9626		1.7122
4	2.9021E−02		3.6449E−02		4.5113E−02	
		5.6516		5.0337		4.9401
8	5.7733E−04		1.1127E−03		1.4695E−03	
		10.7294		10.6812		9.2660
16	3.4006E−07		6.7769E−07		2.3869E−06	
		9.3332		12.6480		12.9991
32	5.2723E−10		1.0558E−10		2.9154E−10	
		19.0193		16.5354		21.5171
64	9.9226E−16		1.1116E−15		9.7145E−17	
		2.6599		5.3237		
128	1.5701E−16		2.7756E−17		NaN	
		2.1781		−3.1102		
256	3.4694E−17		2.3967E−16		NaN	
		−2.1330				
512	1.5218E−16		NaN		NaN	

Table 3.5: $\beta = 0.99 - 0.01i$, $\gamma = 0$, $\rho = 1$

$P_\beta(\mathbf{r}, \mathbf{r}_0) \approx -0.07374153763450 - 0.25888728209860i$ (with $p = 4$, $N = 64$)

$P_\beta(\mathbf{r}, \mathbf{r}_0) \approx -0.07374181647900 - 0.25888793298985i$ (by Gauss–Laguerre quadrature)

NaN indicates that an implementation problem is encountered as described in Section 1.4 due to some x_k evaluating to ± 1 in (3.45).

	$p = 2, \quad 2p = 4.0$		$p = 3, \quad 2p = 6.0$		$p = 4, \quad 2p = 8.0$	
N	$\lvert\beta\rvert \lVert J_N f - J_{2N} f \rVert/\pi$	EOC	$\lvert\beta\rvert \lVert J_N f - J_{2N} f \rVert/\pi$	EOC	$\lvert\beta\rvert \lVert J_N f - J_{2N} f \rVert/\pi$	EOC
2	1.1590E−01	3.0347	1.2870E−01	2.5753	1.4214E−01	2.1938
4	1.4144E−02	7.9751	2.1594E−02	6.9259	3.1068E−02	5.7652
8	5.6212E−05	16.7556	1.7760E−04	15.3008	5.7125E−04	13.8593
16	5.0803E−10	20.1249	4.3998E−09	21.8929	3.8437E−08	22.1249
32	4.4431E−16	1.3960	1.1298E−15	4.3472	8.4042E−15	8.2422
64	1.6883E−16	−0.6745	5.5511E−17	−2.1983	2.7756E−17	−2.0949
128	2.6946E−16	−0.2444	2.5476E−16	−0.6100	1.1857E−16	−1.2288
256	3.1919E−16	−0.0860	3.8883E−16	1.0009	2.7790E−16	−0.8556
512	3.3880E−16		1.9429E−16		5.0287E−16	

	$p = 5, \quad 2p = 10.0$		$p = 6, \quad 2p = 12.0$		$p = 7, \quad 2p = 14.0$	
N	$\lvert\beta\rvert \lVert J_N f - J_{2N} f \rVert/\pi$	EOC	$\lvert\beta\rvert \lVert J_N f - J_{2N} f \rVert/\pi$	EOC	$\lvert\beta\rvert \lVert J_N f - J_{2N} f \rVert/\pi$	EOC
2	1.5465E−01	1.9334	1.6686E−01	1.7508	1.7871E−01	1.6189
4	4.0489E−02	4.9183	4.9582E−02	4.3501	5.8184E−02	3.9348
8	1.3391E−03	12.5982	2.4312E−03	11.5343	3.8045E−03	10.5388
16	2.1596E−07	21.2380	8.1969E−07	23.0027	2.5575E−06	20.4675
32	8.7315E−14	9.0145	9.7531E−14	9.4789	1.7639E−12	14.7947
64	1.6883E−16	0.1946	1.3668E−16	1.1390	6.2063E−17	
128	1.4752E−16		6.2063E−17	−0.4240	NaN	
256	1.4752E−16	−0.1389	8.3267E−17		NaN	
512	1.6244E−16		NaN		NaN	

Table 3.6: $\beta = 0.99 - 0.01i$, $\gamma = 1$, $\rho = 1$

$P_\beta(\mathbf{r}, \mathbf{r}_0) \approx -0.00903780772042 - 0.17497316464342i$ (with $p = 4$, $N = 64$)

$P_\beta(\mathbf{r}, \mathbf{r}_0) \approx -0.00903780769558 - 0.17497316468676i$ (by Gauss–Laguerre quadrature)

NaN indicates that an implementation problem is encountered as described in Section 1.4 due to some x_k evaluating to ± 1 in (3.45).

	$p = 2$, $1p = 2.0$		$p = 3$, $1p = 3.0$		$p = 4$, $1p = 4.0$	
N	$\lvert\beta\rvert \lvert J_N f - J_{2N} f\rvert / \pi$	EOC	$\lvert\beta\rvert \lvert J_N f - J_{2N} f\rvert / \pi$	EOC	$\lvert\beta\rvert \lvert J_N f - J_{2N} f\rvert / \pi$	EOC
2	2.9835E−02		4.0521E−02		5.3142E−02	
		3.4749		2.9109		2.5398
4	2.6834E−03		5.3877E−03		9.1384E−03	
		8.9063		6.5565		5.3946
8	5.5928E−06		5.7242E−05		2.1724E−04	
		12.1892		14.3281		12.0419
16	1.1976E−09		2.7830E−09		5.1520E−08	
		17.4698		15.8912		17.3616
32	6.5974E−15		4.5793E−14		3.0592E−13	
		6.1471		9.6881		14.4281
64	9.3095E−17		5.5511E−17		1.3878E−17	
		0.3169		−0.5000		−3.1699
128	7.4734E−17		7.8505E−17		1.2490E−16	
		−1.1610		−1.3219		−0.1520
256	1.6711E−16		1.9626E−16		1.3878E−16	
		−0.0888		−0.8923		0.6610
512	1.7772E−16		3.6428E−16		8.7771E−17	

	$p = 5$, $1p = 5.0$		$p = 6$, $1p = 6.0$		$p = 7$, $1p = 7.0$	
N	$\lvert\beta\rvert \lvert J_N f - J_{2N} f\rvert / \pi$	EOC	$\lvert\beta\rvert \lvert J_N f - J_{2N} f\rvert / \pi$	EOC	$\lvert\beta\rvert \lvert J_N f - J_{2N} f\rvert / \pi$	EOC
2	6.3383E−02		7.1217E−02		7.7820E−02	
		2.4181		2.3776		2.2894
4	1.1859E−02		1.3704E−02		1.5919E−02	
		4.7332		4.0425		3.5981
8	4.4587E−04		8.3166E−04		1.3145E−03	
		11.4955		10.8915		10.4077
16	1.5442E−07		4.3779E−07		9.6770E−07	
		17.0128		16.0351		16.2904
32	1.1678E−12		6.5195E−12		1.2074E−11	
		15.1996		16.1807		17.0519
64	3.1032E−17		8.7771E−17		8.8861E−17	
		−1.6893		0.5000		
128	1.0007E−16		6.2063E−17		NaN	
		−1.5788		−1.2680		
256	2.9894E−16		1.4947E−16		NaN	
		0.1731				
512	2.6513E−16		NaN		NaN	

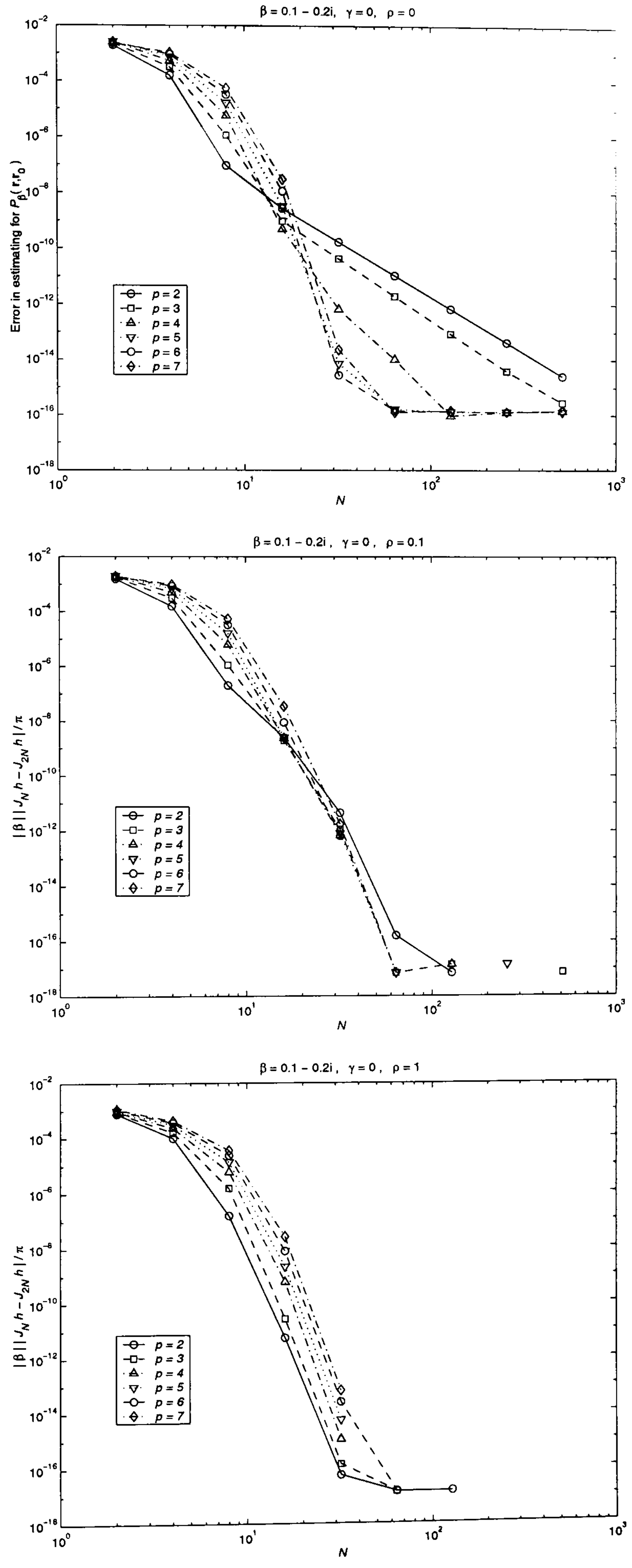


Figure 3.6: Error in estimating $P_\beta(\mathbf{r}, \mathbf{r}_0)$ vs. N, with h given by equation (3.19).

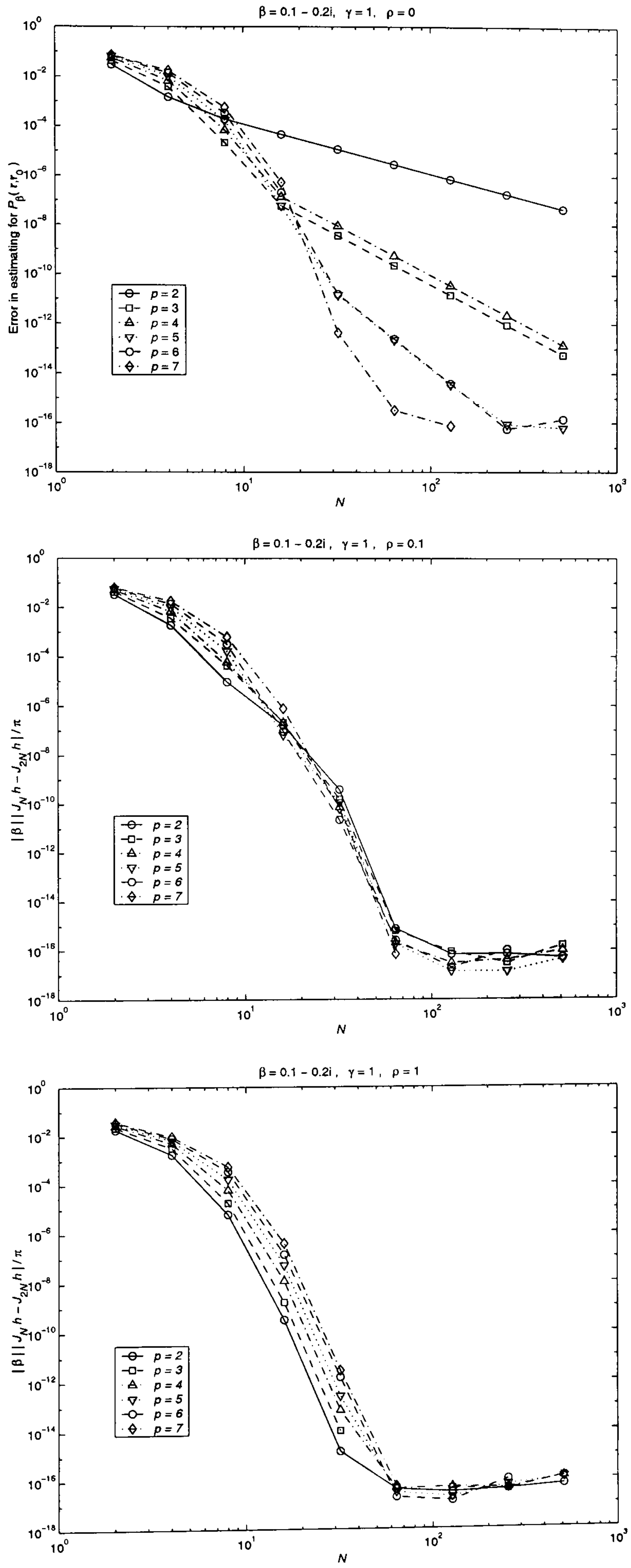


Figure 3.7: Error in estimating $P_\beta(\mathbf{r}, \mathbf{r}_0)$ vs. N, with h given by equation (3.19).

Table 3.7: $\beta = 0.1 - 0.2i$, $\gamma = 0$, $\rho = 0$

$$P_\beta(\mathbf{r}, \mathbf{r}_0) = -0.05700591319878 + 0.08720197355569i$$

NaN indicates that an implementation problem is encountered as described in Section 1.4 due to some x_k evaluating to ± 1 in (3.45).

	$p = 2, \quad 3p/2 = 3.0$		$p = 3, \quad 3p/2 = 4.5$		$p = 4, \quad 3p/2 = 6.0$	
N	ERROR	EOC	ERROR	EOC	ERROR	EOC
2	1.9048E−03		2.2761E−03		2.5404E−03	
		3.5773		2.8413		2.2546
4	1.5957E−04		3.1761E−04		5.3235E−04	
		10.7175		8.1322		6.5105
8	9.4768E−08		1.1320E−06		5.8389E−06	
		5.0949		10.1674		13.4792
16	2.7729E−09		9.8440E−10		5.1132E−10	
		3.9922		4.4905		9.5842
32	1.7424E−10		4.3791E−11		6.6615E−13	
		3.9981		4.4945		6.0037
64	1.0905E−11		1.9428E−12		1.0382E−14	
		3.9995		4.4952		5.8371
128	6.8177E−13		8.6146E−14		1.8161E−16	
		4.0001		4.5024		3.7100
256	4.2608E−14		3.8008E−15		1.3878E−17	
		4.0025		4.6247		1.0000
512	2.6584E−15		1.5407E−16		6.9389E−18	

	$p = 5, \quad 3p/2 = 7.5$		$p = 6, \quad 3p/2 = 9.0$		$p = 7, \quad 3p/2 = 10.5$	
N	ERROR	EOC	ERROR	EOC	ERROR	EOC
2	2.5942E−03		2.4856E−03		2.2905E−03	
		1.8168		1.4498		1.1239
4	7.3634E−04		9.0991E−04		1.0510E−03	
		5.4902		4.7701		4.2228
8	1.6382E−05		3.3347E−05		5.6289E−05	
		12.2658		11.4836		10.8319
16	3.3266E−09		1.1645E−08		3.0882E−08	
		18.8498		22.0045		20.3599
32	7.0412E−15		2.7677E−15		2.2950E−14	
		8.8259				11.6915
64	1.5516E−17		0		6.9389E−18	
128	1.5516E−17		1.3878E−17		0	
256	0		0		NaN	
512	0		6.9389E−18		NaN	

Table 3.8: $\beta = 0.1 - 0.2i$, $\gamma = 1$, $\rho = 0$

$$P_\beta(\mathbf{r}, \mathbf{r}_0) = -0.05700591319878 + 0.08720197355569i$$

NaN indicates that an implementation problem is encountered as described in Section 1.4 due to some x_k evaluating to ± 1 in (3.45).

N	$p=2$, $1p=2.0$ ERROR	EOC	$p=3$, $1p=3.0$ ERROR	EOC	$p=4$, $1p=4.0$ ERROR	EOC
2	2.9776E−02		4.3840E−02		5.6486E−02	
		4.3090		3.5215		3.0558
4	1.5022E−03		3.8178E−03		6.7929E−03	
		2.9719		7.4750		6.6209
8	1.9147E−04		2.1459E−05		6.9017E−05	
		2.0484		8.5295		8.9884
16	4.6289E−05		5.8074E−08		1.3589E−07	
		1.9988		3.9801		3.9077
32	1.1582E−05		3.6801E−09		9.0542E−09	
		1.9997		4.0008		4.0004
64	2.8960E−06		2.2988E−10		5.6572E−10	
		1.9999		4.0012		4.0001
128	7.2403E−07		1.4356E−11		3.5354E−11	
		2.0000		4.0010		4.0000
256	1.8101E−07		8.9664E−13		2.2096E−12	
		2.0000		4.0009		3.9995
512	4.5253E−08		5.6006E−14		1.3815E−13	

N	$p=5$, $1p=5.0$ ERROR	EOC	$p=6$, $1p=6.0$ ERROR	EOC	$p=7$, $1p=7.0$ ERROR	EOC
2	6.4872E−02		6.9932E−02		7.2931E−02	
		2.6639		2.3434		2.0801
4	1.0236E−02		1.3779E−02		1.7248E−02	
		5.8995		5.3492		4.9121
8	1.7148E−04		3.3804E−04		5.7287E−04	
		11.5119		10.6908		10.0639
16	5.8720E−08		2.0450E−07		5.3522E−07	
		11.9972		13.6470		20.2262
32	1.4363E−11		1.5942E−11		4.3636E−13	
		6.0026		6.0017		10.4866
64	2.2402E−13		2.4880E−13		3.0413E−16	
		5.9872		6.0055		1.6319
128	3.5315E−15		3.8728E−15		9.8131E−17	
		5.6411		5.4457		
256	7.0763E−17		8.8861E−17		NaN	
		0.1803		−0.3324		
512	6.2450E−17		1.1189E−16		NaN	

Table 3.9: $\beta = 0.1 - 0.2i$, $\gamma = 0$, $\rho = 0.1$

$P_\beta(\mathbf{r}, \mathbf{r}_0) \approx -0.06676531983090 + 0.08144988555515i$ (with $p = 3$, $N = 64$)

$P_\beta(\mathbf{r}, \mathbf{r}_0) \approx -0.06677901439626 + 0.08146750512402i$ (by Gauss–Laguerre quadrature)

NaN indicates that an implementation problem is encountered as described in Section 1.4 due to some x_k evaluating to ± 1 in (3.45).

	$p = 2$, $3p/2 = 3.0$		$p = 3$, $3p/2 = 4.5$		$p = 4$, $3p/2 = 6.0$	
N	$\lvert\beta\rvert\lvert J_N h - J_{2N} h\rvert/\pi$	EOC	$\lvert\beta\rvert\lvert J_N h - J_{2N} h\rvert/\pi$	EOC	$\lvert\beta\rvert\lvert J_N h - J_{2N} h\rvert/\pi$	EOC
2	1.5349E−03		1.7471E−03		1.9040E−03	
4	1.5652E−04	3.2938	3.0937E−04	2.4976	5.0486E−04	1.9151
8	2.0109E−07	9.6043	1.0960E−06	8.1409	6.2164E−06	6.3437
16	2.4897E−09	6.3357	1.9530E−09	9.1324	2.3681E−09	11.3582
32	4.5035E−12	9.1107	1.1161E−12	10.7731	6.9255E−13	11.7395
64	1.5838E−16	14.7953	6.9389E−18	17.2953	0	
128	6.9389E−18	4.5126	1.3878E−17	−1.0000	1.3878E−17	
256	0		0		0	
512	0		6.9389E−18		0	

	$p = 5$, $3p/2 = 7.5$		$p = 6$, $3p/2 = 9.0$		$p = 7$, $3p/2 = 10.5$	
N	$\lvert\beta\rvert\lvert J_N h - J_{2N} h\rvert/\pi$	EOC	$\lvert\beta\rvert\lvert J_N h - J_{2N} h\rvert/\pi$	EOC	$\lvert\beta\rvert\lvert J_N h - J_{2N} h\rvert/\pi$	EOC
2	1.9549E−03		1.9491E−03		1.9466E−03	
4	6.8930E−04	1.5039	8.4590E−04	1.2043	9.7868E−04	0.9921
8	1.6234E−05	5.4081	3.2653E−05	4.6952	5.4340E−05	4.1707
16	2.5230E−09	12.6515	8.9251E−09	11.8370	3.4570E−08	10.6183
32	8.1987E−13	11.5875	6.5972E−13	13.7237	1.7398E−12	14.2783
64	6.9389E−18	16.8503	0		6.9389E−18	17.9358
128	0		0		NaN	
256	1.3878E−17		0		NaN	
512	0		NaN		NaN	

Table 3.10: $\beta = 0.1 - 0.2i$, $\gamma = 1$, $\rho = 0.1$

$P_\beta(\mathbf{r}, \mathbf{r}_0) \approx -0.07167929633026 + 0.06548823755866i$ (with $p = 3$, $N = 64$)

$P_\beta(\mathbf{r}, \mathbf{r}_0) \approx -0.07112801617726 + 0.06473200539844i$ (by Gauss–Laguerre quadrature)

NaN indicates that an implementation problem is encountered as described in Section 1.4 due to some x_k evaluating to ± 1 in (3.45).

	$p = 2, \quad 1p = 2.0$		$p = 3, \quad 1p = 3.0$		$p = 4, \quad 1p = 4.0$	
N	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC
2	3.2972E−02		4.2688E−02		4.9651E−02	
		4.1242		3.5763		2.8747
4	1.8908E−03		3.5788E−03		6.7697E−03	
		7.6518		6.3653		6.8064
8	9.4022E−06		4.3411E−05		6.0482E−05	
		5.8401		7.6510		8.1559
16	1.6412E−07		2.1598E−07		2.1206E−07	
		8.6877		10.3980		11.4441
32	3.9802E−10		1.6007E−10		7.6107E−11	
		18.9584		17.9157		18.4799
64	7.8136E−16		6.4737E−16		2.0817E−16	
		3.4932		2.8650		2.7459
128	6.9389E−17		8.8861E−17		3.1032E−17	
		−0.0283		1.5178		−0.4240
256	7.0763E−17		3.1032E−17		4.1633E−17	
		0.5000		−2.3502		−1.2370
512	5.0037E−17		1.5823E−16		9.8131E−17	

	$p = 5, \quad 1p = 5.0$		$p = 6, \quad 1p = 6.0$		$p = 7, \quad 1p = 7.0$	
N	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC
2	5.4629E−02		5.8954E−02		6.3113E−02	
		2.4424		2.1025		1.8157
4	1.0051E−02		1.3728E−02		1.7928E−02	
		5.9081		5.4115		4.8332
8	1.6737E−04		3.2254E−04		6.2890E−04	
		11.3028		11.7514		9.6420
16	6.6250E−08		9.3551E−08		7.8714E−07	
		9.1149		12.0159		13.5201
32	1.1949E−10		2.2590E−11		6.7005E−11	
		19.2916		16.3885		19.8528
64	1.8619E−16		2.6331E−16		7.0763E−17	
		3.7459		3.7459		
128	1.3878E−17		1.9626E−17		NaN	
				−2.3502		
256	1.3878E−17		1.0007E−16		NaN	
		−1.6610				
512	4.3885E−17		NaN		NaN	

Table 3.11: $\beta = 0.1 - 0.2i$, $\gamma = 0$, $\rho = 1$

$P_\beta(\mathbf{r}, \mathbf{r}_0) \approx -0.11043681502955 - 0.00957558987026i$ (with $p = 3$, $N = 64$)

$P_\beta(\mathbf{r}, \mathbf{r}_0) \approx -0.11043681502854 - 0.00957558987042i$ (by Gauss–Laguerre quadrature)

NaN indicates that an implementation problem is encountered as described in Section 1.4 due to some x_k evaluating to ± 1 in (3.45).

	$p = 2, \quad 3p/2 = 3.0$		$p = 3, \quad 3p/2 = 4.5$		$p = 4, \quad 3p/2 = 6.0$	
N	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC
2	7.6687E−04		8.5025E−04		9.2003E−04	
4	1.0118E−04	2.9221	1.6099E−04	2.4009	2.3333E−04	1.9793
8	1.5895E−07	9.3141	1.5346E−06	6.7130	5.9452E−06	5.2945
16	5.6205E−12	14.7875	2.7834E−11	15.7506	6.1647E−10	13.2354
32	5.5511E−17	16.6276	1.3947E−16	17.6065	1.0999E−15	19.0962
64	1.3878E−17	2.0000	1.3878E−17	3.3291	0	
128	1.3878E−17		0		0	
256	0		0		0	
512	0		0		0	

	$p = 5, \quad 3p/2 = 7.5$		$p = 6, \quad 3p/2 = 9.0$		$p = 7, \quad 3p/2 = 10.5$	
N	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC
2	9.8189E−04		1.0531E−03		1.1313E−03	
4	3.0202E−04	1.7009	3.6562E−04	1.5262	4.2444E−04	1.4143
8	1.3599E−05	4.4730	2.3916E−05	3.9343	3.6224E−05	3.5505
16	2.1890E−09	12.6010	8.0964E−09	11.5284	2.7300E−08	10.3738
32	5.6043E−15	18.5753	2.5009E−14	18.3045	6.6095E−14	18.6559
64	0		1.3878E−17	10.8154	0	
128	0		1.3878E−17		NaN	
256	0		0		NaN	
512	0		NaN		NaN	

Table 3.12: $\beta = 0.1 - 0.2i$, $\gamma = 1$, $\rho = 1$

$P_\beta(\mathbf{r}, \mathbf{r}_0) \approx -0.05861168261500 - 0.03230345478596i$ (with $p = 3$, $N = 64$)

$P_\beta(\mathbf{r}, \mathbf{r}_0) \approx -0.05861167719527 - 0.03230345153251i$ (by Gauss–Laguerre quadrature)

NaN indicates that an implementation problem is encountered as described in Section 1.4 due to some x_k evaluating to ± 1 in (3.45).

	$p = 2, \quad 1p = 2.0$		$p = 3, \quad 1p = 3.0$		$p = 4, \quad 1p = 4.0$	
N	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC
2	1.8393E−02		2.2545E−02		2.7086E−02	
		3.3932		2.8203		2.4432
4	1.7507E−03		3.1918E−03		4.9806E−03	
		8.1311		7.4507		6.3245
8	6.2445E−06		1.8245E−05		6.2148E−05	
		14.2609		13.4500		12.3394
16	3.1809E−10		1.6305E−09		1.1992E−08	
		17.7265		17.2924		17.4112
32	1.4667E−15		1.0157E−14		6.8801E−14	
		5.1386				10.6145
64	4.1633E−17		0		4.3885E−17	
		0.4240				−0.1893
128	3.1032E−17		4.3885E−17		5.0037E−17	
		−0.3390		0.1610		0.1893
256	3.9252E−17		3.9252E−17		4.3885E−17	
		−0.5850		−1.6610		−1.4339
512	5.8878E−17		1.2413E−16		1.1857E−16	

	$p = 5, \quad 1p = 5.0$		$p = 6, \quad 1p = 6.0$		$p = 7, \quad 1p = 7.0$	
N	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC	$\lvert\beta\rvert \lvert J_N h - J_{2N} h\rvert/\pi$	EOC
2	3.0868E−02		3.4079E−02		3.7003E−02	
		2.2420		2.0926		1.9445
4	6.5255E−03		7.9902E−03		9.6136E−03	
		5.2683		4.5030		4.1133
8	1.6932E−04		3.5239E−04		5.5546E−04	
		11.6805		11.2759		10.4242
16	5.1584E−08		1.4211E−07		4.0424E−07	
		17.5968		16.5393		17.1402
32	2.6023E−13		1.4921E−12		2.7985E−12	
		13.0338		16.2143		15.6215
64	3.1032E−17		1.9626E−17		5.5511E−17	
		0.6610		0.5000		
128	1.9626E−17		1.3878E−17		NaN	
		−1.5850		−2.8074		
256	5.8878E−17		9.7145E−17		NaN	
		−0.9262				
512	1.1189E−16		NaN		NaN	

3.4 Conclusions

As mentioned in Section 3.2, we restrict our attention to the case when the relative surface admittance β is in the range $|\beta| \leq 1$, which range of β includes most values of interest in outdoor sound propagation. From Section 3.2, we have two expressions for $P_\beta(\mathbf{r}, \mathbf{r}_0)$ which are complementary, and which we present using the notation in Chapter 2, that

$$J\Psi := \int_{-\infty}^{+\infty} e^{-\rho s^2} \Psi(s^2)\, ds.$$

For $|\beta| \leq 1$ and $|1-\beta| \leq 0.1$,

$$P_\beta(\mathbf{r}, \mathbf{r}_0) = -\frac{\beta e^{i\rho}}{\pi} Jf, \tag{3.46}$$

where

$$f(t) = -\frac{\beta + \gamma(1+it)}{(t-2i)^{1/2}\,(t-ia_+)(t-ia_-)},$$

$$\gamma = \cos\theta_0\,,$$

$$a_\pm = 1 + \beta\gamma \mp (1-\beta^2)^{1/2}(1-\gamma^2)^{1/2},$$

with $\mathrm{Re}\left\{(1-\beta^2)^{1/2}\right\}, \mathrm{Re}\left\{(t-2i)^{1/2}\right\} > 0$. For $\mathrm{Re}\,\beta > 0$, $|\beta| \leq 1$, and $|1-\beta| \geq 0.1$,

$$\begin{aligned} P_\beta(\mathbf{r}, \mathbf{r}_0) = & -\frac{\beta e^{i\rho}}{\pi} Jh + \frac{\beta e^{i\rho(1-\tilde{a}_+)}\sqrt{a_+}}{2(1-\beta^2)^{1/2}\sqrt{\tilde{a}_+}} \,\mathrm{erfc}\,(e^{-i\pi/4}\sqrt{\rho}\sqrt{\tilde{a}_+}) \\ & - \frac{\beta e^{i\rho(1-a_+)}}{2(1-\beta^2)^{1/2}} \,\mathrm{erfc}\,(e^{-i\pi/4}\sqrt{\rho}\sqrt{a_+}), \end{aligned} \tag{3.47}$$

where

$$h(t) = f(t) + \frac{e^{i\pi/4}(1-\mathrm{Re}\,a_+)\sqrt{a_+}}{2(1-\beta^2)^{1/2}(t-ia_+)(t-i\tilde{a}_+)},$$

$$\tilde{a}_+ = 1 + i\mathrm{Im}\,a_+,$$

with $\mathrm{Re}\sqrt{a_+}, \mathrm{Re}\left\{(1-\beta^2)^{1/2}\right\} > 0$. In other words, expression (3.46) is suitable when β is near 1, and expression (3.47) is suitable when β is bounded away from 1.

Applying the quadrature rule approximation (2.13), $J_N f$, to evaluate Jf in (3.46) and Jh in (3.47), we obtain the error bounds in Theorems 3.3 and 3.4, respectively. The complementary error functions in (3.47) have been evaluated in this thesis by using the code in Appendix A.

From Theorems 3.3 and 3.4, we can see that the quadrature rule approximation (2.13) is predicted to be an accurate numerical quadrature method, even for fairly small values of N, for the evaluation of Jf and Jh, provided $\rho \geq 0$ is not too large.

We demonstrate the numerical analysis results of Theorems 3.3 and 3.4 by plotting the error in estimating $P_\beta(\mathbf{r}, \mathbf{r}_0)$ against ρ, depicting it in Figures 3.8–3.9 ($\beta = 0.99 - 0.01i$ and $\gamma = 0, 1$) and Figures 3.10–3.11 ($\beta = 0.1 - 0.02i$ and $\gamma = 0, 1$), respectively. We can see that, for $N = 64$ and $p = 6$ or $p = 7$, the results are accurate, with error not more than 10^{-15} when $\gamma = 0$, not more than 10^{-10} when $\gamma = 1$, for $0 < \rho \leq 10$.

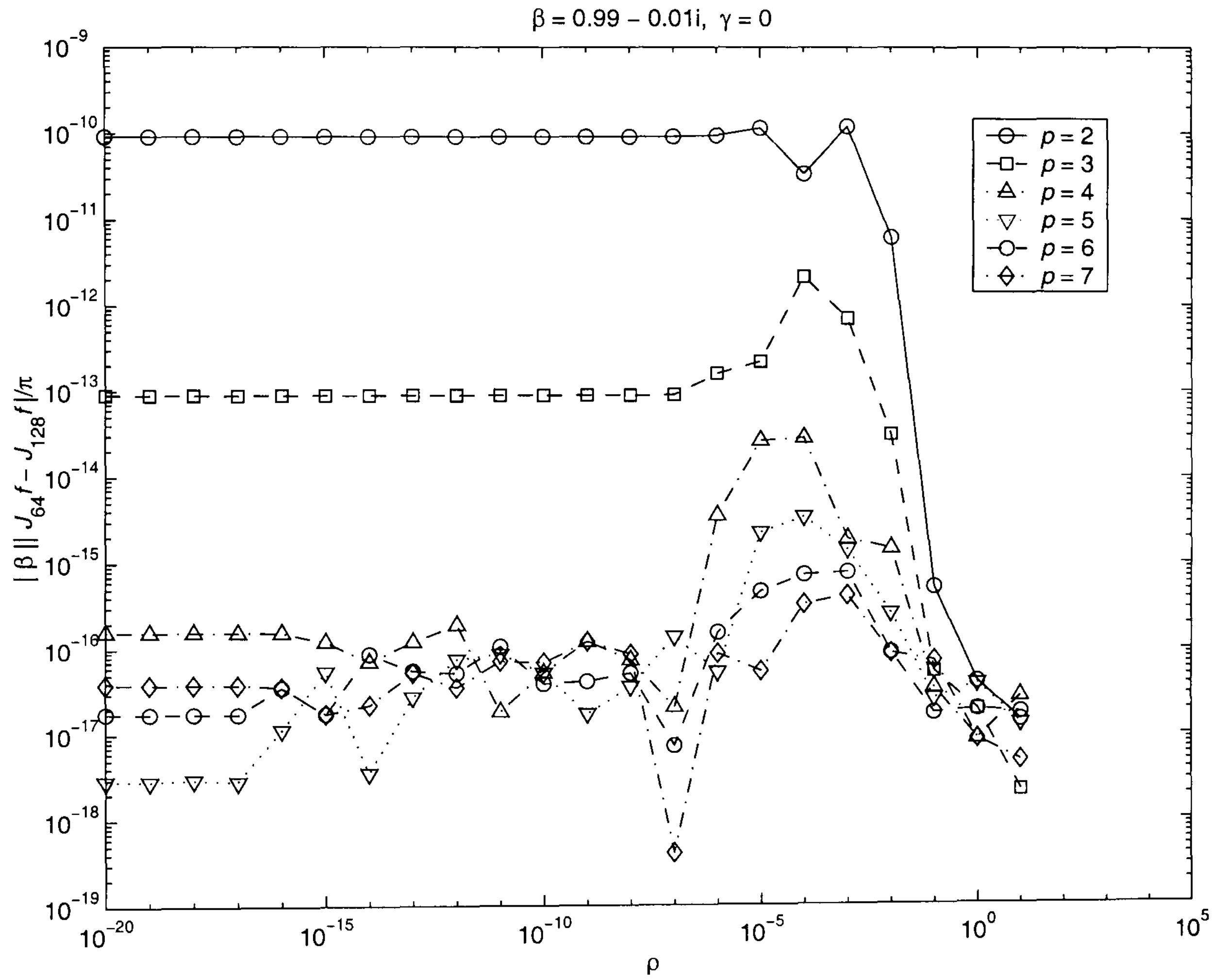


Figure 3.8: Error in estimating $P_\beta(\mathbf{r}, \mathbf{r}_0)$ vs. ρ, with f given by equation (3.10).

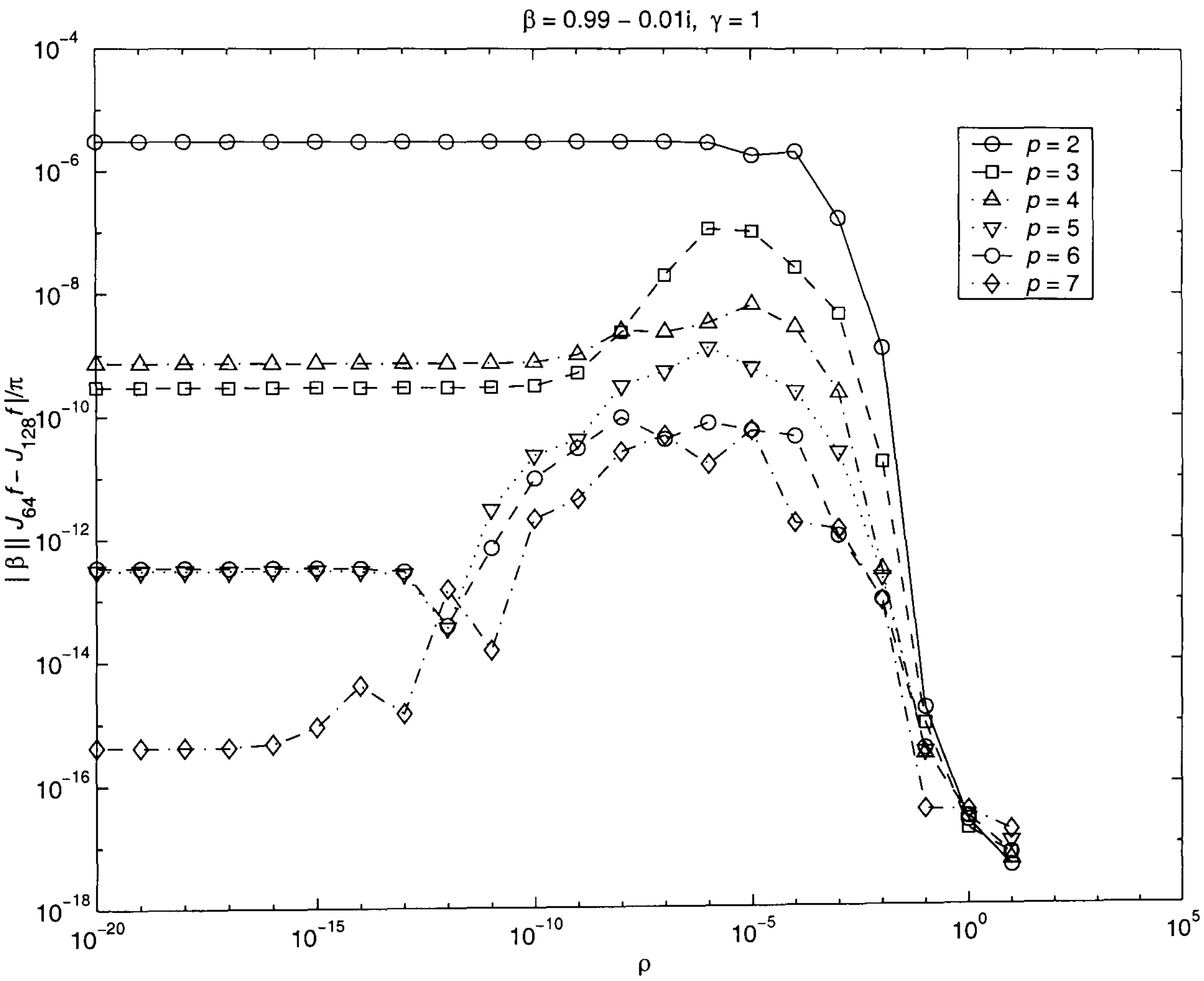


Figure 3.9: Error in estimating $P_\beta(\mathbf{r}, \mathbf{r}_0)$ vs. ρ, with f given by equation (3.10).

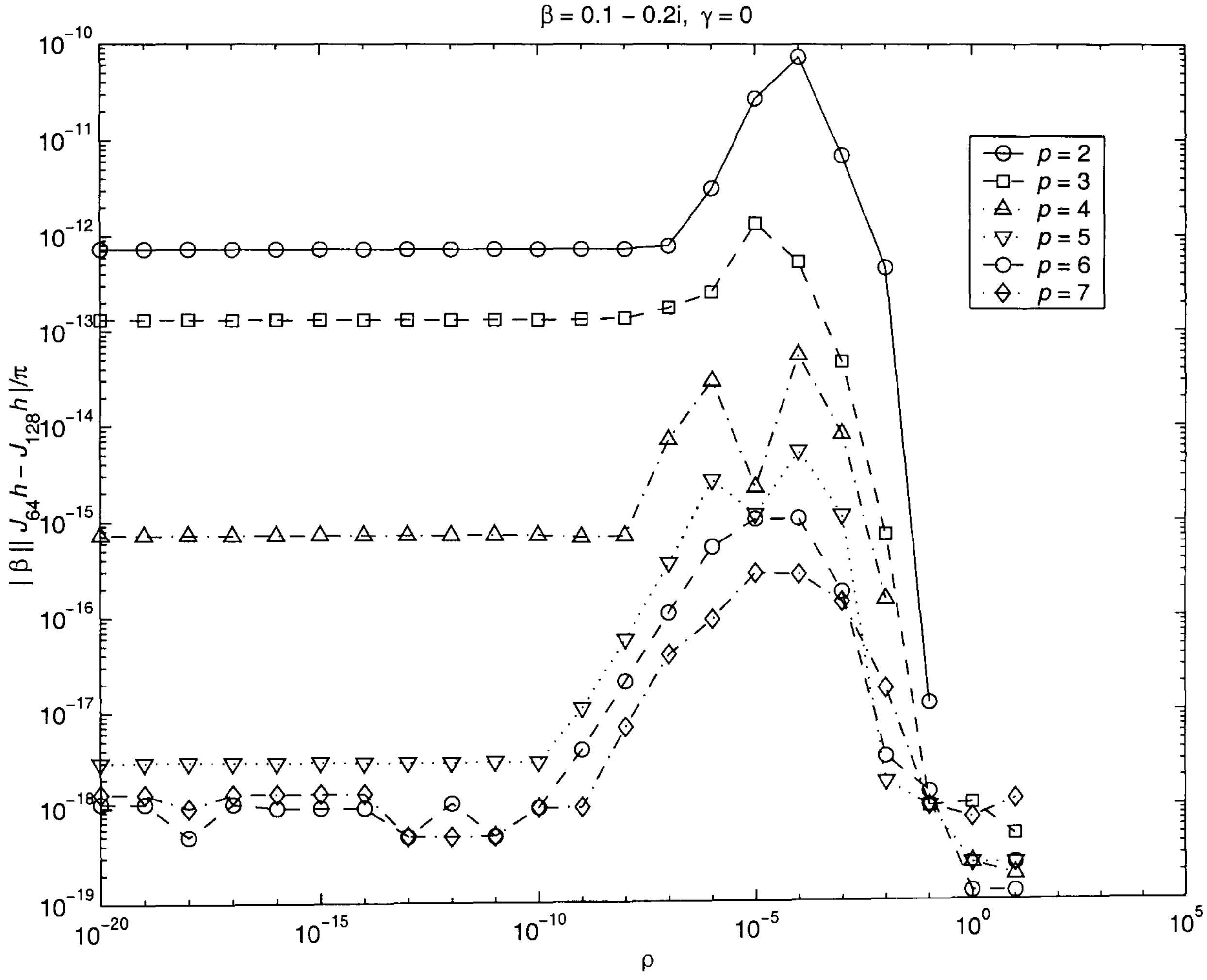


Figure 3.10: Error in estimating $P_\beta(\mathbf{r}, \mathbf{r}_0)$ vs. ρ, with h given by equation (3.19).

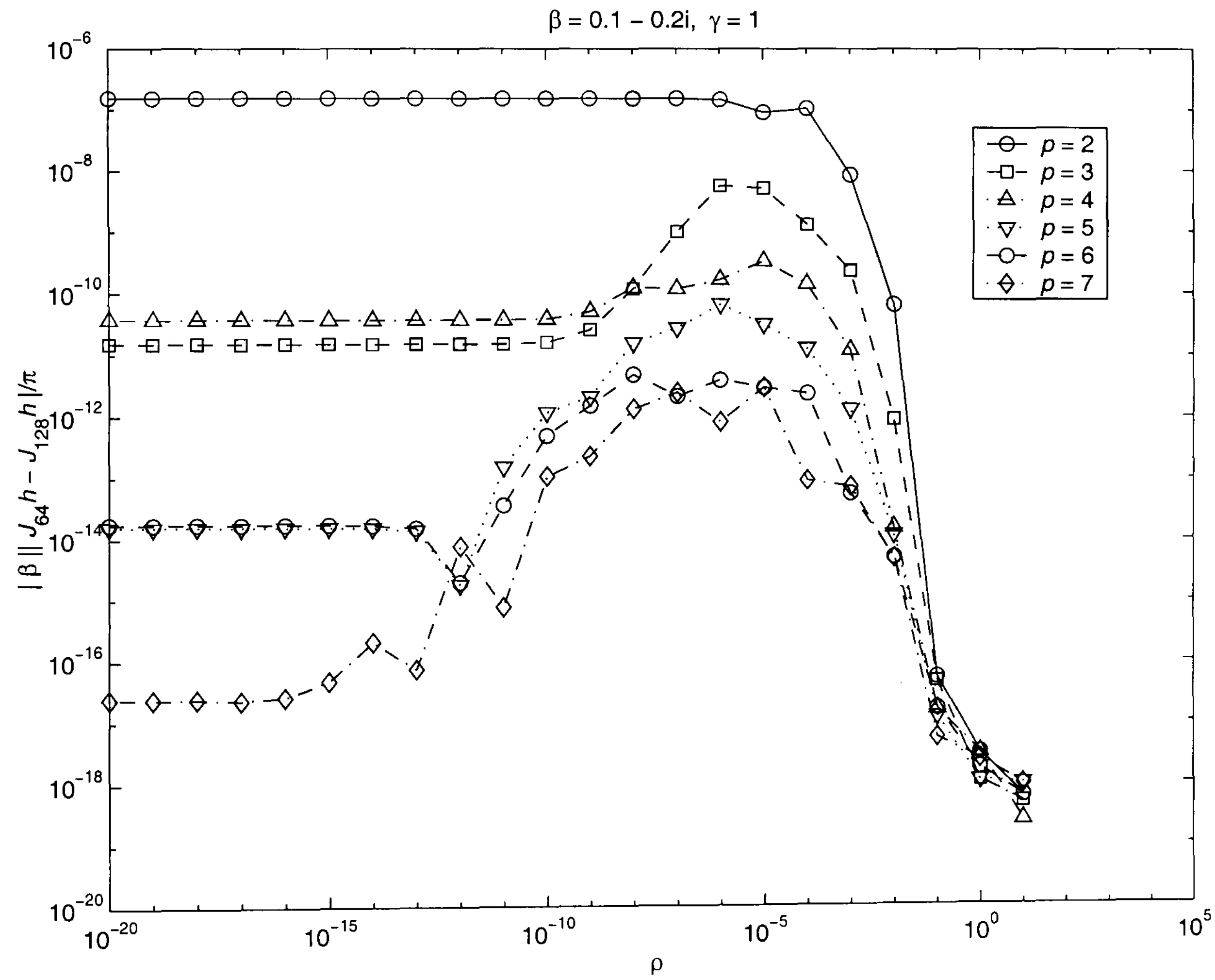


Figure 3.11: Error in estimating $P_\beta(\mathbf{r}, \mathbf{r}_0)$ vs. ρ, with h given by equation (3.19).

Chapter 4

A Numerical Quadrature Method for Integrals on Finite Intervals with Branch Point Singularities near the Interval of Integration

In this chapter, we will apply the quadrature method and error analysis in Chapter 1 to numerically evaluate If, where f may have a branch point singularity near or on the interval of integration. We consider functions f satisfying the following assumptions.

Assumption 4.1 *For some $q \in \mathbb{N}$ and b_r with $-1 < b_r < 1$ it holds that $f \in C^q(-1, b_r) \cap C^q(b_r, 1)$, and that there exist $c > 0$ and α with $0 < \alpha \leq 1$ such that, for $j = 0, 1, \ldots, q$,*

$$|f^{(j)}(t)| \leq \begin{cases} c\left[\dfrac{(1+t)|t-b_r|}{1+b_r}\right]^{\alpha-1-j}, & -1 < t < b_r, \\ \\ c\left[\dfrac{(1-t)|t-b_r|}{1-b_r}\right]^{\alpha-1-j}, & b_r < t < 1. \end{cases} \tag{4.1}$$

Note that, in particular, the inequality (4.1) holds if $f^{(j)}$ satisfies the simpler bound

$$|f^{(j)}(t)| \leq c\,|t-b_r|^{\alpha-1-j}, \qquad t \in (-1, b_r) \cap (b_r, 1).$$

It follows from this observation that Assumption 4.1 holds when f is analytic except for a branch point singularity at $b \in \mathbb{C}$ with $\operatorname{Re} b = b_r$, precisely if f satisfies the following assumption.

Assumption 4.1′ *For some $\varepsilon > 0$, and $b = b_r + ib_i \in \mathbb{C}$ with $b_i \geq 0$, the function f is analytic in $\mathcal{D}_{\varepsilon,b}$, where (see Figure 4.1)*

$$\mathcal{D}_{\varepsilon,b} := \Big\{z \in \mathbb{C} : \operatorname{dist}(z, [-1,1]) < \varepsilon\Big\} \backslash \Big\{b_r + it : t \geq b_i\Big\}.$$

Further, for some $\widetilde{c} > 0$ and α with $0 < \alpha \leq 1$,

$$|f(z)| \leq \widetilde{c}\,|z - b|^{\alpha-1}, \qquad z \in \mathcal{D}_{\varepsilon,b}.$$

Lemma 4.1 *Let f satisfy Assumption 4.1′. Then, for $j = 0, 1, \ldots,$*

$$|f^{(j)}(t)| \leq \widetilde{c}\,C_j |t - b_r|^{\alpha-1-j}, \qquad t \in [-1,1]\backslash\{b_r\}, \tag{4.2}$$

where

$$C_j := \frac{j!}{\widetilde{\theta}^j (1 - \widetilde{\theta}\,)^{1-\alpha}}$$

and

$$\widetilde{\theta} := \min\left\{\frac{\varepsilon}{R}, \frac{j}{j+1-\alpha}\right\}.$$

Thus, in the case $-1 < b_r < 1$, f satisfies Assumption 4.1 for every $q \in \mathbb{N}$, with

$$c = \widetilde{c} \max_{j=0,\ldots,q} C_j.$$

Proof. Let $t \in [-1,1]\backslash\{b_r\}$, $R = |t - b|$, and $0 < \theta < \min\{1, \varepsilon/R\}$. From Cauchy's integral formula with circular contour $C_{R\theta}(t)$, the circle of radius $R\theta$ centred at t (see Figure 4.2),

$$\begin{aligned}
|f^{(j)}(t)| &= \left|\frac{j!}{2\pi i}\int_{C_{R\theta}(t)} \frac{f(z)}{(z-t)^{j+1}}\,dz\right| \\
&\leq \frac{j!}{R^j\theta^j}\max_{z\in C_{R\theta}(t)} |f(z)| \\
&\leq \frac{j!\,\widetilde{c}}{R^j\theta^j}\max_{z\in C_{R\theta}(t)} |z - b|^{\alpha-1} \\
&= \frac{j!\,\widetilde{c}}{R^j\theta^j}\big[R(1-\theta)\big]^{\alpha-1} \\
&= \frac{j!\,\widetilde{c}\,|t-b|^{\alpha-1-j}}{\theta^j(1-\theta)^{1-\alpha}} \\
&\leq \frac{j!\,\widetilde{c}\,|t-b_r|^{\alpha-1-j}}{\theta^j(1-\theta)^{1-\alpha}}.
\end{aligned}$$

In the case that $\varepsilon/R < 1$, taking the limit $\theta \to \frac{\varepsilon}{R}^-$ we see that this bound holds also for $\theta = \varepsilon/R$. Then setting $\theta = \widetilde{\theta}$ (to minimise $[\theta^j(1-\theta)^{1-\alpha}]^{-1}$), we obtain (4.2). ∎

Before applying the quadrature method developed in Chapter 1 to $If = \int_{-1}^{+1} f(x)dx$, in the case when f satisfies Assumption 4.1, we write If as

$$If = \int_{-1}^{b_r} f(x)\,dx + \int_{b_r}^{+1} f(x)\,dx,$$

and make a linear substitution to change the intervals of integration to $[-1,1]$. This gives

$$If = \int_{-1}^{+1} \widetilde{f}(t)\,dt = I\widetilde{f}, \tag{4.3}$$

where

$$\widetilde{f}(t) = f_1(t) + f_2(t), \tag{4.4}$$

$$f_1(t) = \left(\frac{1+b_r}{2}\right) f\left(\frac{1+b_r}{2}t - \frac{1-b_r}{2}\right), \quad -1 < t < 1, \tag{4.5}$$

$$f_2(t) = \left(\frac{1-b_r}{2}\right) f\left(\frac{1-b_r}{2}t + \frac{1+b_r}{2}\right), \quad -1 < t < 1. \tag{4.6}$$

The singularities of $\widetilde{f}$ are thus just at ± 1. To apply Theorem 1.3 and apply the numerical quadrature method of Chapter 1 to evaluate $I\widetilde{f}$, it is sensible to check that $\widetilde{f} \in \mathcal{S}^{\widetilde{q},\widetilde{\alpha}}[-1,1]$ for some $\widetilde{q} \in \mathbb{N}$ and $\widetilde{\alpha} > 0$, and to estimate $\|\widetilde{f}\|_{\widetilde{q},\widetilde{\alpha}}$. From equations (4.4) to (4.6),

$$\widetilde{f}^{(j)}(t) = \left(\frac{1+b_r}{2}\right)^{j+1} f^{(j)}\left(\frac{1+b_r}{2}t - \frac{1-b_r}{2}\right) + \left(\frac{1-b_r}{2}\right)^{j+1} f^{(j)}\left(\frac{1-b_r}{2}t + \frac{1+b_r}{2}\right)$$

so that, recalling that $0 < \alpha \le 1$ in Assumption 4.1,

$$\begin{aligned} |\widetilde{f}^{(j)}(t)| &\le c\,2^{j+1-2\alpha}(1+b_r)^\alpha(1-t^2)^{\alpha-1-j} + c\,2^{j+1-2\alpha}(1-b_r)^\alpha(1-t^2)^{\alpha-1-j} \\ &= c\,2^{j+1-2\alpha}[(1+b_r)^\alpha + (1-b_r)^\alpha](1-t^2)^{\alpha-1-j} \\ &\le c\,2^{j+2(1-\alpha)}(1-t^2)^{\alpha-1-j}. \end{aligned} \tag{4.7}$$

Hence, we have shown that if Assumption 4.1 holds then $\widetilde{f} \in \mathcal{S}^{\widetilde{q},\widetilde{\alpha}}[-1,1]$, and, comparing (4.7) with (1.10),

$$\|\widetilde{f}\|_{\widetilde{q},\widetilde{\alpha}} \le c\,2^{q+2(1-\alpha)}. \tag{4.8}$$

Our numerical method for evaluation of If, in the case that Assumption 4.1 holds, will be to approximate If by $I_N\widetilde{f}$, where the numerical integration rule I_N is defined by

(1.26), with some function w satisfying Assumption 1.1. Explicitly

$$If \approx I_N \widetilde{f} = \sum_{k=1-N}^{N-1} a_k \widetilde{f}(x_k), \tag{4.9}$$

where, for $k = 1-N, \ldots, N-1$,

$$a_k = \frac{1}{N} w'\left(\frac{k}{N}\right), \qquad x_k = w\left(\frac{k}{N}\right),$$

and $\widetilde{f}$ is given by (4.4). The error in this approximation is bounded in the next theorem.

Throughout the following error estimate, we let $C > 0$ denote a generic constant, whose value depends at most on the values of q, α in Assumption 4.1, p in Assumption 1.1, and on the choice of the function w.

Theorem 4.1 *Suppose that w satisfies Assumption 1.1, f satisfies Assumption 4.1, $q \in \mathbb{N}$, and $1 < \alpha p \le q$. Then, if $\alpha p \notin \mathbb{N}$, the error in the quadrature (4.9) can be bounded by*

$$|If - I_N \widetilde{f}| \le cCN^{-\alpha p},$$

where the constant C depends only on q, α and on the function w. If $\alpha p = q$, then

$$|If - I_N \widetilde{f}| \le c_\delta c C N^{\delta - q},$$

for every $\delta > 0$, where $c_\delta > 0$ depends only on δ.

Proof. This result follows from Theorem 1.3, (4.3), and (4.8). ■

Combining Theorem 4.1 with Lemma 4.1, we obtain the following corollary.

Corollary 4.1 *Suppose that w satisfies Assumption 1.1, f satisfies Assumption 4.1′, $q \in \mathbb{N}$, and $1 < \alpha p \le q$. Then, if $\alpha p \notin \mathbb{N}$, the error in the quadrature (4.9) can be bounded by*

$$|If - I_N \widetilde{f}| \le \frac{\widetilde{c}C}{\widetilde{\theta}^q (1-\widetilde{\theta})^{1-\alpha}} N^{-\alpha p}$$

with

$$\widetilde{\theta} := \min\left\{\frac{\varepsilon}{R}, \frac{j}{j+1-\alpha}\right\},$$

where the constant C depends only on q, α and on the function w. If $\alpha p = q$, then

$$|If - I_N \widetilde{f}| \le \frac{c_\delta \widetilde{c} C}{\widetilde{\theta}^q (1-\widetilde{\theta})^{1-\alpha}} N^{\delta - q},$$

for every $\delta > 0$, where $c_\delta > 0$ depends only on δ.

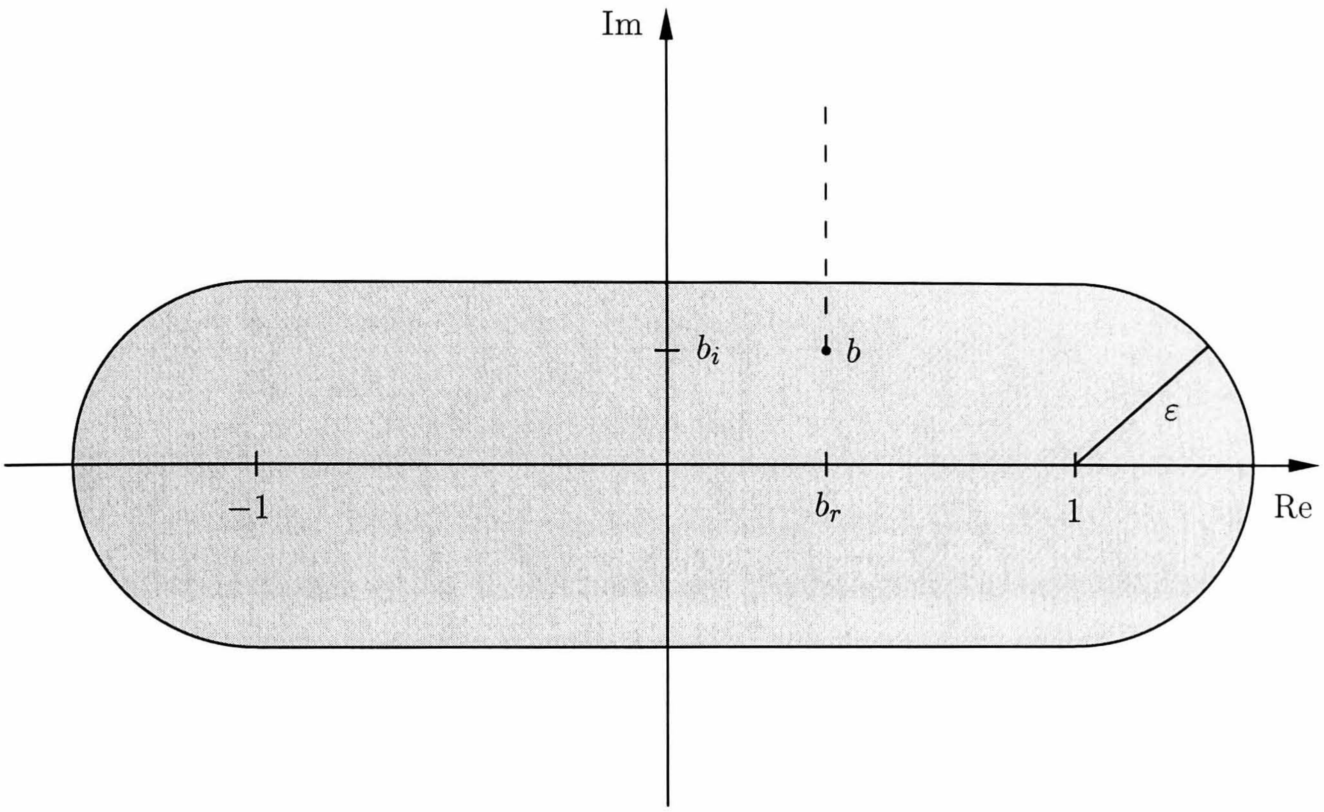


Figure 4.1: $\mathcal{D}_{\varepsilon,b}$ in Assumption 4.1′.

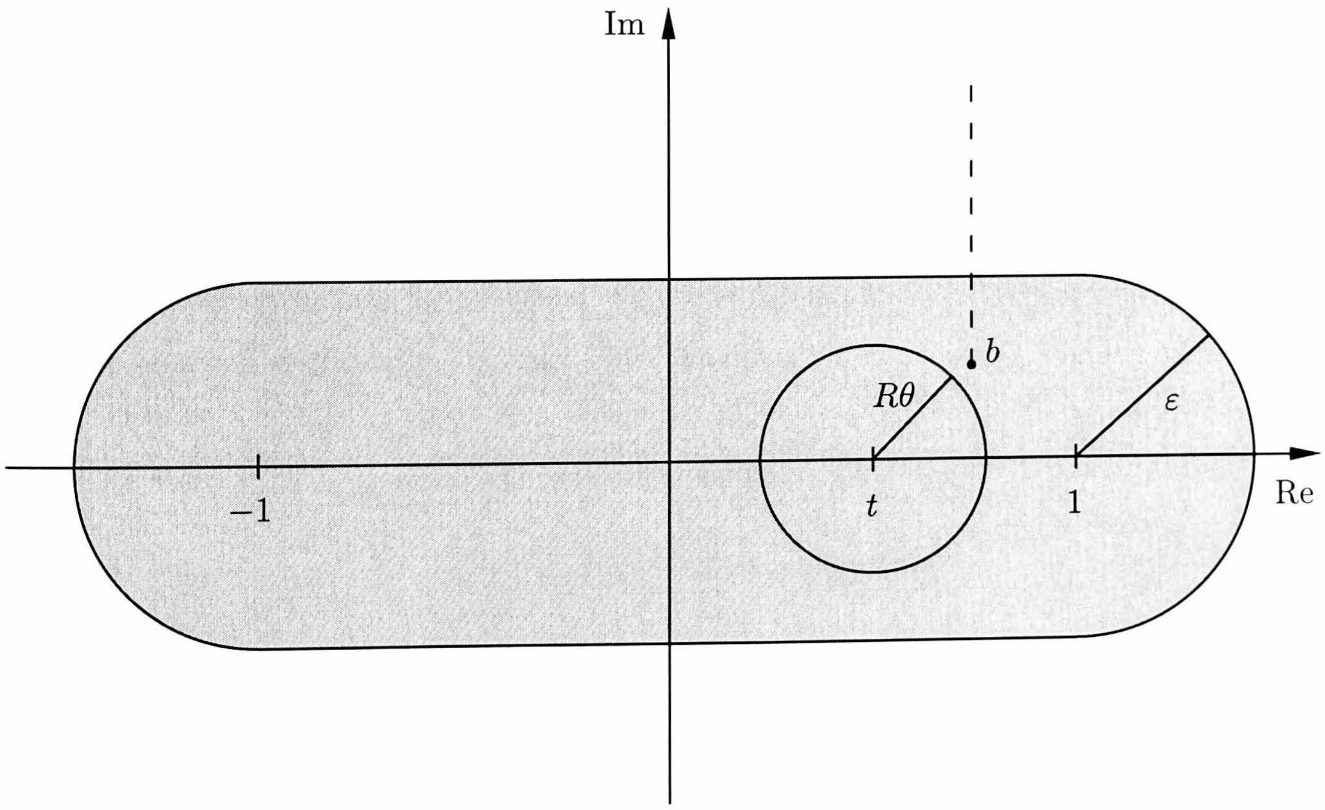


Figure 4.2: $\mathcal{D}_{\varepsilon,b}$ and the circular contour $C_{R\theta}(t)$ used in the proof of Lemma 4.1.

4.1 Numerical Examples

Example 1

Let

$$f(z) = (z-b)^{-1/2} \tag{4.10}$$

where $b = b_r + ib_i \in \mathbb{C}$ with $-1 < b_r < 1$, and $b_i \geq 0$. Then

$$If = \int_{-1}^{+1} f(t)\,dt = 2\big[(1-b_r-ib_i)^{1/2} - i(1+b_r+ib_i)^{1/2}\big].$$

We will illustrate the numerical scheme introduced above by using it to compute values of If for different choices of $b \in \mathbb{C}$. All numerical computations in this example have been carried out using the Kress form of the function w satisfying Assumption 1.1, given by equations (1.31) and (1.33).

If $b_i > 0$, then a suitable approximation for If is $I_N f$, given by (1.26). For, if $b_i > 0$, then $f \in \mathcal{C}^\infty[-1,1] \subset \mathcal{S}^{q,\alpha}[-1,1]$ for every $q \in \mathbb{N}$ and $0 < \alpha \leq 1$, so that Theorem 1.3 predicts that

$$|If - I_N f| \leq c_\delta C \|f\|_{q,\alpha} N^{\delta-\alpha p} \tag{4.11}$$

for every $\delta > 0$ and every α with $0 < \alpha \leq 1$, if w satisfies Assumption 1.1, where C, here and below, denotes a constant which depends only on q, α, p, w, and c_δ a constant which depends only on δ. Thus, by suitable choice of w, convergence of $I_N f$ to If at an arbitrarily high order can be achieved. Further, for $|b_r| \geq 1$, it follows from Lemma 4.1, applied with $\alpha = 1/2$ and $\varepsilon = 1$, that, for $j = 0, 1, \ldots,$

$$\begin{aligned} |f^{(j)}(t)| &\leq \tilde{c} C_j |t-b_r|^{-1/2-j} \\ &\leq \tilde{c} 2^{1/2+j} C_j (1-t^2)^{-1/2-j}. \end{aligned} \tag{4.12}$$

Thus

$$\|f\|_{q,1/2} \leq \tilde{c} 2^{1/2+q} \max_{j=0,\ldots,q} C_j$$

so that, applying Theorem 1.3 with $\alpha = 1/2$,

$$|If - I_N f| \leq c_\delta \tilde{c} C N^{\delta - p/2}. \tag{4.13}$$

However, for $-1 < b_r < 1$, from (1.10),

$$\begin{aligned}\|f\|_{q,\alpha} &\geq \sup_{-1<t<1} |f'(t)|(1-t^2)^{2-\alpha} \\ &= \frac{1}{2} \sup_{-1<t<1} |t - b_r - ib_i|^{-3/2}(1-t^2)^{2-\alpha} \\ &\geq \widetilde{C}\, b_i^{-3/2},\end{aligned}$$

where $\widetilde{C} > 0$ depends only on b_r and α, so that the bound on the right hand side of (4.11) blows up as $b_i \to 0$. This suggests that applying the numerical quadrature of Chapter 1 to If will be inaccurate for small b_i.

As an approximation which is accurate uniformly in b_r and b_i for $-1 < b_r < 1$ and $b_i \geq 0$, $I_N\widetilde{f}$ will be used to evaluate If. We can see that f satisfies Assumption 4.1′ with $\alpha = 1/2$, $\widetilde{c} = 1$, and $\varepsilon = 1$. Thus, by Lemma 4.1, for $-1 < b_r < 1$, $b_i \geq 0$, f satisfies Assumption 4.1 for every $q \in \mathbb{N}$, with a constant $c > 0$ in (4.1) dependent only on q. So, if also w satisfies Assumption 1.1, applying Theorem 4.1,

$$|If - I_N\widetilde{f}\,| \leq c_\delta C N^{\delta - p/2}, \tag{4.14}$$

for every $\delta > 0$, where $c_\delta > 0$ depends only on δ and $C > 0$ depends only on p and w.

As a numerical example to show that finding the numerical value of If by $I_N\widetilde{f}$ rather than I_Nf will improve the error in estimating the integral If, we have carried out computations as follows.

Firstly, we vary b_r in the range $-1 < b_r < 1$ and choose $b_i = 0.001$, evaluating the error in estimating If with I_Nf (see Figure 4.3). These results, coupled with those of Figure 4.4, show that, for $-1 < b_r < 1$, estimating If by I_Nf is inaccurate for small b_i.

Secondly, to show that the error in estimating If with $I_N\widetilde{f}$ is much smaller, and also to show the fact, as predicted by Theorem 4.1, that the error in estimating If with $I_N\widetilde{f}$ tends to zero as $N \to \infty$, uniformly in b_r and b_i, we repeat calculations of Figures 4.3 and 4.4 but with I_Nf replaced by the more accurate estimate, $I_N\widetilde{f}$. The results are depicted in Figures 4.5 and 4.6. We can see that, for each p, the error in estimating If with $I_{128}\widetilde{f}$, is bounded uniformly in b_r and b_i, as predicted by Theorem 4.1. To see that the error in estimating If with $I_N\widetilde{f}$ tends to zero as $N \to \infty$, we depict the result in Figure 4.8.

To summarise the numerical schemes used for different ranges of b_r, we illustrate both schemes in Figure 4.7, and see that $I_N\widetilde{f}$ is a suitable numerical quadrature method for

$-1 < b_r < 1$, as predicted by (4.14). For $|b_r| \geq 1$, $I_N f$ can be used to estimate the integral If, as suggested by (4.13).

To illustrate the rate of convergence, $\delta - p/2$ for arbitrary $\delta > 0$, in estimating If by $I_N \widetilde{f}$ predicted by (4.14), we choose $b_r = 0$ and $b_i = 0$. Results are depicted and tabulated in Figure 4.8 and Table 4.1, respectively.

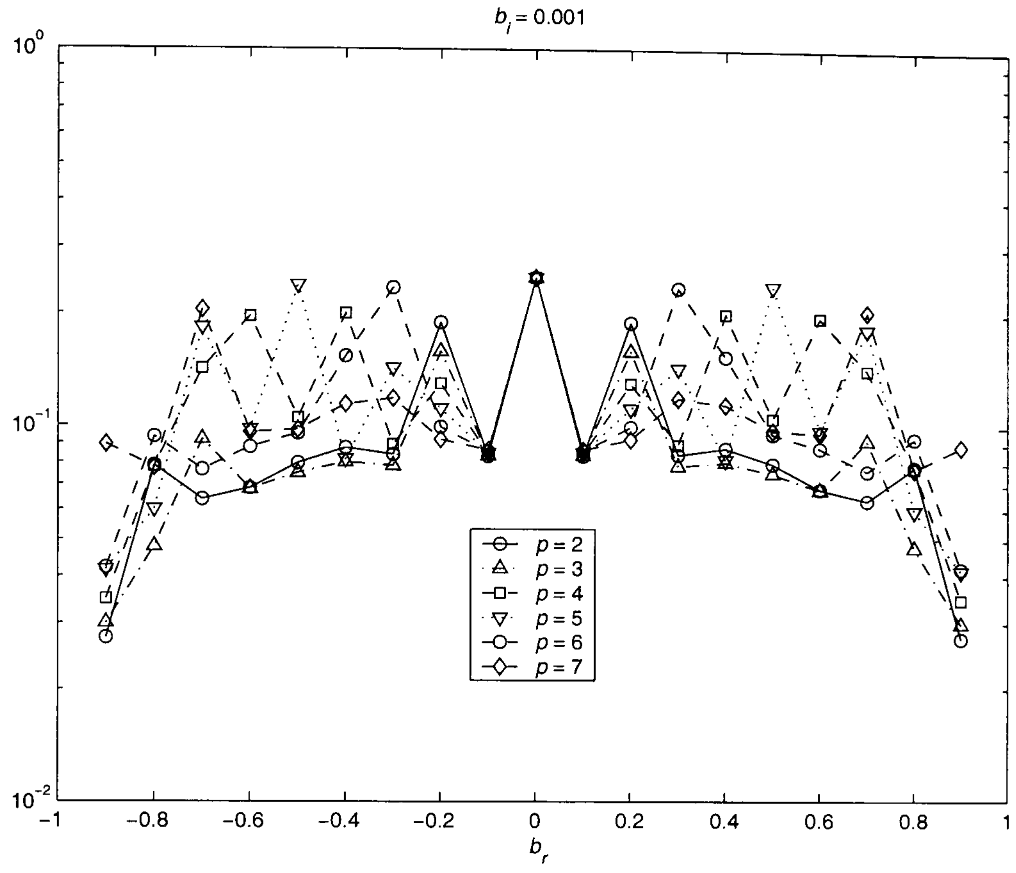


Figure 4.3: Error, $|If - I_{128}f|$, for $p = 2, \dots, 7$.

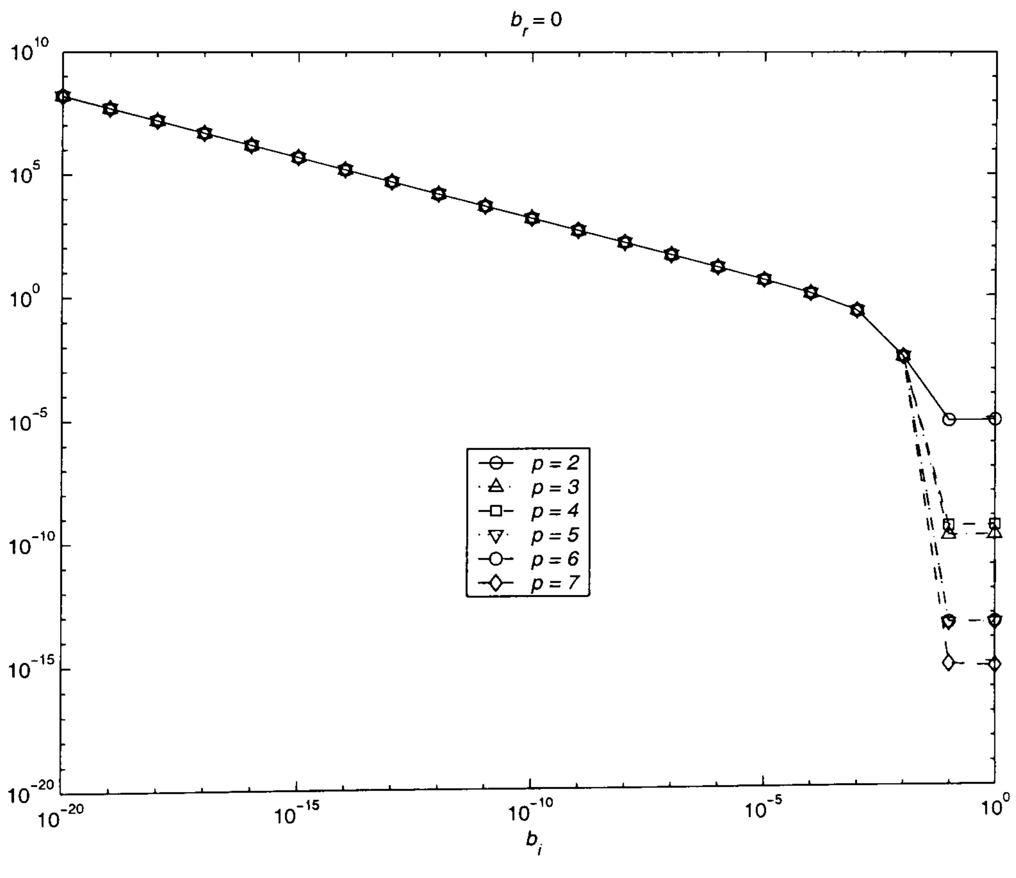


Figure 4.4: Error, $|If - I_{128}f|$, for $p = 2, \dots, 7$.

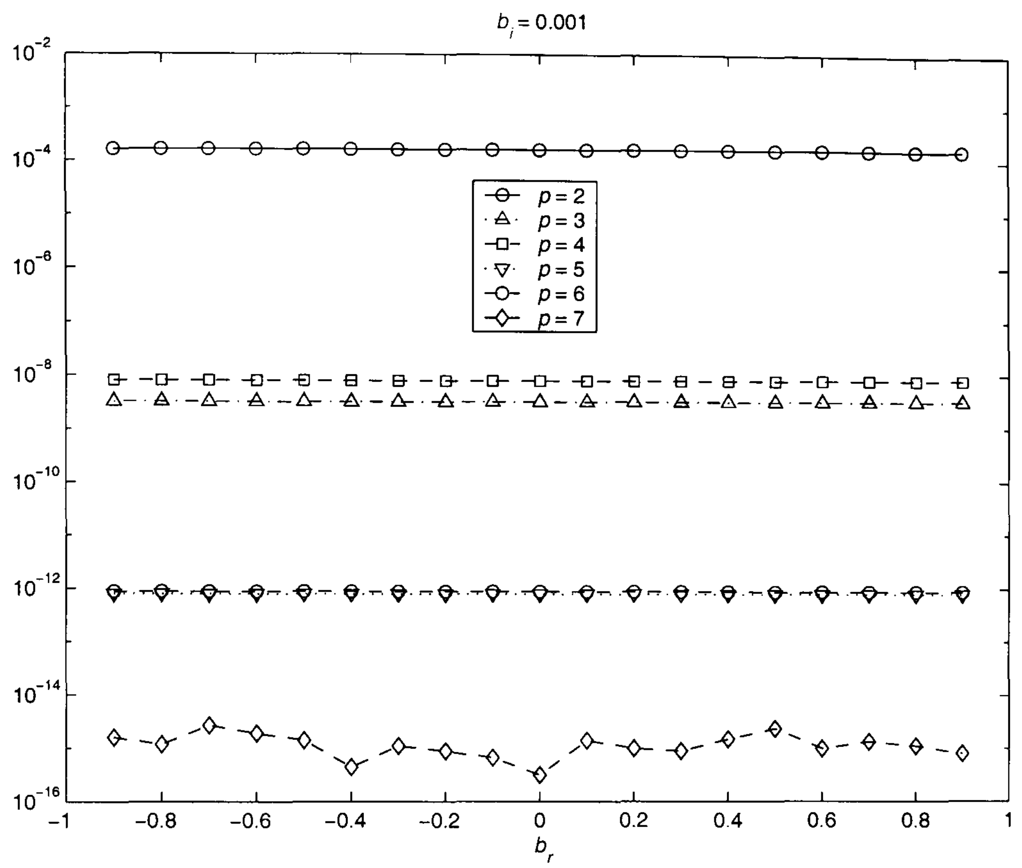


Figure 4.5: Error, $|If - I_{128}\widetilde{f}\,|$, for $p = 2, \ldots, 7$.

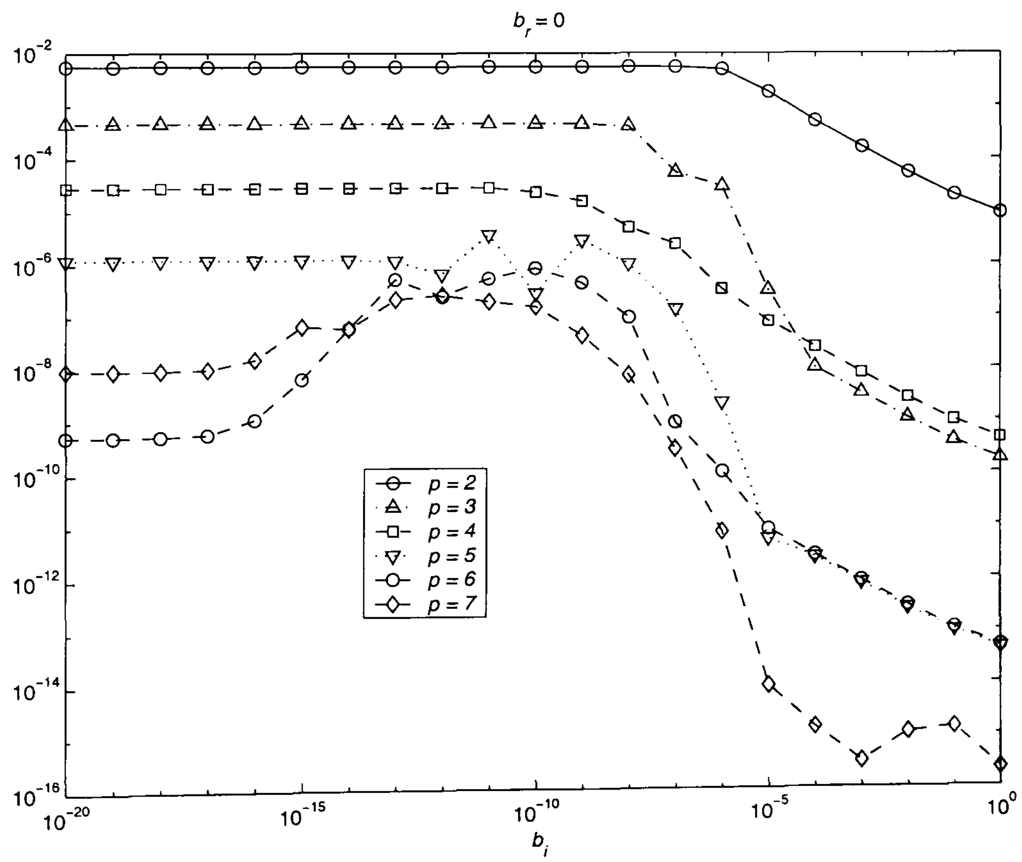


Figure 4.6: Error, $|If - I_{128}\widetilde{f}\,|$, for $p = 2, \ldots, 7$.

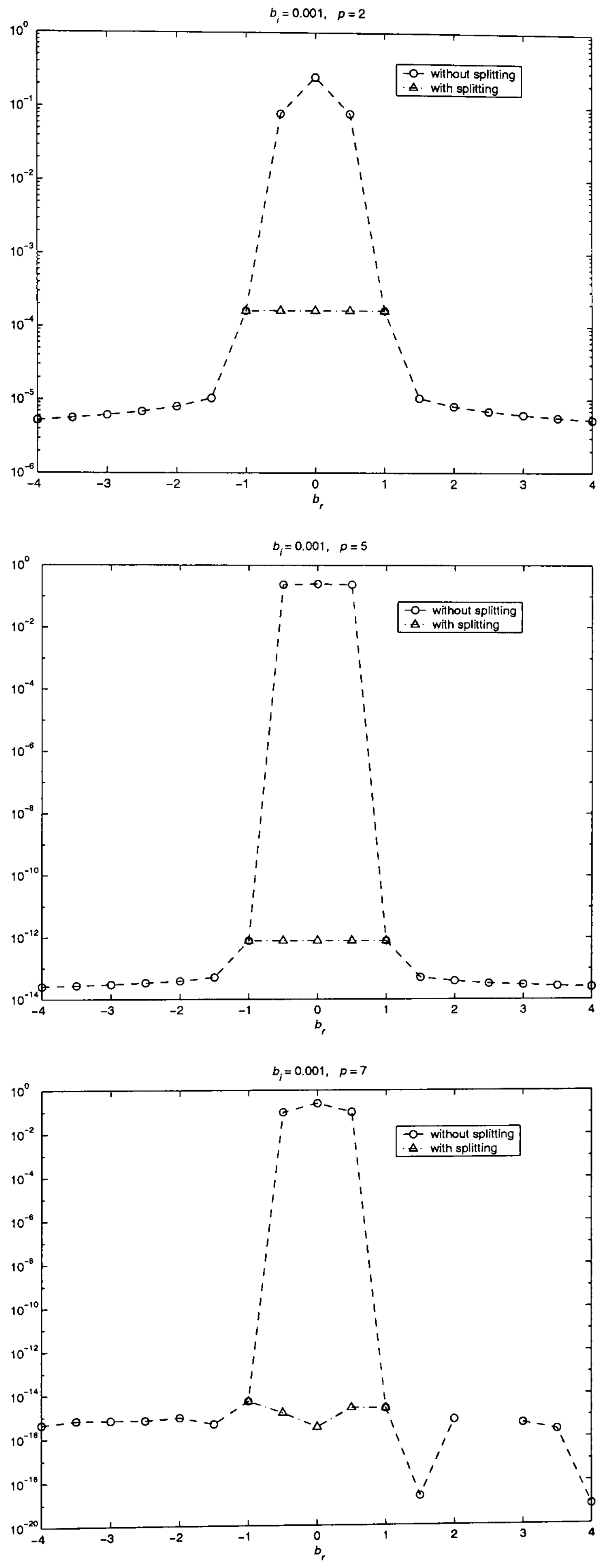


Figure 4.7: Errors, $|If - I_{128}f|$ (the curves labelled "without splitting") and $|If - I_{128}\tilde{f}|$ (the curves labelled "with splitting"), for $p = 2, 5, 7$.

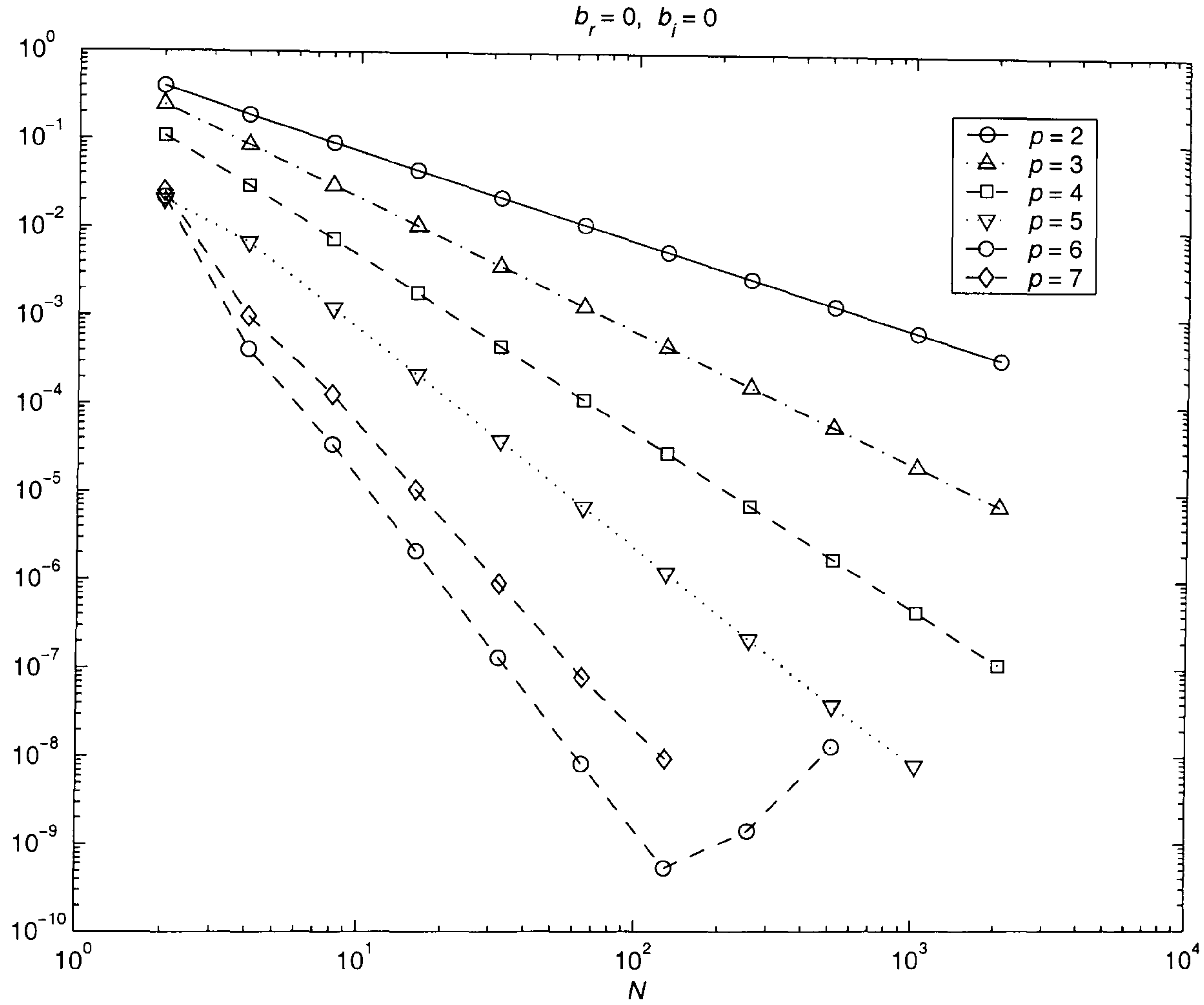


Figure 4.8: Error, $|If - I_N\widetilde{f}\,|$, for $p = 2, \ldots, 7$.

Table 4.1: $b_r = 0$, $b_i = 0$, $If = 2(1-i)$

NaN indicates that an implementation problem is encountered as described in Section 1.4 due to some quadrature points evaluating to ± 1.

	$p=2, \quad p/2=1.0$		$p=3, \quad p/2=1.5$		$p=4, \quad p/2=2.0$	
N	$\lvert If - I_N\tilde{f}\rvert$	EOC	$\lvert If - I_N\tilde{f}\rvert$	EOC	$\lvert If - I_N\tilde{f}\rvert$	EOC
2	3.9734E−01		2.4481E−01		1.0826E−01	
4	1.8781E−01	1.0811	8.5386E−02	1.5196	2.9425E−02	1.8793
8	9.1150E−02	1.0430	2.9920E−02	1.5129	7.3641E−03	1.9985
16	4.4885E−02	1.0220	1.0531E−02	1.5065	1.8413E−03	1.9998
32	2.2270E−02	1.0111	3.7148E−03	1.5032	4.6035E−04	1.9999
64	1.1092E−02	1.0056	1.3119E−03	1.5016	1.1509E−04	2.0000
128	5.5351E−03	1.0028	4.6357E−04	1.5008	2.8772E−05	2.0000
256	2.7648E−03	1.0014	1.6385E−04	1.5004	7.1931E−06	2.0000
512	1.3817E−03	1.0007	5.7922E−05	1.5002	1.7983E−06	2.0000
1024	6.9070E−04	1.0004	2.0477E−05	1.5001	4.4957E−07	2.0000
2048	3.4531E−04	1.0002	7.2395E−06	1.5000	1.1206E−07	2.0043

	$p=5, \quad p/2=2.5$		$p=6, \quad p/2=3.0$		$p=7, \quad p/2=3.5$	
N	$\lvert If - I_N\tilde{f}\rvert$	EOC	$\lvert If - I_N\tilde{f}\rvert$	EOC	$\lvert If - I_N\tilde{f}\rvert$	EOC
2	2.0157E−02		2.1672E−02		2.5046E−02	
4	6.6462E−03	1.6007	4.1290E−04	5.7139	9.7753E−04	4.6793
8	1.2149E−03	2.4517	3.4358E−05	3.5871	1.2725E−04	2.9414
16	2.1890E−04	2.4725	2.1277E−06	4.0133	1.0670E−05	3.5761
32	3.9081E−05	2.4857	1.3268E−07	4.0033	9.1973E−07	3.5362
64	6.9436E−06	2.4927	8.3273E−09	3.9940	7.9885E−08	3.5252
128	1.2306E−06	2.4963	5.3165E−10	3.9693	9.5389E−09	3.0660
256	2.1774E−07	2.4987	1.4256E−09	−1.4230	NaN	
512	3.8649E−08	2.4941	1.3119E−08	−3.2020	NaN	
1024	7.9458E−09	2.2822	NaN		NaN	
2048	NaN		NaN		NaN	

Example 2

Let

$$f(z) = (z - b)^{1/3} \tag{4.15}$$

where $b = b_r + ib_i \in \mathbb{C}$ with $-1 < b_r < 1$, and $b_i \geq 0$. Then

$$If = \int_{-1}^{+1} f(t)\,dt = 0.75\big[\,(1 - b_r - ib_i)^{4/3} - (-1 - b_r - ib_i)^{4/3}\,\big].$$

We carry out identical calculations to those of Example 1, except that the exponent in the definition of f is $1/3$ rather than $-1/2$, again illustrating the numerical scheme introduced in this chapter by using it to compute values of If for different choices of $b \in \mathbb{C}$.

As in the case of Example 1, Theorem 1.3 predicts that the bound (4.11) holds for every $\delta > 0$ and every α with $0 < \alpha \leq 1$, if w satisfies Assumption 1.1. Thus, by suitable choice of w, convergence of $I_N f$ to If at an arbitrarily high order can be achieved. Further, for $|b_r| \geq 1$, it follows from Lemma 4.1, applied with $\alpha = 1$ and $\varepsilon = 1$, that, for $j = 0, 1, \ldots$,

$$\begin{aligned} |f^{(j)}(t)| &\leq \tilde{c}C_j|t - b_r|^{-j} \\ &\leq \tilde{c}2^jC_j(1 - t^2)^{-j}. \end{aligned}$$

Thus

$$\|f\|_{q,1} \leq \tilde{c}2^q \max_{j=0,\ldots,q} C_j$$

so that, applying Theorem 1.3 with $\alpha = 1$,

$$|If - I_N f| \leq c_\delta \tilde{c} C N^{\delta - p}.$$

However, for $-1 < b_r < 1$, from (1.10),

$$\|f\|_{q,\alpha} \geq \sup_{-1<t<1} |f'(t)|(1 - t^2)^{2-\alpha} \geq \widetilde{C}\, b_i^{-2/3},$$

where $\widetilde{C} > 0$ depends only on b_r and α, so that the bound on the right hand side of (4.11) blows up as $b_i \to 0$. Again, this suggests that applying the numerical quadrature of Chapter 1 to If will be inaccurate for small b_i.

As in Example 1, the approximation $I_N \widetilde{f}$ can be shown to be accurate in the limit $b_i \to 0$. For $-1 < b_r < 1$, $b_i \geq 0$, and if w satisfies Assumption 1.1, it follows from Theorem 4.1 that

$$|If - I_N \widetilde{f}\,| \leq c_\delta C N^{\delta - p} \tag{4.16}$$

for every $\delta > 0$, where $c_\delta > 0$ depends only on δ and $C > 0$ depends only on p and w.

The numerical results show similar trends to those of Example 1, with some differences due to the weaker singularity of f in this second example. Comparing Figures 4.9 and 4.10 with Figures 4.11 and 4.12, we see that $I_N\tilde{f}$ is much more accurate than $I_N f$ when b_i is small. The approximation $I_N f$ is not so bad as in Example 1, however. In particular it no longer holds that $|If - I_N f| \to \infty$ as $b_i \to 0$. Figure 4.14 and Table 4.2 show that the convergence rate predicted by (4.16) is achieved: in fact, a convergence rate of $p + 1$ rather than p is achieved for $p = 3$ and $p = 5$. Comparing Table 4.1 with Table 4.2, we see that for the milder singularity of Example 2 there is no problem with rounding errors (see the discussion at the end of Chapter 1). In particular, $I_N\tilde{f}$ can be computed for all N and p, in contrast to Example 1, and errors of approximating the size of machine precision are achieved, whereas no errors are smaller than 5×10^{-8} in Table 4.1.

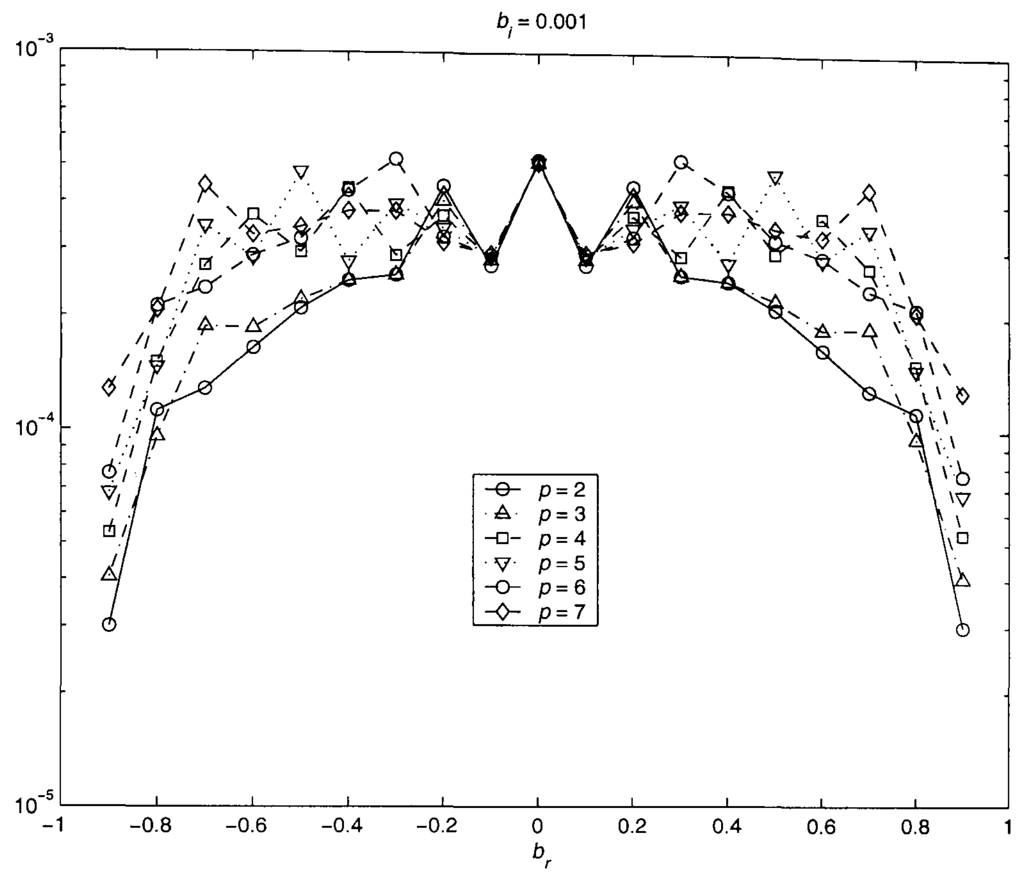


Figure 4.9: Error, $|If - I_{128}f|$, for $p = 2, \ldots, 7$.

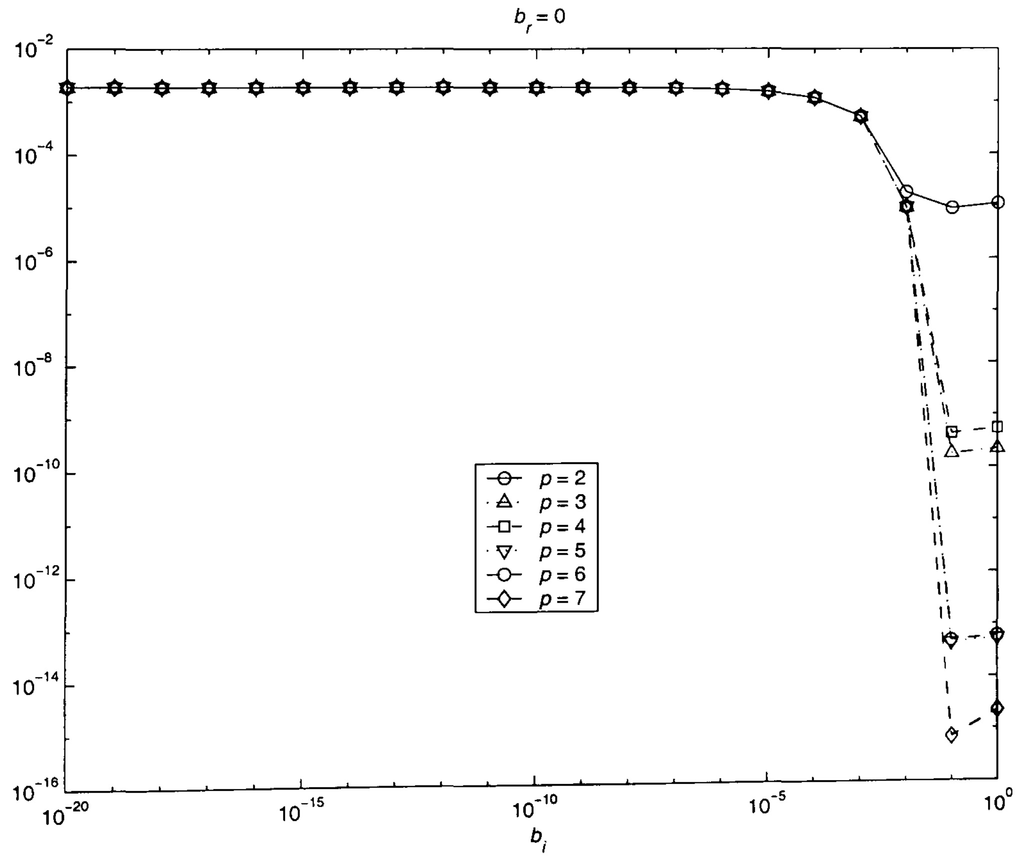


Figure 4.10: Error, $|If - I_{128}f|$, for $p = 2, \ldots, 7$.

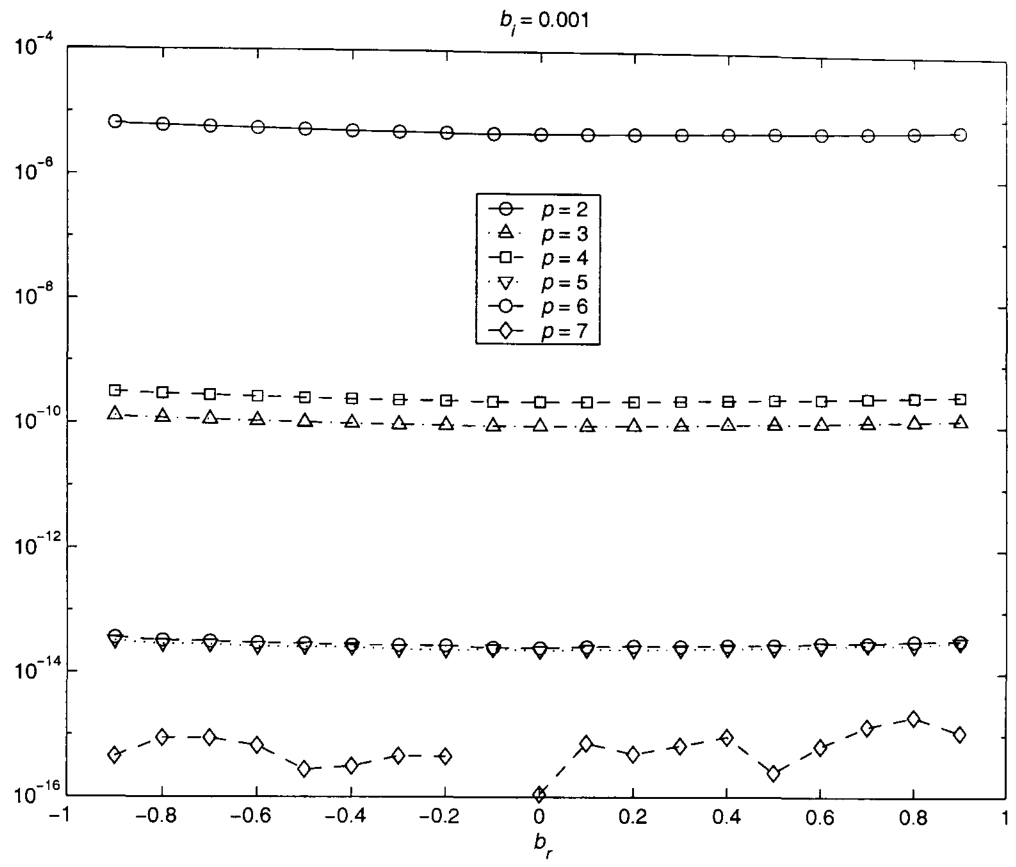


Figure 4.11: Error, $|If - I_{128}\widetilde{f}\,|$, for $p = 2, \ldots, 7$.

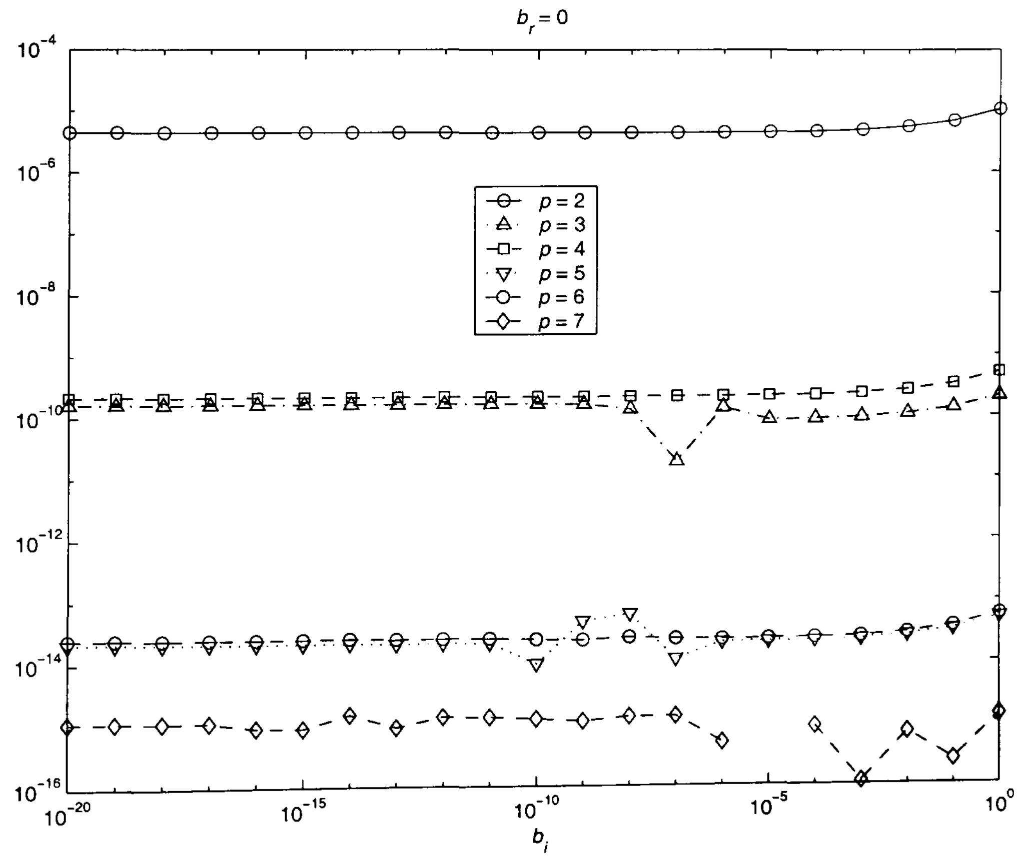


Figure 4.12: Error, $|If - I_{128}\widetilde{f}\,|$, for $p = 2, \ldots, 7$.

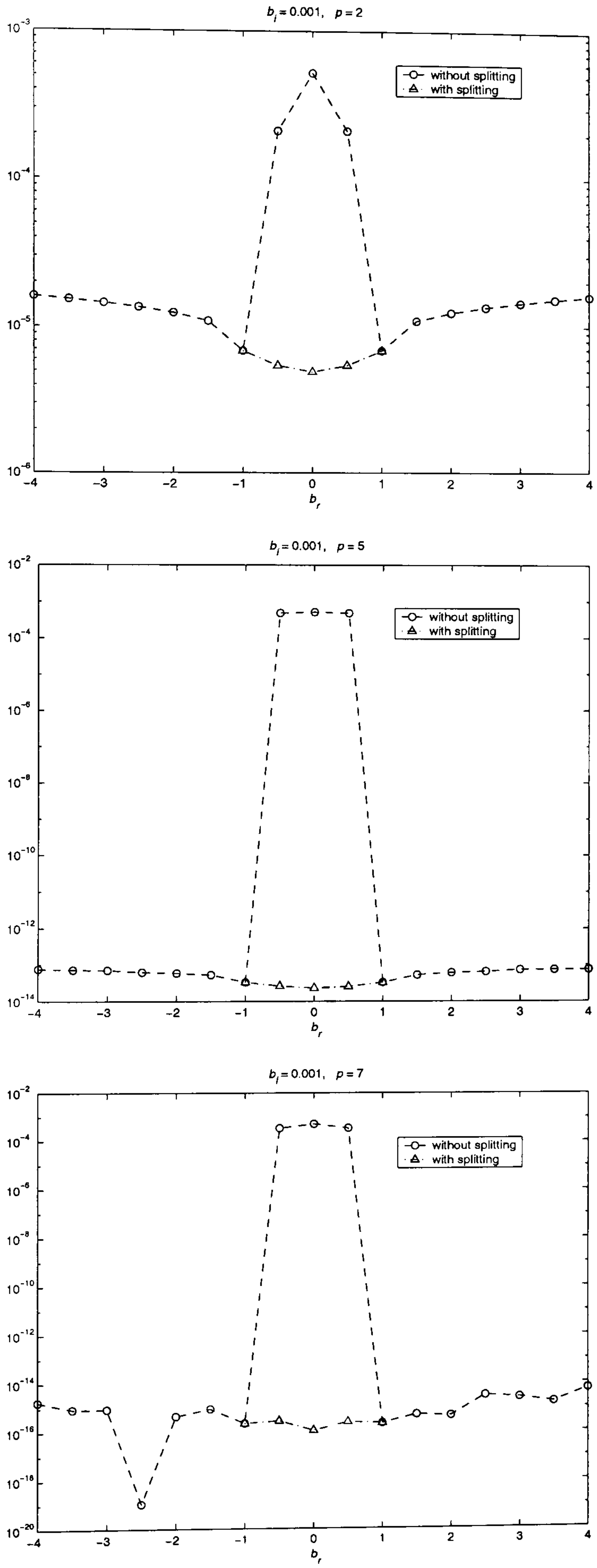


Figure 4.13: Errors, $|If - I_{128}f|$ (the curves labelled "without splitting") and $|If - I_{128}\tilde{f}|$ (the curves labelled "with splitting"), for $p = 2, 5, 7$.

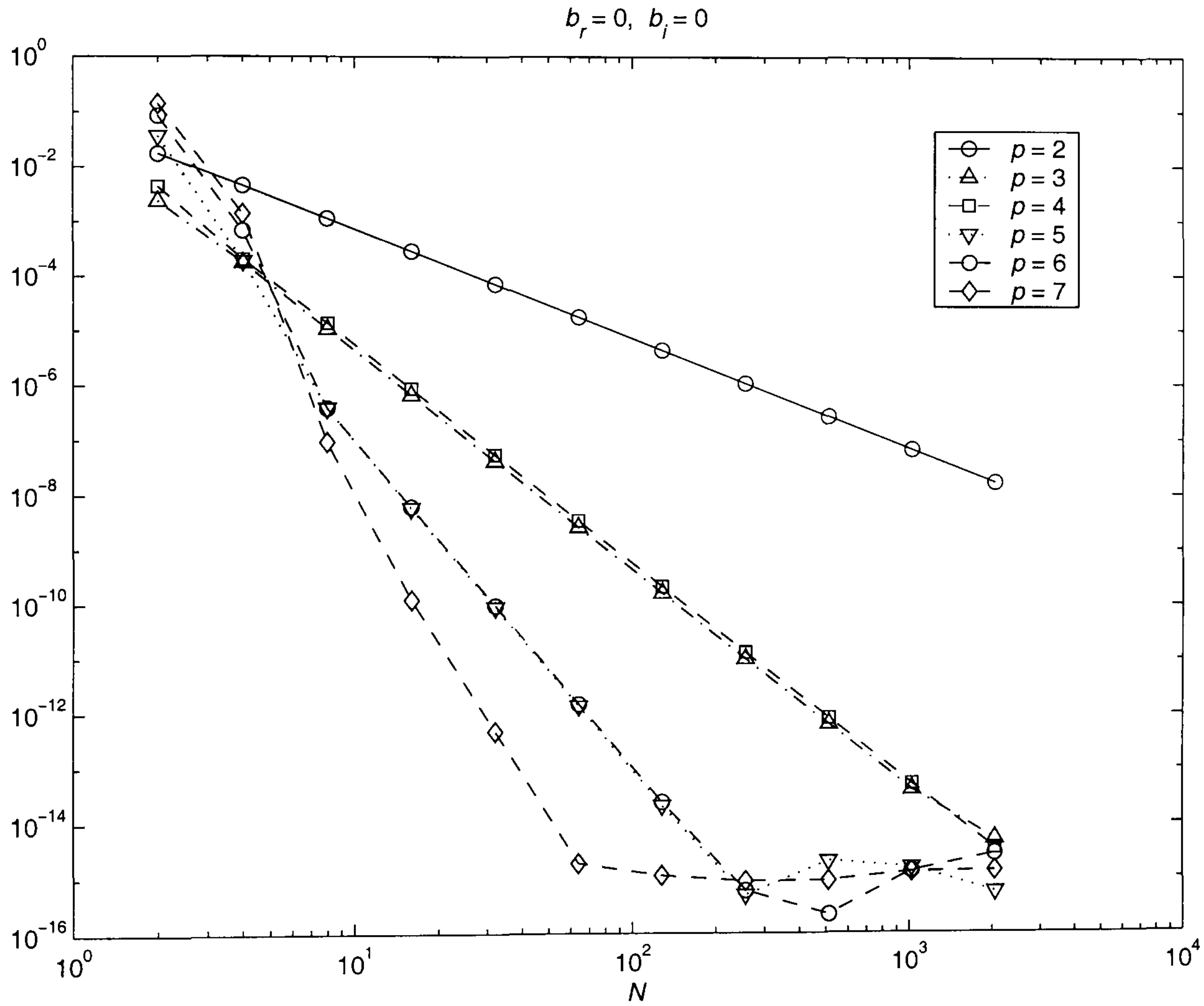


Figure 4.14: Error, $|If - I_N\widetilde{f}\,|$, for $p = 2, \ldots, 7$.

Table 4.2: $b_r = 0$, $b_i \approx 0$, $If = 1.125 + 0.64951905283833i$

N	$p=2$: $\lvert If - I_N\tilde{f}\rvert$	$p=2$: EOC	$p=3$: $\lvert If - I_N\tilde{f}\rvert$	$p=3$: EOC	$p=4$: $\lvert If - I_N\tilde{f}\rvert$	$p=4$: EOC
2	1.7380E−02		2.3838E−03		4.4170E−03	
		1.9120		3.7416		4.4345
4	4.6182E−03		1.7821E−04		2.0427E−04	
		2.0031		4.0316		3.8801
8	1.1520E−03		1.0896E−05		1.3873E−05	
		2.0087		4.0088		3.9859
16	2.8628E−04		6.7690E−07		8.7561E−07	
		2.0074		4.0022		3.9948
32	7.1203E−05		4.2241E−08		5.4925E−08	
		2.0052		4.0006		3.9979
64	1.7736E−05		2.6391E−09		3.4378E−09	
		2.0035		4.0001		3.9991
128	4.4235E−06		1.6492E−10		2.1499E−10	
		2.0022		4.0001		3.9997
256	1.1042E−06		1.0307E−11		1.3440E−11	
		2.0014		4.0006		3.9983
512	2.7577E−07		6.4393E−13		8.4098E−13	
		2.0009		3.9726		4.0024
1024	6.8899E−08		4.1018E−14		5.2473E−14	
		2.0006		3.0044		3.9163
2048	1.7218E−08		5.1119E−15		3.4755E−15	

N	$p=5$: $\lvert If - I_N\tilde{f}\rvert$	$p=5$: EOC	$p=6$: $\lvert If - I_N\tilde{f}\rvert$	$p=6$: EOC	$p=7$: $\lvert If - I_N\tilde{f}\rvert$	$p=7$: EOC
2	3.6466E−02		8.4690E−02		1.4102E−01	
		7.5851		6.9441		6.6512
4	1.8991E−04		6.8777E−04		1.4030E−03	
		8.9324		10.7822		13.8519
8	3.8872E−07		3.9054E−07		9.4887E−08	
		6.0513		5.9804		9.5920
16	5.8616E−09		6.1857E−09		1.2295E−10	
		6.0267		5.9977		8.0150
32	8.9906E−11		9.6803E−11		4.7529E−13	
		6.0158		5.9994		7.9688
64	1.3895E−12		1.5131E−12		1.8971E−15	
		6.0320		5.9468		0.7447
128	2.1234E−14		2.4531E−14		1.1322E−15	
		5.4184		5.3586		0.3390
256	4.9651E−16		5.9787E−16		8.9509E−16	
		−2.0626		1.4290		−0.0325
512	2.0741E−15		2.2204E−16		9.1551E−16	
		0.4016		−2.6047		−0.5053
1024	1.5701E−15		1.3506E−15		1.2995E−15	
		1.5000		−1.0391		−0.0606
2048	5.5511E−16		2.7756E−15		1.3552E−15	

Chapter 5

Numerical Quadrature Methods for Integrals on the Real Line of Laplace Type with Branch Point Singularities near the Path of Integration

In this chapter, we will consider the problem of evaluating numerically the integral

$$\bar{J}f := \int_0^\infty e^{-\rho t} f(t)\, dt, \tag{5.1}$$

where $\rho \geq 0$, i.e., the Laplace transform of f, developing methods which are accurate and efficient for cases when function f is analytic but with a branch point singularity near the positive real axis. Our results will apply in the case when f satisfies the following assumption.

Assumption 5.1 *For some $q \in \mathbb{N}$ and $B_r > 0$, it holds that $f \in C^q[0, B_r) \cap C^q(B_r, \infty)$, and that there exist $\widehat{c} > 0$ and α with $0 < \alpha \leq 1$ such that, for $n = 0, 1, \ldots, q$,*

$$|f^{(n)}(t)| \leq \widehat{c}\,|t - B_r|^{\alpha-1-n}(1+t)^{-2\alpha}, \qquad t \in [0, B_r) \cup (B_r, \infty).$$

Assumption 5.1 holds in particular when the following assumption on f is satisfied.

Assumption 5.1′ *For some* $\varepsilon > 0$, $\theta \in (0, \pi/2]$, *and* $B = B_r + iB_i \in \mathbb{C}$ *with* $B_i \geq 0$, *the function* f *is analytic in (see Figure 5.1)*

$$\mathcal{D}_{\varepsilon,\theta,B} := \mathcal{D}_{\varepsilon,\theta} \backslash \Big\{ B_r + it : t \geq B_i \Big\},$$

where $\mathcal{D}_{\varepsilon,\theta}$ *is defined by (see Figure 2.1)*

$$\mathcal{D}_{\varepsilon,\theta} := \Big\{ z \in \mathbb{C} : |\arg(z+\varepsilon)| < \theta \Big\}.$$

Further, for some $\widetilde{c} > 0$ *and* $\alpha > 0$,

$$|f(z)| \leq \widetilde{c}\, |z - B|^{\alpha-1}(1+|z|)^{-2\alpha}, \qquad z \in \mathcal{D}_{\varepsilon,\theta,B}.$$

Lemma 5.1 *Let* f *satisfy Assumption 5.1′. Then, for* $n = 0, 1, \ldots$,

$$|f^{(n)}(t)| \leq \widetilde{c}\, C_n |t - B_r|^{\alpha-1-n}(1+t)^{-2\alpha}, \qquad t \in [0,\infty)\backslash\{B_r\}, \tag{5.2}$$

where

$$C_n := \frac{n!\, 2^{2\alpha}}{\widetilde{\omega}^n (1-\widetilde{\omega})^{1-\alpha}}$$

and

$$\widetilde{\omega} := \min\left\{ \frac{\eta}{R}, \frac{n}{n+1-\alpha} \right\}.$$

Thus, in the case $B_r \in [0,\infty)$, f *satisfies Assumption 5.1 for every* $q \in \mathbb{N}$, *with*

$$\widehat{c} = \widetilde{c} \max_{n=0,\ldots,q} C_n.$$

Proof. Let $t \in [0,\infty)\backslash\{B_r\}$, $R = |t - B|$, $\bar{\varepsilon} = \min\{\varepsilon, 1\}$, $\eta = \frac{1}{2}(\bar{\varepsilon} + t)\sin\theta$, and $0 < \omega < \min\{1, \eta/R\}$. From Cauchy's integral formula with circular contour $C_{R\omega}(t)$, the circle of radius $R\omega$ centred at t (see Figure 5.2),

$$\begin{aligned}
|f^{(n)}(t)| &\leq \frac{n!}{R^n \omega^n} \max_{z \in C_{R\omega}(t)} |f(z)| \\
&\leq \frac{n!\,\widetilde{c}}{R^n \omega^n} \max_{z \in C_{R\omega}(t)} |z - B|^{\alpha-1}(1+|z|)^{-2\alpha}.
\end{aligned}$$

Now $\eta \leq \frac{1}{2}(1+t)$ so that, for $z \in C_{R\omega}(t)$, $1 + |z| \geq 1 + t - R\omega \geq 1 + t - \eta \geq \frac{1}{2}(1+t)$. Thus

$$\begin{aligned}
|f^{(n)}(t)| &\leq \frac{n!\,\widetilde{c}}{R^n \omega^n}[R(1-\omega)]^{\alpha-1}[(1+t)/2]^{-2\alpha} \\
&= \frac{n!\,\widetilde{c}\,2^{2\alpha}}{\omega^n(1-\omega)^{1-\alpha}}|t - B|^{\alpha-1-n}(1+t)^{-2\alpha} \\
&\leq \frac{n!\,\widetilde{c}\,2^{2\alpha}}{\omega^n(1-\omega)^{1-\alpha}}|t - B_r|^{\alpha-1-n}(1+t)^{-2\alpha}.
\end{aligned}$$

In the case that $\eta/R < 1$, taking the limit $\omega \to \frac{\eta}{R}^-$ we see that this bound holds also for $\omega = \eta/R$. Then setting $\omega = \widetilde{\omega}$ (to minimise $[\omega^n(1-\omega)^{1-\alpha}]^{-1}$), we obtain (5.2). ■

To apply the results and methods from Chapter 4, we make a substitution in (5.1) to bring the range of integration to $[-1,1]$. Define the homeomorphism $\widehat{P} : [-1,1) \to [0,\infty)$ by

$$\widehat{P}(u) := \frac{1+u}{1-u}, \qquad -1 \le u < 1.$$

Substituting $t = \widehat{P}(u)$ into (5.1), we see that

$$\bar{J}f = \int_{-1}^{+1} \widehat{F}(u)\,du = I\widehat{F}, \tag{5.3}$$

where

$$\widehat{F}(u) := \frac{2f(\widehat{P}(u))e^{-\rho\widehat{P}(u)}}{(1-u)^2}, \qquad -1 \le u < 1.$$

Further, we write $I\widehat{F}$ as

$$I\widehat{F} = \int_{-1}^{b_r} \widehat{F}(u)\,du + \int_{b_r}^{+1} \widehat{F}(u)\,du,$$

where $b_r = \widehat{P}^{-1}(B_r) = (B_r - 1)/(B_r + 1)$, and make a linear substitution to change the intervals of integration to $[-1,1]$. This gives

$$I\widehat{F} = \int_{-1}^{+1} \widetilde{F}(u)\,du = I\widetilde{F}, \tag{5.4}$$

where

$$\widetilde{F}(u) = \widetilde{F}_1(u) + \widetilde{F}_2(u), \tag{5.5}$$

$$\widetilde{F}_1(u) = \left(\frac{1+b_r}{2}\right)\widehat{F}\left(\frac{1+b_r}{2}u - \frac{1-b_r}{2}\right), \qquad -1 < u < 1, \tag{5.6}$$

$$\widetilde{F}_2(u) = \left(\frac{1-b_r}{2}\right)\widehat{F}\left(\frac{1-b_r}{2}u + \frac{1+b_r}{2}\right), \qquad -1 < u < 1. \tag{5.7}$$

Our numerical method will be to approximate $\bar{J}f$ by $I_N\widetilde{F}$, defined by (1.26). To apply the result of Theorem 4.1 to bound

$$|\bar{J}f - I_N\widetilde{F}| = |I\widetilde{F} - I_N\widetilde{F}|,$$

we have to show that $\widetilde{F}$ satisfies Assumption 4.1. So we will pause to find the jth derivative of $\widehat{F}$ by arguing similarly to Section 2.2 to show that if f satisfies Assumption 5.1, then for $j = 0, 1, \ldots, q$ and some $C > 0$,

$$|\widehat{F}^{(j)}(u)| \le \begin{cases} C\left[\dfrac{(1+u)|u-b_r|}{1+b_r}\right]^{\alpha-1-j}, & -1 < u < b_r, \\[2ex] C\left[\dfrac{(1-u)|u-b_r|}{1-b_r}\right]^{\alpha-1-j}, & b_r < u < 1. \end{cases}$$

The jth derivative of $\widehat{F}(u)$, for $-1 \le u < 1$, is

$$\widehat{F}^{(j)}(u) = \sum_{k=0}^{j} \left\{ \binom{j}{k} \widehat{F}_1^{(j-k)}(u) \left[\sum_{n=0}^{k} \binom{k}{n} \widehat{F}_2^{(k-n)}(u) \widehat{F}_3^{(n)}(u) \right] \right\}, \tag{5.8}$$

where

$$\widehat{F}_1(u) := 2(1-u)^{-2}, \qquad \widehat{F}_2(u) := e^{-\rho \widehat{P}(u)}, \qquad \widehat{F}_3(u) := f(\widehat{P}(u)).$$

For $\widehat{F}_1$ and its derivatives, it can be shown that, for $m = 0, 1, \ldots,$

$$\left|\widehat{F}_1^{(m)}(u)\right| = C_m(1-u)^{-2-m}, \qquad -1 \le u < 1. \tag{5.9}$$

(Here and below C_m denotes a constant whose value depends only on m, not necessary the same constant at each occurrence.) The proofs of Lemmas 5.2–5.4 below are simple modifications of those of Lemmas 2.2–2.4, and are left as exercises for the reader.

Lemma 5.2 *For $m = 0, 1, \ldots,$ $\widehat{P}^{(m)}(u)$ has a pole of order not more than $m+1$ at 1, so that*

$$|\widehat{P}^{(m)}(u)| \le C_m(1-u)^{-m-1}, \qquad -1 \le u < 1.$$

For $m = 0, 1, \ldots,$ and $j = 0, 1, \ldots, m$, let $\widehat{U}_j^m$ be defined recursively by

$$\widehat{U}_0^0(u) = 1,$$

$$\widehat{U}_j^{m+1}(u) = \begin{cases} \dfrac{d\widehat{U}_0^m(u)}{du}, & \text{if } j = 0, \\[2ex] \dfrac{d\widehat{U}_j^m(u)}{du} + \widehat{U}_{j-1}^m(u)\widehat{P}'(u), & \text{if } j = 1, 2, \ldots, m, \\[2ex] \widehat{U}_m^m(u)\widehat{P}'(u), & \text{if } j = m+1. \end{cases}$$

Lemma 5.3 *For $m = 0, 1, \ldots,$ and $j = 0, 1, \ldots, m$, $\widehat{U}_j^m(u)$ has a pole of order not more than $m+j$ at 1, so that*

$$|\widehat{U}_j^m(u)| \le C_m(1-u)^{-m-j}, \qquad -1 \le u < 1.$$

Lemma 5.4 *If $g \in \mathcal{C}^\infty[-1,1)$ and $G(u) := g(\widehat{P}(u))$ then, for $m = 0,1,\ldots,$*

$$G^{(m)}(u) = \sum_{j=0}^{m} \widehat{U}_j^m(u)\, g^{(j)}(\widehat{P}(u)), \qquad -1 \le u < 1.$$

Using Lemma 5.4 and Lemma 5.3, since $\widehat{F}_2(u) = e^{-\rho\widehat{P}(u)}$ for $-1 \le u < 1$ and $\widehat{P}(u) \ge 0$, then, for $m = 0,1,\ldots,$

$$\begin{aligned}
\left|\widehat{F}_2^{(m)}(u)\right| &\le \sum_{j=0}^{m} \left|\widehat{U}_j^m(u)\right| \rho^j e^{-\rho\widehat{P}(u)} \\
&\le C_m\,(1-u)^{-m} \sum_{j=0}^{m} \rho^j\,(1-u)^{-j}\, e^{-\rho\widehat{P}(u)} \\
&= C_m\,(1-u)^{-m} \sum_{j=0}^{m} \widehat{s}^{\,j}\,(1+u)^{-j}\, e^{-\widehat{s}}
\end{aligned}$$

where $\widehat{s} := \rho\widehat{P}(u) = \rho(1+u)/(1-u)$. Thus, and since $\widehat{s}^{\,j}e^{-\widehat{s}}$ is bounded on $[0,\infty)$ for every j and $\sum_{j=0}^{m}\rho^j(1-u)^j e^{-\rho\widehat{P}(u)} \le \sum_{j=0}^{m}(2\rho)^j < (m+1)(1+(2\rho)^m)$ for $-1 < u \le 0$, we see that

$$\left|\widehat{F}_2^{(m)}(u)\right| \le \begin{cases} C_m(1+\rho^m)(1-u)^{-m}, & -1 \le u \le 0, \\[2ex] C_m(1-u)^{-m}, & 0 \le u < 1, \end{cases}$$

so that

$$\left|\widehat{F}_2^{(m)}(u)\right| \le C_m(1+\rho^m)(1-u)^{-m}, \qquad -1 \le u < 1. \tag{5.10}$$

Similarly, using Lemma 5.4 and Lemma 5.3, since $\widehat{F}_3(u) = f(\widehat{P}(u))$ for $-1 \le u < 1$ and $\widehat{P}(u) \ge 0$, and Assumption 5.1 holds, then, for $m = 0, 1, \ldots,$

$$
\begin{aligned}
\left|\widehat{F}_3^{(m)}(u)\right| &\le \sum_{j=0}^{m} \left|\widehat{U}_j^m(u) f^{(j)}(\widehat{P}(u))\right| \\
&\le \widehat{c}C_m \sum_{j=0}^{m} (1-u)^{-m-j} \left|\frac{1+u}{1-u} - B_r\right|^{\alpha-1-j} \left(1 + \frac{1+u}{1-u}\right)^{-2\alpha} \\
&= \widehat{c}C_m \sum_{j=0}^{m} (1-u)^{-m-j} \left|\frac{1+u}{1-u} - \frac{1+b_r}{1-b_r}\right|^{\alpha-1-j} \left(\frac{2}{1-u}\right)^{-2\alpha} \\
&= \widehat{c}C_m 2^{-\alpha-1} (1-u)^{\alpha+1-m} \left(\frac{|u-b_r|}{1-b_r}\right)^{\alpha-1} \sum_{j=0}^{m} \left(\frac{1-b_r}{2|u-b_r|}\right)^j \\
&\le \widehat{c}C_m (1-u)^{\alpha+1-m} \left[\left(\frac{|u-b_r|}{1-b_r}\right)^{\alpha-1} + \left(\frac{|u-b_r|}{1-b_r}\right)^{\alpha-1-m}\right] \qquad (5.11)
\end{aligned}
$$

since

$$
\sum_{j=0}^{m} \left(\frac{1-b_r}{2|u-b_r|}\right)^j \le (m+1) \max_{0 \le j \le m} \left(\frac{1-b_r}{2|u-b_r|}\right)^j \le (m+1)\left[1 + \left(\frac{1-b_r}{|u-b_r|}\right)^m\right].
$$

Lemma 5.5 *If Assumption 5.1 holds then, for $j = 0, 1, \ldots, q$,*

$$
|\widehat{F}^{(j)}(u)| \le \widehat{c}C(1+\rho^q)(1-b_r)^{1-\alpha}\left[|u-b_r|^j + (1-b_r)^j\right]\left[(1-u)|u-b_r|\right]^{\alpha-1-j}
$$

for $u \in [-1, b_r) \cup (b_r, 1)$, where $b_r = (B_r - 1)/(B_r + 1) \in (-1, 1)$, and the constant $C > 0$ depends only on q and α.

Proof. Using (5.8) to (5.11), we find that

$$
\begin{aligned}
|\widehat{F}^{(j)}(u)| &\le \widehat{c}C(1+\rho^q)(1-b_r)^{1-\alpha}(1-u)^{\alpha-1-j}|u-b_r|^{\alpha-1} \sum_{k=0}^{j}\sum_{n=0}^{k} \left[1 + \left(\frac{1-b_r}{|u-b_r|}\right)^n\right] \\
&\le \widehat{c}C(1+\rho^q)(1-b_r)^{1-\alpha}(1-u)^{\alpha-1-j}|u-b_r|^{\alpha-1} \left[1 + \left(\frac{1-b_r}{|u-b_r|}\right)^j\right] \\
&= \widehat{c}C(1+\rho^q)(1-b_r)^{1-\alpha}\left[|u-b_r|^j + (1-b_r)^j\right]\left[(1-u)|u-b_r|\right]^{\alpha-1-j}.
\end{aligned}
$$

■

Corollary 5.1 *If Assumption 5.1 holds then, for* $j = 0, 1, \ldots, q$,

$$|\widehat{F}^{(j)}(u)| \leq \begin{cases} \widehat{c}C(1+\rho^q)\left[\dfrac{(1+u)|u-b_r|}{1+b_r}\right]^{\alpha-1-j}, & -1 < u < b_r, \\ \widehat{c}C(1+\rho^q)\left[\dfrac{(1-u)|u-b_r|}{1-b_r}\right]^{\alpha-1-j}, & b_r < u < 1, \end{cases}$$

where $b_r = (B_r - 1)/(B_r + 1) \in (-1, 1)$, *and the constant* $C > 0$ *depends only on* q *and* α, *so that* $\widehat{F}$ *satisfies Assumption 4.1 with* $c = \widehat{c}C(1+\rho^q)$.

Proof. For $u \in (b_r, 1)$, we can see that $|u - b_r| < 1 - b_r$. Then, from Lemma 5.5,

$$|\widehat{F}^{(j)}(u)| \leq \widehat{c}C(1+\rho^q)\left[\frac{(1-u)|u-b_r|}{1-b_r}\right]^{\alpha-1-j}.$$

For $u \in (-1, b_r)$, we can see that $|u - b_r| < 1 - u$, and $1 - b_r < 1 - u$. Then, from Lemma 5.5 and together with $1 + u < 1 + b_r$,

$$|\widehat{F}^{(j)}(u)| \leq \widehat{c}C(1+\rho^q)|u-b_r|^{\alpha-1-j} \leq \widehat{c}C(1+\rho^q)\left[\frac{(1+u)|u-b_r|}{1+b_r}\right]^{\alpha-1-j}.$$

■

Choosing $w \in C^\infty[-1,1]$ which satisfies Assumption 1.1 and applying the quadrature rule (1.26) to (5.4), we get that

$$\bar{J}f \approx I_N\widetilde{F} := \sum_{k=1-N}^{N-1} a_k\,\widetilde{F}(x_k), \tag{5.12}$$

where, for $k = 1-N, \ldots, N-1$,

$$a_k = \frac{1}{N}w'\left(\frac{k}{N}\right), \qquad x_k = w\left(\frac{k}{N}\right),$$

and $\widetilde{F}$ is given by equation (5.5). Now, from Corollary 5.1, we can apply Theorem 4.1 with $c = \widehat{c}C(1+\rho^q)$, and obtain the following error estimate.

Throughout the following error estimate, we let $C > 0$ denote a generic constant, whose value depends at most on the values of q, α in Assumption 5.1, p in Assumption 1.1, and on the choice of the function w.

Theorem 5.1 *Suppose that w satisfies Assumption 1.1, f satisfies Assumption 5.1. $q \in \mathbb{N}$, and $1 < \alpha p < q$. Then, for $\alpha p \notin \mathbb{N}$, the error in the quadrature (5.12) can be bounded by*

$$|\bar{J}f - I_N \widetilde{F}\,| \leq \widehat{c}\,C(1+\rho^q)N^{-\alpha p},$$

where the constant C depends only on q, α, and on the function w. If $\alpha p = q$, then

$$|\bar{J}f - I_N \widetilde{F}\,| \leq c_\delta \widehat{c}\,C(1+\rho^q)N^{\delta - q},$$

for every $\delta > 0$, where $c_\delta > 0$ depends only on δ.

Combining Theorem 5.1 with Lemma 5.1, we obtain the following corollary.

Corollary 5.2 *Suppose that w satisfies Assumption 1.1, f satisfies Assumption 5.1′, $q \in \mathbb{N}$, and $1 < \alpha p < q$. Then, for $\alpha p \notin \mathbb{N}$, the error in the quadrature (5.12) can be bounded by*

$$|\bar{J}f - I_N \widetilde{F}\,| \leq \frac{\widetilde{c}\,C(1+\rho^q)}{\widetilde{\omega}^q(1-\widetilde{\omega}\,)^{1-\alpha}}\,N^{-\alpha p}$$

with

$$\widetilde{\omega} = \min\left\{\frac{\eta}{R}, \frac{n}{n+1-\alpha}\right\}.$$

where the constant C depends only on q, α, and on the function w. If $\alpha p = q$, then

$$|\bar{J}f - I_N \widetilde{F}\,| \leq \frac{c_\delta \widetilde{c}\,C(1+\rho^q)}{\widetilde{\omega}^q(1-\widetilde{\omega}\,)^{1-\alpha}}\,N^{\delta - q},$$

for every $\delta > 0$, where $c_\delta > 0$ depends only on δ.

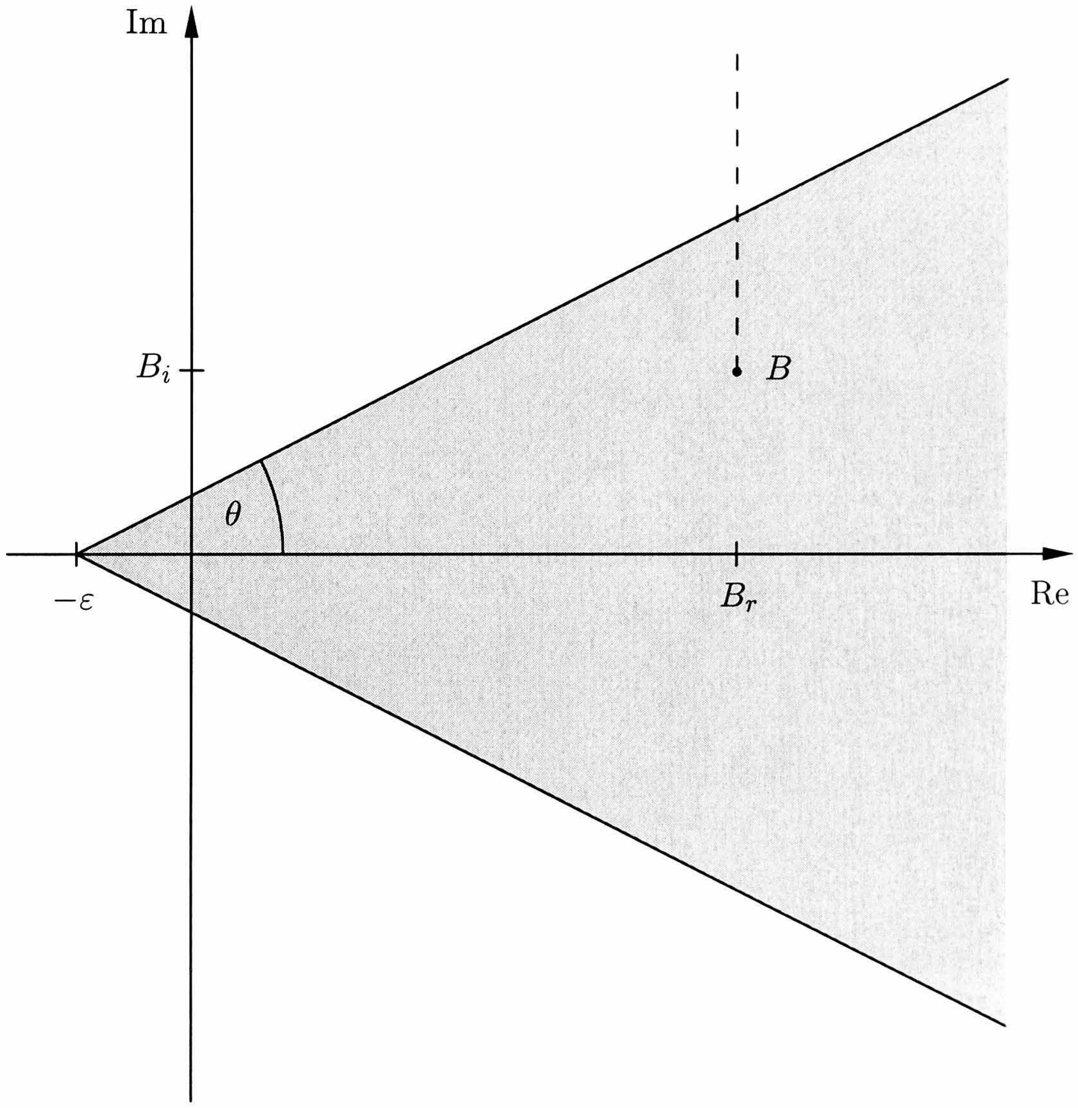


Figure 5.1: $\mathcal{D}_{\varepsilon,\theta,B}$ in Assumption 5.1′.

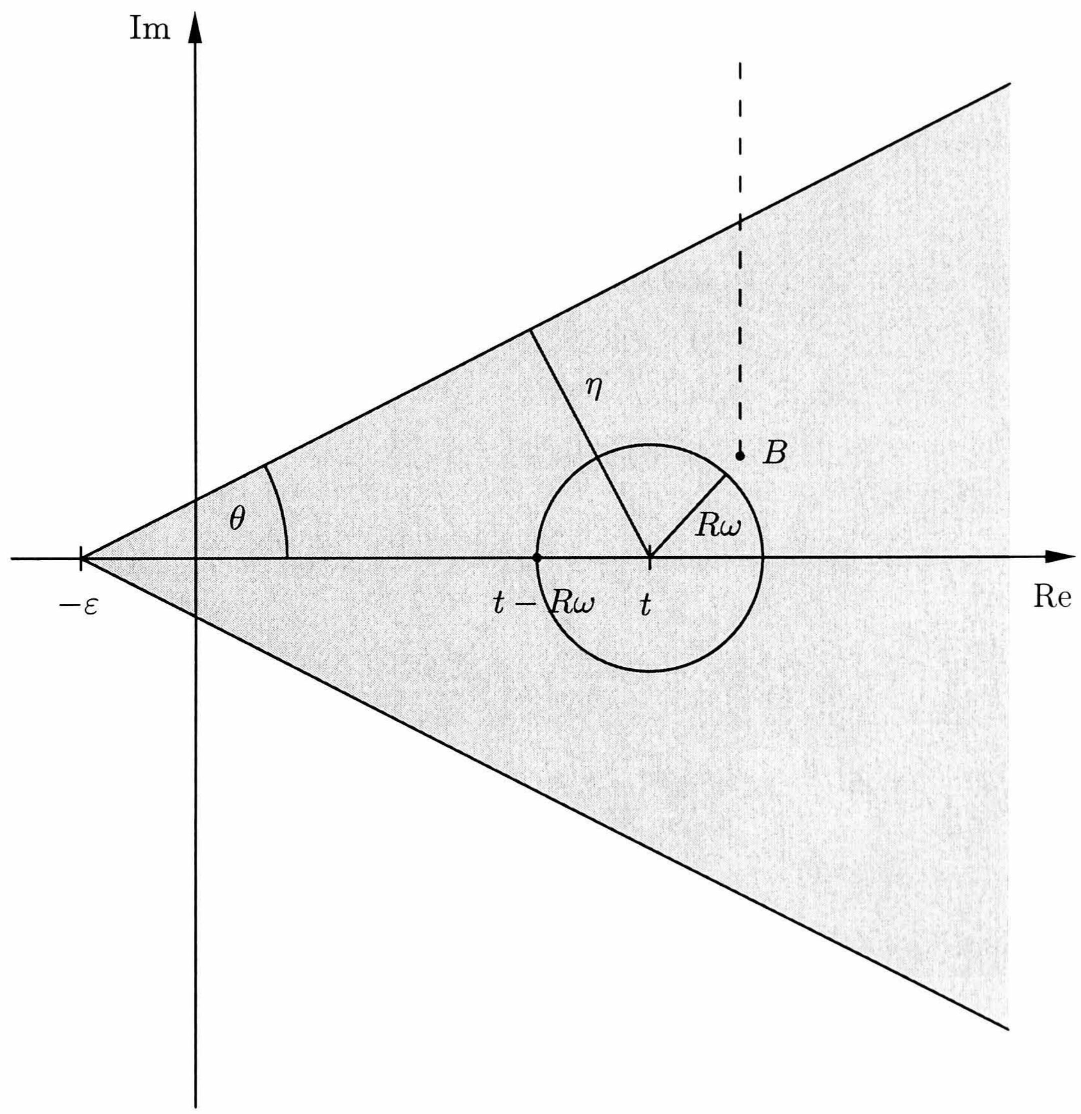


Figure 5.2: $\mathcal{D}_{\varepsilon,\theta,B}$ and the circular contour $C_{R\omega}(t)$ used in the proof of Lemma 5.1.

5.1 Numerical Examples

Let

$$f(z) = \frac{1}{(1+z)\sqrt{z-B}} \tag{5.13}$$

where $B = B_r + iB_i \in \mathbb{C}$ with $B_i \geq 0$. We will consider the problem of finding the numerical value of

$$\bar{J}f = \int_0^\infty e^{-\rho t} f(t)\, dt \tag{5.14}$$

for $\rho = 0, 0.00001, 1$. Substituting $t = \widehat{P}(u) = (1+u)/(1-u)$ in (5.14) and following the steps leading from (5.3) to (5.4), we have

$$\bar{J}f = I\widetilde{F} = \int_{-1}^{+1} \widetilde{F}(u)\, du, \tag{5.15}$$

where, for $-1 < u < 1$,

$$\widetilde{F}(u) = \widetilde{F}_1(u) + \widetilde{F}_2(u),$$

$$\widetilde{F}_1(u) = \left(\frac{1+b_r}{2}\right)\widehat{F}\left(\frac{1+b_r}{2}u - \frac{1-b_r}{2}\right),$$

$$\widetilde{F}_2(u) = \left(\frac{1-b_r}{2}\right)\widehat{F}\left(\frac{1-b_r}{2}u + \frac{1+b_r}{2}\right),$$

$$\widehat{F}(u) := \frac{2f(\widehat{P}(u))e^{-\rho\widehat{P}(u)}}{(1-u)^2}.$$

Again substituting $u = w(x)$ where, for some integer $p \geq 2$,

$$w(x) := \frac{V(x) - V(-x)}{V(x) + V(-x)}, \qquad -1 \leq x \leq 1, \tag{5.16}$$

$$V(x) := \left[\left(\frac{1}{2} - \frac{1}{p}\right)x^3 + \frac{1}{p}x + \frac{1}{2}\right]^p, \qquad -1 \leq x \leq 1, \tag{5.17}$$

in (5.15), we see that

$$\bar{J}f = I\widetilde{F} = \int_{-1}^{+1} w'(x)\widetilde{F}(w(x))dx. \tag{5.18}$$

In the following results, the integral $\bar{J}f$ is estimated by $I_N\widetilde{F}$, the quadrature rule approximation (5.12), with $2N-1$ points, i.e., we approximate (5.18) by the trapezium rule with $2N$ panels. Explicitly, this approximation is

$$\bar{J}f \approx I_N\widetilde{F} = \sum_{k=1-N}^{N-1} a_k\, \widetilde{F}(x_k). \tag{5.19}$$

where, for $k = 1 - N, \ldots, N-1$,

$$a_k = \frac{1}{N} w'\left(\frac{k}{N}\right), \qquad x_k = w\left(\frac{k}{N}\right).$$

For f given by (5.13), for $\rho = 0$, the exact value of the integral (5.14) is

$$\bar{J}f = \sqrt{2}\left[\pi/2 - \arctan\left(i/\sqrt{2}\,\right)\right].$$

For $\rho = 0.00001, 1$, we do not know the exact values of the integral $\bar{J}f$. But we need these values to compare with the numerical values from quadrature rule approximation (5.19), so we choose $I_{128}\widetilde{F}$ together with $p = 7$ for the mapping function (5.16) and (5.17) as our approximation to the exact values of $\bar{J}f$ for the cases $\rho = 0.00001, 1$.

As predicted by Theorem 5.1, the error in estimating $\bar{J}f$ with $I_N\widetilde{F}$ tends to zero as $N \to \infty$, and uniformly in B_r and B_i. In Figures 5.3–5.4, we can see that, for each p, the error in estimating $\bar{J}f$ with $I_N\widetilde{F}$ is bounded uniformly in B_r and B_i, as predicted by Theorem 5.1. To see that the error in estimating $\bar{J}f$ with $I_N\widetilde{F}$ tends to zero as $N \to \infty$, we depict the results in Figures 5.5–5.7 for $\rho = 0, 0.00001, 1$, respectively.

To illustrate the rate of convergence, predicted as $\delta - p/2$ for arbitrary $\delta > 0$, in estimating $\bar{J}f$ by $I_N\widetilde{F}$, we choose $B_r = 1$, $B_i = 0$, and $\rho = 0, 0.00001, 1$. Results are depicted and tabulated in Figures 5.5–5.7 and Tables 5.1–5.3, respectively. In our example $f(x) = \frac{1}{(1+x)\sqrt{x - B_r}}$, the parameter α in Assumption 5.1 is 1/2. Recall that we compute the error in estimating $\bar{J}f$ with $I_N\widetilde{F}$ given by (5.19). So we calculate and tabulate the EOC given by (1.45) in these tables. We also show at the top of each column the value of $\alpha p = p/2$.

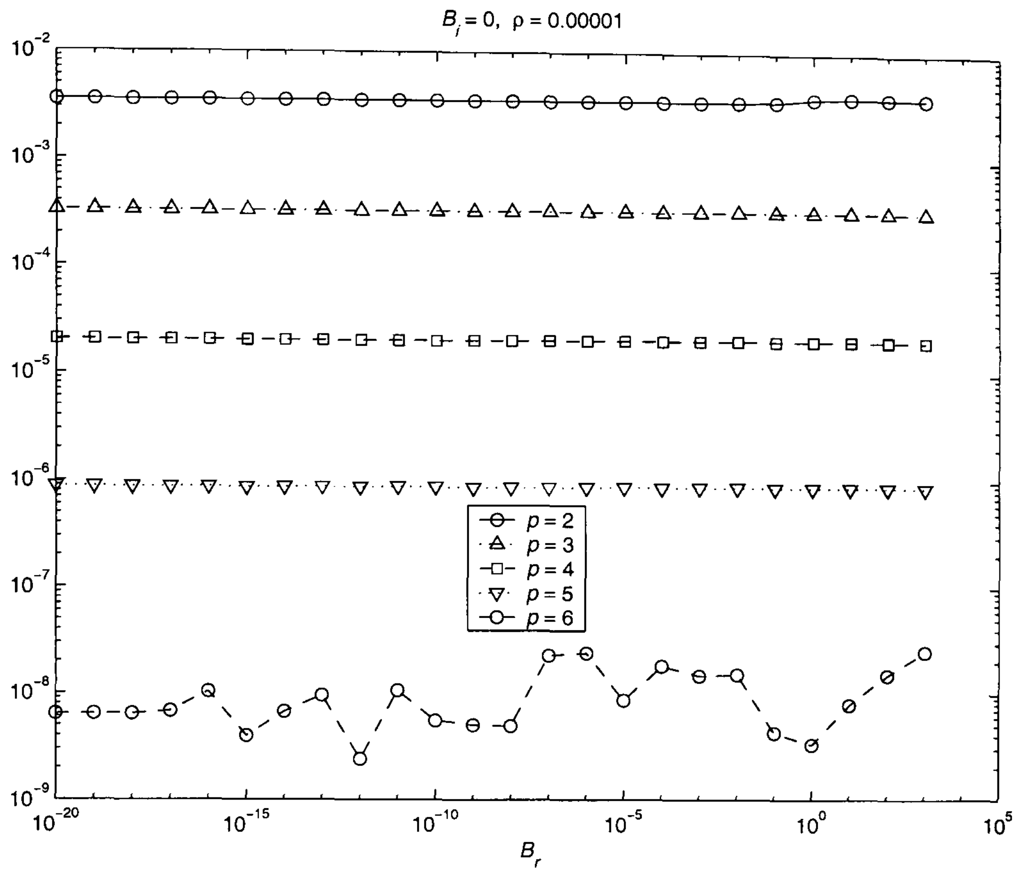


Figure 5.3: Error, $|\bar{J}f - I_{128}\widetilde{F}|$, for $p = 2, \ldots, 6$.

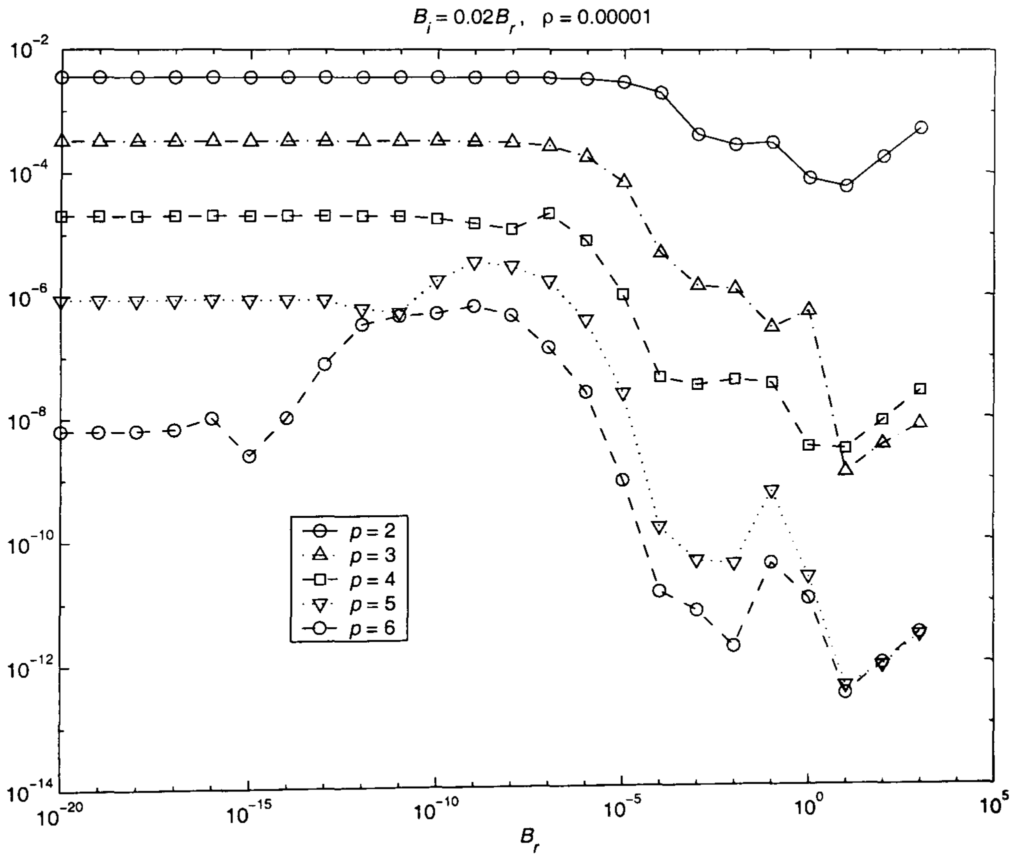


Figure 5.4: Error, $|\bar{J}f - I_{128}\widetilde{F}|$, for $p = 2, \ldots, 6$.

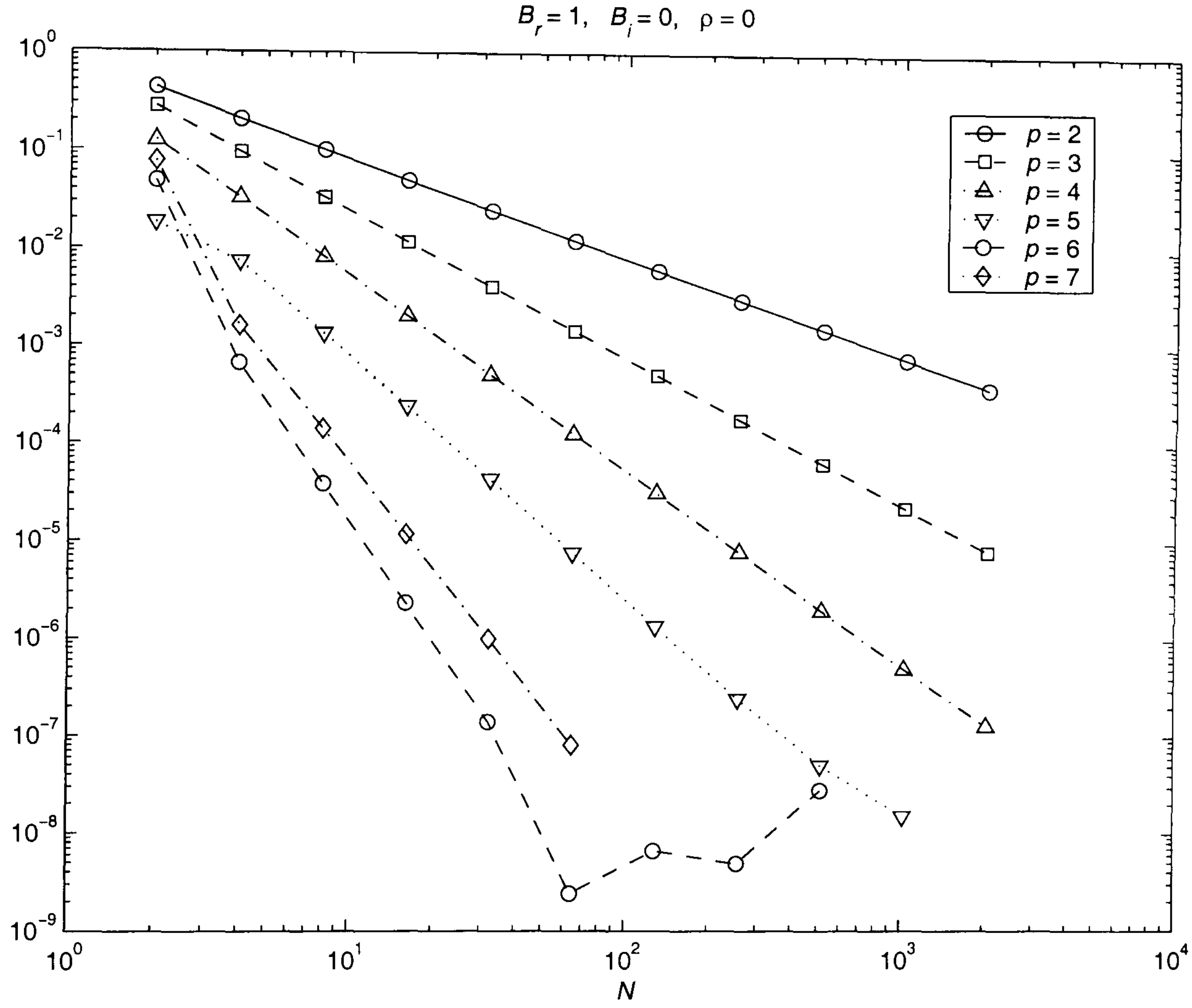


Figure 5.5: Error, $|\bar{J}f - I_{128}\widetilde{F}|$, with $\rho = 0$ and for $p = 2, \ldots, 7$.

Table 5.1: $B_r = 1,\ B_i = 0,\ \rho = 0$

$$\bar{J}f = \sqrt{2}\left[\pi/2 - \arctan\left(i/\sqrt{2}\,\right)\right] \approx 2.22144146907918 - 1.24645048028046i$$

NaN indicates that an implementation problem is encountered as described in Section 1.4 due to some x_k evaluating to ± 1 in (5.19).

	$p=2,\quad p/2=1.0$		$p=3,\quad p/2=1.5$		$p=4,\quad p/2=2.0$	
N	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC
2	4.3055E−01		2.7523E−01		1.2606E−01	
		1.0603		1.5265		1.9301
4	2.0646E−01		9.5535E−02		3.3081E−02	
		1.0312		1.5138		2.0045
8	1.0103E−01		3.3456E−02		8.2444E−03	
		1.0158		1.5066		2.0012
16	4.9962E−02		1.1774E−02		2.0594E−03	
		1.0080		1.5033		2.0003
32	2.4843E−02		4.1533E−03		5.1474E−04	
		1.0040		1.5016		2.0000
64	1.2387E−02		1.4668E−03		1.2868E−04	
		1.0020		1.5008		1.9998
128	6.1849E−03		5.1830E−04		3.2175E−05	
		1.0010		1.5004		1.9991
256	3.0903E−03		1.8320E−04		8.0490E−06	
		1.0005		1.5001		1.9963
512	1.5446E−03		6.4766E−05		2.0174E−06	
		1.0002		1.4998		1.9854
1024	7.7218E−04		2.2901E−05		5.0949E−07	
		1.0001		1.4993		1.9474
2048	3.8606E−04		8.1009E−06		1.3211E−07	

	$p=5,\quad p/2=2.5$		$p=6,\quad p/2=3.0$		$p=7,\quad p/2=3.5$	
N	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC
2	1.8331E−02		4.8379E−02		7.7183E−02	
		1.3133		6.1746		5.5825
4	7.3762E−03		6.6976E−04		1.6107E−03	
		2.4414		4.1124		3.5014
8	1.3580E−03		3.8721E−05		1.4223E−04	
		2.4722		4.0260		3.5765
16	2.4474E−04		2.3768E−06		1.1922E−05	
		2.4855		4.0695		3.5450
32	4.3701E−05		1.4157E−07		1.0214E−06	
		2.4917		5.8730		3.6366
64	7.7700E−06		2.4156E−09		8.2124E−08	
		2.4904		−1.4567		
128	1.3827E−06		6.6304E−09		0	
		2.4648		0.4142		
256	2.5046E−07		4.9758E−09		NaN	
		2.2906		−2.5030		
512	5.1191E−08		2.8205E−08		NaN	
		1.7407				
1024	1.5317E−09		NaN		NaN	
2048	NaN		NaN		NaN	

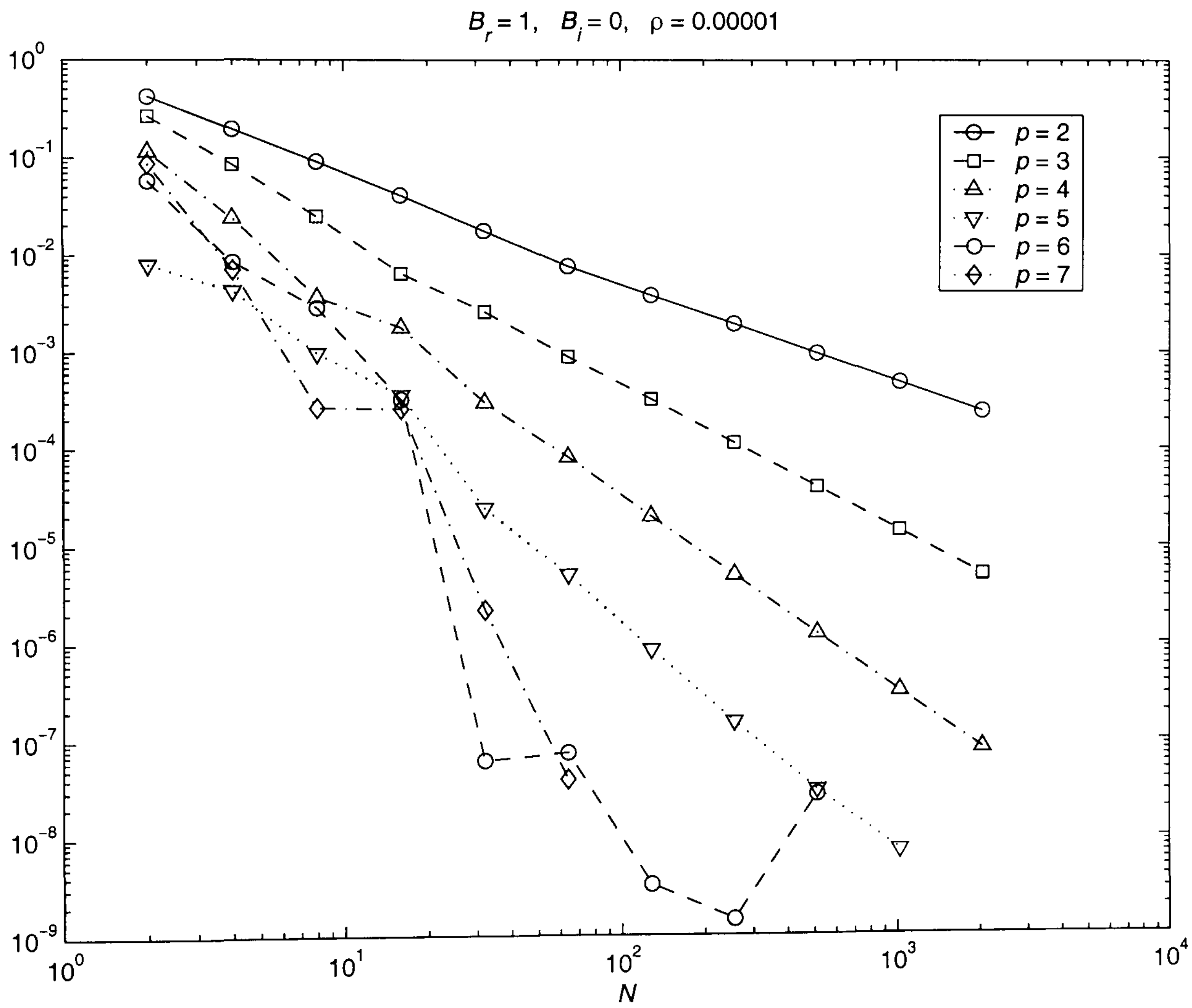


Figure 5.6: Error, $|\bar{J}f - I_{128}\widetilde{F}|$, with $\rho = 0.00001$ and for $p = 2, \ldots, 7$.

Table 5.2: $B_r = 1,\ B_i = 0,\ \rho = 0.00001$

$\bar{J}f \approx I_{128}\widetilde{F} \approx 2.21025366523428 - 1.24644294787069i$ (estimated with $p = 7$)

NaN indicates that an implementation problem is encountered as described in Section 1.4 due to some x_k evaluating to ± 1 in (5.19).

	$p = 2,\quad p/2 = 1.0$		$p = 3,\quad p/2 = 1.5$		$p = 4,\quad p/2 = 2.0$	
N	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC
2	4.2074E−01	1.0960	2.6540E−01	1.6233	1.1618E−01	2.2528
4	1.9683E−01	1.1008	8.6147E−02	1.7700	2.4378E−02	2.7237
8	9.1774E−02	1.1460	2.5258E−02	1.9588	3.6905E−03	1.0377
16	4.1471E−02	1.2214	6.4978E−03	1.3122	1.7977E−03	2.5683
32	1.7786E−02	1.2236	2.6166E−03	1.5483	3.0310E−04	1.8770
64	7.6162E−03	0.9878	8.9467E−04	1.4503	8.2518E−05	2.0199
128	3.8404E−03	0.9726	3.2740E−04	1.4987	2.0347E−05	1.9992
256	1.9571E−03	1.0021	1.1586E−04	1.5001	5.0894E−06	1.9973
512	9.7710E−04	1.0005	4.0960E−05	1.4999	1.2747E−06	1.9892
1024	4.8837E−04	1.0001	1.4483E−05	1.4995	3.2107E−07	1.9622
2048	2.4416E−04		5.1222E−06		8.2398E−08	

	$p = 5,\quad p/2 = 2.5$		$p = 6,\quad p/2 = 3.0$		$p = 7,\quad p/2 = 3.5$	
N	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC
2	7.9820E−03	0.8883	5.8059E−02	2.7564	8.7015E−02	3.6116
4	4.3122E−03	2.1464	8.5925E−03	1.5784	7.1186E−03	4.7334
8	9.7402E−04	1.4325	2.8772E−03	3.1480	2.6760E−04	0.0383
16	3.6086E−04	3.8691	3.2460E−04	12.3236	2.6059E−04	6.8595
32	2.4696E−05	2.2645	6.3323E−08	−0.2555	2.2441E−06	5.8052
64	5.1397E−06	2.5571	7.5589E−08	4.5114	4.0133E−08	
128	8.7330E−07	2.4734	3.3143E−09	1.2006	0	
256	1.5725E−07	2.3318	1.4420E−09	−4.2714	NaN	
512	3.1235E−08	2.0912	2.7848E−08		NaN	
1024	7.3306E−09		NaN		NaN	
2048	NaN		NaN		NaN	

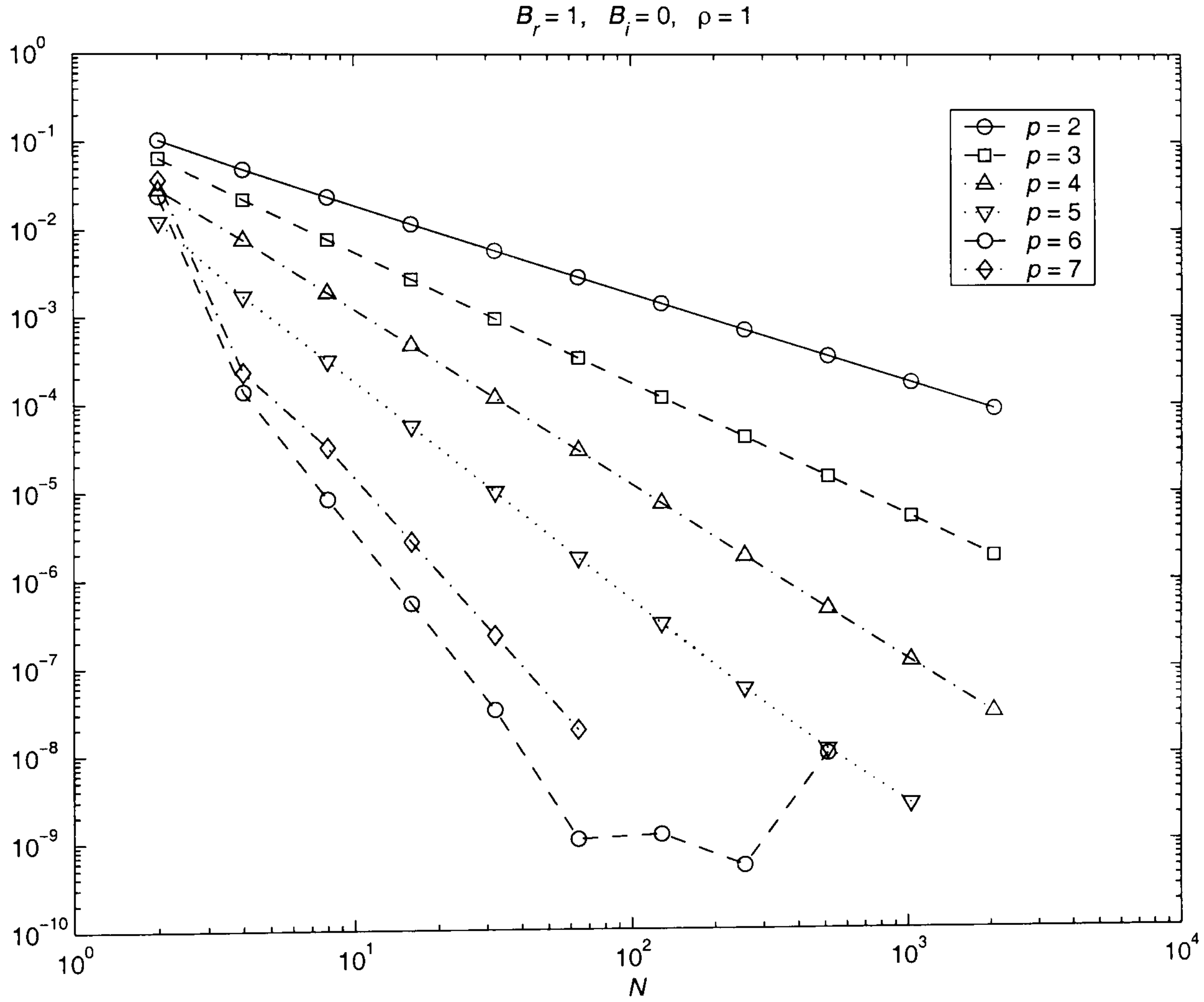


Figure 5.7: Error, $|\bar{J}f - I_{128}\widetilde{F}|$, with $\rho = 1$ and for $p = 2, \ldots, 7$.

Table 5.3: $B_r = 1$, $B_i = 0$, $\rho = 1$

$$\bar{J}f \approx I_{128}\widetilde{F} \approx 0.27475352508090 - 0.71667612129770i \text{ (estimated with } p = 7)$$

NaN indicates that an implementation problem is encountered as described in Section 1.4 due to some x_k evaluating to ± 1 in (5.19).

	$p = 2, \quad p/2 = 1.0$		$p = 3, \quad p/2 = 1.5$		$p = 4, \quad p/2 = 2.0$	
N	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC
2	1.0479E−01		6.4675E−02		2.8493E−02	
		1.1021		1.5427		1.8979
4	4.8814E−02		2.2199E−02		7.6454E−03	
		1.0423		1.5121		1.9966
8	2.3703E−02		7.7831E−03		1.9158E−03	
		1.0218		1.5065		1.9999
16	1.1674E−02		2.7394E−03		4.7899E−04	
		1.0110		1.5032		2.0000
32	5.7925E−03		9.6634E−04		1.1975E−04	
		1.0055		1.5016		1.9999
64	2.8851E−03		3.4127E−04		2.9939E−05	
		1.0028		1.5008		1.9998
128	1.4398E−03		1.2059E−04		7.4857E−06	
		1.0014		1.5004		1.9993
256	7.1921E−04		4.2624E−05		1.8723E−06	
		1.0007		1.5001		1.9973
512	3.5943E−04		1.5068E−05		4.6896E−07	
		1.0003		1.4999		1.9892
1024	1.7967E−04		5.3279E−06		1.1812E−07	
		1.0002		1.4995		1.9622
2048	8.9826E−05		1.8844E−06		3.0312E−08	

	$p = 5, \quad p/2 = 2.5$		$p = 6, \quad p/2 = 3.0$		$p = 7, \quad p/2 = 3.5$	
N	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC	$\lvert\bar{J}f - I_N\widetilde{F}\rvert$	EOC
2	1.2264E−02		2.3968E−02		3.6579E−02	
		2.8238		7.4265		7.3024
4	1.7320E−03		1.3933E−04		2.3173E−04	
		2.4530		4.0455		2.8346
8	3.1632E−04		8.4381E−06		3.2484E−05	
		2.4738		3.9333		3.5493
16	5.6943E−05		5.5232E−07		2.7747E−06	
		2.4856		4.0497		3.5429
32	1.0167E−05		3.3351E−08		2.3808E−07	
		2.4920		4.9533		3.6069
64	1.8074E−06		1.0765E−09		1.9540E−08	
		2.4920		−0.1776		
128	3.2128E−07		1.2175E−09		0	
		2.4735		1.1992		
256	5.7849E−08		5.3022E−10		NaN	
		2.3318		−4.2722		
512	1.1491E−08		1.0245E−08		NaN	
		2.0913				
1024	2.6965E−09		NaN		NaN	
2048	NaN		NaN		NaN	

5.2 Efficient Evaluation of the Half-Space Impedance Green's Function for the Helmholtz Equation

In Section 3.1, representations for the half-plane impedance Green's function for the Helmholtz equation have been obtained in terms of Laplace-type integrals of the form

$$\int_0^\infty t^{-1/2} e^{-\rho t} f(t)\, dt.$$

This Green's function solves the problem of outdoor sound propagation with a coherent line source parallel to a homogeneous impedance plane. So this is a two-dimensional problem in the plane perpendicular to the line source.

In this section we consider the corresponding three-dimensional problem of a point source above a homogeneous impedance plane. The solution to this problem is given by (3.5) but now with $G_0(\mathbf{r}, \mathbf{r}_0)$, the solution for the case $\beta = 0$, given by

$$G_0(\mathbf{r}, \mathbf{r}_0) = -\frac{1}{4\pi R} e^{ikR} - \frac{1}{4\pi R'} e^{ikR'},$$

where R and R' are as in Figure 3.1. A derivation of a formula for $P_\beta(\mathbf{r}, \mathbf{r}_0)$ can be obtained similarly to that in Section 3.1. Following steps leading to equation (3.9), it is found that (cf. Kawai *et al.* [30])

$$P_\beta(\mathbf{r}, \mathbf{r}_0) = -\frac{k\beta e^{i\rho}}{4\pi} \int_0^\infty t^{-1/2} e^{-\rho t} F(t)\, dt, \qquad \operatorname{Im}\beta \geq 0 \text{ or } \operatorname{Re} a_+ > 0,$$

where $\rho = kR'$,

$$F(t) = -\frac{G(\sqrt{t}) + G(-\sqrt{t})}{2(t - 2i)^{1/2}(t - ia_+)(t - ia_-)},$$

the constants $a_\pm$ are given by (3.11),

$$G(s) := e^{-ikr\sin\psi}((1 + is^2)\gamma + s(s^2 - 2i)^{1/2}(1 - \gamma^2)^{1/2} + \beta)\, \mathrm{H}_0^{(1)}(kr\sin\psi)\sin\psi,$$

$$\sin\psi = (1 + is^2)(1 - \gamma^2)^{1/2} + s(s^2 - 2i)^{1/2}\gamma, \qquad \operatorname{Re}\left\{(s^2 - 2i)^{1/2}\right\} > 0.$$

A simpler and in many ways more suitable representation of $P_\beta(\mathbf{r}, \mathbf{r}_0)$ for numerical integration purposes, given by Thomasson [51], is

$$P_\beta(\mathbf{r}, \mathbf{r}_0) = \frac{k\beta e^{i\rho}}{2\pi} \int_0^\infty e^{-\rho t} f(t)\, dt + P_\beta^s, \tag{5.20}$$

where

$$P_\beta^s = \begin{cases} \dfrac{k\beta}{2}\mathrm{H}_0^{(1)}\left(kr(1-\beta^2)^{1/2}\right)e^{-ik\beta(z+z_0)}, & \mathrm{Im}\,\beta < 0 \ \text{ and } \ \mathrm{Re}\,a_+ \le 0, \\ 0, & \text{otherwise} \end{cases} \tag{5.21}$$

with $r = (\,(x-x_0)^2 + (y-y_0)^2\,)^{1/2}$,

$$f(t) = \begin{cases} \dfrac{i}{\sqrt{-W(t)}}, & \mathrm{Im}\,\beta < 0 \ \text{ and } \ \mathrm{Re}\,a_+ < 0, \\ \dfrac{1}{\sqrt{W(t)}}, & \text{otherwise} \end{cases} \tag{5.22}$$

with

$$W(t) = -(t - ia_+)(t - ia_-), \tag{5.23}$$

and where the square roots in (5.22) are taken with argument in the range $(-\pi/2, \pi/2)$.

In order to obtain an integrand that decreases more rapidly when $t \to \infty$, especially important when ρ is small, and which satisfies that $r > 1$ in Assumption 5.1′ (note that $f(t) = O(t^{-1})$ as $t \to \infty$), we write P_β as

$$P_\beta = (P_\beta - \beta P_1) + \beta P_1. \tag{5.24}$$

From (5.20), (5.22) and (5.23) (see Chandler-Wilde [10]),

$$P_1(\mathbf{r}, \mathbf{r}_0) = -\frac{ike^{i\rho}}{2\pi}\int_0^\infty \frac{e^{-\rho t}}{t - i(1+\gamma)}\,dt = -\frac{ike^{-i\gamma\rho}}{2\pi}\mathrm{E}_1(-i(1+\gamma)\rho), \tag{5.25}$$

where $\mathrm{E}_1(z) := \int_z^\infty \frac{e^{-t}}{t}\,dt$ is the exponential integral. Clearly, from (5.20), (5.24) and (5.25),

$$P_\beta = \frac{k\beta e^{i\rho}}{2\pi}\int_0^\infty e^{-\rho t}\left[f(t) - \frac{1}{i(t - i(1+\gamma))}\right]dt - \frac{ik\beta e^{-i\gamma\rho}}{2\pi}\mathrm{E}_1(-i(1+\gamma)\rho) + P_\beta^s\,. \tag{5.26}$$

Using the notation in Section 5.1 that

$$\bar{J}F = \int_0^\infty e^{-\rho t}F(t)\,dt,$$

we rewrite (5.26) as

$$P_\beta = \frac{k\beta e^{i\rho}}{2\pi}\bar{J}g - \frac{ik\beta e^{-i\gamma\rho}}{2\pi}\mathrm{E}_1(-i(1+\gamma)\rho) + P_\beta^s\,, \tag{5.27}$$

where

$$g(t) = f(t) - \frac{1}{i(t - i(1+\gamma))},$$

and have that $g(t) = O\big(t^{-2}\big)$ as $t \to \infty$. To apply the results in Section 5.1, the function g is explicitly written as

$$|g(t)| = \left| \frac{1}{\sqrt{(t-ia_+)}\sqrt{(t-ia_-)}} + \frac{1}{\sqrt{(t-i(1+\gamma))^2}} \right|$$

$$= \left| \frac{\sqrt{(t-i(1+\gamma))^2} + \sqrt{(t-ia_+)}\sqrt{(t-ia_-)}}{\sqrt{(t-ia_+)}\sqrt{(t-ia_-)}\sqrt{(t-i(1+\gamma))^2}} \right|$$

$$= \left| \frac{(t-i(1+\gamma))^2 - (t-ia_+)(t-ia_-)}{\sqrt{(t-ia_+)}\sqrt{(t-ia_-)}\sqrt{(t-i(1+\gamma))^2}\left[\sqrt{(t-i(1+\gamma))^2} - \sqrt{(t-ia_+)}\sqrt{(t-ia_-)}\right]} \right|$$

$$= \left| \frac{i2\gamma(\beta-1)t - (1+\gamma)^2 + (\beta+\gamma)^2}{\sqrt{(t-ia_+)}\sqrt{(t-ia_-)}\sqrt{(t-i(1+\gamma))^2}\left[\sqrt{(t-i(1+\gamma))^2} - \sqrt{(t-ia_+)}\sqrt{(t-ia_-)}\right]} \right|$$

$$\leq \frac{2\gamma|1-\beta||t| + (1+\gamma)^2 + |\beta+\gamma|^2}{|\sqrt{(t-ia_+)}||\sqrt{(t-ia_-)}||\sqrt{(t-i(1+\gamma))^2}|\,|\sqrt{(t-i(1+\gamma))^2} - \sqrt{(t-ia_+)}\sqrt{(t-ia_-)}|}, \tag{5.28}$$

and then shown that function g satisfies Assumption 5.1′ in the following theorem.

Theorem 5.2 *For $0 \leq \gamma \leq 1$, $|\beta| \leq 1$, $|1-\beta| \leq 0.1$, the function g, given by (5.28), satisfies Assumption 5.1′ with $\varepsilon = 1/4$, $\theta = \pi/6$, $r = 2$ and $\widetilde{c} = 1806$. If $\gamma = 0$, $|\beta| \leq 1$, $|1-\beta| \leq 0.1$, then Assumption 5.1′ is satisfied with $\varepsilon = 1/4$, $\theta = \pi/6$, $r = 3$ and $\widetilde{c} = 452$.*

Proof. We use the same facts from Theorem 3.1, it follows that function g is analytic on $\mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}$. For $t \in \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}$, we find that

$$2\gamma|1-\beta||t| + (1+\gamma)^2 + |\beta+\gamma|^2 \leq \begin{cases} 8(1+|t|), & \text{if } \ 0 \leq \gamma \leq 1, \\ 2, & \text{if } \ \gamma = 0, \end{cases} \tag{5.29}$$

$$|t - ia_+| \geq \frac{9}{164}(1+|t|), \tag{5.30}$$

$$|t - ia_-| \geq \frac{57}{367}(1+|t|), \tag{5.31}$$

except that, for $0 \leq \gamma \leq 1$,

$$|t - i(1+\gamma)| \geq |t - i| \geq \frac{4\sqrt{3}-1}{8} > 0.74. \tag{5.32}$$

Applying this bound with $A = 1$, $B = 0.74$ and $K = 2$, we see from (3.27) and (5.32) that, for $t \in \mathcal{D}_{\frac{1}{4},\frac{\pi}{6}}$,

$$|t - i(1+\gamma)| \geq \frac{0.74}{1+0.74+1}(1+|t|)$$

$$= \frac{37}{137}(1+|t|). \tag{5.33}$$

Combining inequalities (5.29) to (5.31), and (5.33), for $0 \leq \gamma \leq 1$,

$$|g(t)| \leq 8\left(\frac{9}{164}\right)^{-1/2}\left(\frac{57}{367}\right)^{-1/2}\left(\frac{37}{137}\right)^{-1}\left[\frac{37}{137} - \left(\frac{9}{164}\right)^{1/2}\left(\frac{57}{367}\right)^{1/2}\right]^{-1}(1+|t|)^{-2}$$

$$< 1806(1+|t|)^{-2}.$$

Arguing in the same way for $\gamma = 0$, except that we use $2\gamma|1-\beta||t| + (1+\gamma)^2 + |\beta+\gamma|^2 \leq 2$ in this case, we obtain

$$|g(t)| \leq 452(1+|t|)^{-3}.$$

■

Chapter 6

Conclusions

In this thesis we have been concerned with the development, design, and analysis of simple and efficient quadrature methods, based on the Euler–Maclaurin formula, for different types of integrals with singularities, near or on the interval of integration. As example applications we have considered the problems of efficient evaluation of the impedance Green's function for the Helmholtz equation in a half-plane and half-space, important problems of acoustic propagation.

In Chapter 1 we have developed a numerical quadrature method for approximating the integral $\int_{-1}^{+1} f(t)\,dt$, where f may have endpoint singularities. The classical method is Gaussian quadrature, but this method requires knowing the singularity exactly, factorising out the singularity to leave a smooth remainder, and requires a relatively complicated calculation of weights and abscissae. By contrast we consider a numerical quadrature method, *the variable transformation method*, that it is robust with respect to the nature of the singularity, and whose weights and abscissae are easily generated. This numerical quadrature method requires, in brief, substituting $t = w(x)$, where $w : [-1,1] \to [-1,1]$ is a smooth bijection with all or many derivatives vanishing at the endpoints, and then applying the trapezium rule. The quadrature method and analysis developed in this chapter have been applied throughout the other chapters of this thesis. The rates of convergence we established match those seen in the numerical experiments carried out. in nearly all cases, and our convergence analysis improves somewhat and sharpens previous analysis of Kress [32, 33].

In Chapter 2 the problem of evaluating numerically the integral $\int_{-\infty}^{+\infty} e^{-\rho s^2}\Phi(s)\,ds$, for $\rho \geq 0$, has been considered. The magnitude of ρ is crucial for the choice of numerical quadrature method. For ρ not too small, Gauss–Hermite quadrature is an appropriate and standard method, but this quadrature method is not appropriate if $\rho = 0$ or ρ is small. For ρ small, we have proposed to change the interval of integration from $(-\infty, +\infty)$ to $[-1, 1]$ via a suitable substitution, and then applied the quadrature method and analysis developed in Chapter 1. A complete analysis of this procedure is given showing that, with appropriate choice of substitution $t = w(x)$, arbitrarily high orders of convergence can be obtained as $N \to \infty$, where N is the number of quadrature points, uniformly in ρ with $\rho = O(1)$. These theoretical predictions have been confirmed by numerical experiments.

As an application in Chapter 3 we apply the quadrature method and analysis developed in Chapter 2 to evaluate numerically the impedance Green's function for the Helmholtz equation in a half-plane. This Green's function is represented in terms of integrals of the form $\int_{-\infty}^{+\infty} e^{-\rho s^2}\Phi(s)\,ds$. In this chapter, we establish error bounds that show that the numerical quadrature approximations proposed are accurate for ranges of β (the relative surface admittance) and γ (the cosine of the angle of incidence) which cover the full physical ranges of interest, provided $\rho \geq 0$ (the dimensionless distance from image to receiver) is not too large.

In Chapter 4 we have considered the problem of finding the numerical value of the integral $\int_{-1}^{+1} f(t)\,dt$, where f may have a branch point singularity at $b = b_r + ib_i \in \mathbb{C}$ with $-1 < b_r < 1$ and $b_i \geq 0$. To apply the numerical quadrature method developed in Chapter 1, we decompose the interval of integration at the branch point singularity and then make a linear substitution to change the intervals of integration to $[-1, 1]$. The analysis shows that the error estimated by this procedure tends to zero as $N \to \infty$, where N is the number of quadrature points, uniformly in b_r and b_i. The theoretical predictions have been illustrated and supported through numerical experiments.

As an application of the numerical quadrature method developed in Chapter 4, we have considered in Chapter 5 the problem of evaluating numerically the integral $\int_0^\infty e^{-\rho t} f(t)\,dt$, where $\rho \geq 0$ and f has a branch point singularity at $B = B_r + iB_i \in \mathbb{C}$ with $B_r \in [0, \infty)$ and $B_i \geq 0$. To apply the results in Chapter 4, we have proposed to change the interval of integration from $[0, \infty)$ to $[-1, 1]$, decomposed the interval of integration at the branch point singularity, and then made a linear substitution to change the intervals of integration to $[-1, 1]$. With appropriate choice of the substitution $t = w(x)$, the analysis shows that arbitrarily high orders of convergence can be obtained as $N \to \infty$, where N is the number of quadrature points, uniformly in ρ and B, with $\rho = O(1)$, $B = O(1)$. The theoretical predictions have been illustrated and supported through numerical experiments.

Several questions remain unanswered at the end of this thesis. In Chapter 1 (see Section 1.4 and the numerical results) and intermittenly throughout the remainder of the thesis we have encountered problems of rounding errors limiting the accuracy of some calculations. In particular the accurate calculation of $\int_{-1}^{+1} f(t)\,dt$ is limited to some extent by rounding errors whenever $f(t) \to \infty$ as $t \to \pm 1$, essentially due to $f(t)$ evaluating as $f(\pm 1)$ whenever we evaluate $g(s) := w'(s)f(w(s))$ and $w(s)$ is closer than machine precision to ± 1. This might be cured by special schemes for evaluating the product $w_k f(x_k)$ accurately when the abscissa x_k is close to ± 1 and the weight w_k is very small. We have not taken any steps in this direction in this thesis.

An intriguing point which has arisen in the analysis throughout this thesis is that, although our measured convergence rates match the theoretical error estimates in most cases, whenever a convergence $O(N^{-3})$ is predicted the observed convergence is $O(N^{-4})$. There is some evidence also that the predicted $O(N^{-5})$ is actually $O(N^{-6})$. It would have been interesting to pursue this discrepancy, perhaps with a view to using insights obtained to design still more accurate schemes.

Appendix A

Matlab Code for the Complementary Error Function

In this appendix we list the *Matlab* code used in the thesis for computations of $w(z) = e^{-z^2}\operatorname{erfc}(-iz)$, for $z \in \mathbb{C}$, where erfc is the complementary error function. This code, based on Padé approximations at 0 and ∞ in the first quadrant, $0 \leq \arg z \leq \pi/2$, and symmetry relations to generate $w(z)$ throughout the complex plane, is a conversion from Fortran of the code in Appendix B of [10].

```
function w = was(z)
% was(z) is an approximation to w(z) = exp(-z^2)*erfc(-i*z)
a1 = [1.128379167096,-.1977549371215,.06234968803838,-.005716150768281,
     .000757964511326,-.00004483357225467,.000003330432838151,
     -1.356221892408E-7,6.152777066963E-9,-1.723902793323E-10,
     4.748868498218E-12,-8.523479440253E-14,1.264689471534E-15,
     -1.133411083999E-17,5.249830524266E-20] ;
b1 = [1.,.4914109167483,.1161965834987,.01754614733595,.001893019337148,
     .0001545988226598,.00000987240868436,5.016861789005E-7,
     2.042710590219E-8,6.646171668219E-10,1.704983966924E-11,
     3.352980251996E-13,4.792337044353E-15, 4.470542726687E-17,
     2.061112405395E-19] ;
a2 = [.5641895835478,-58.95781351972,2503.309361429,-56180.59450901,
     726510.9174498, -5538647.253308,24468845.77449,-59099294.32842,
     69059183.20797,-29890482.50154,2047332.214518] ;
```

```
b2 = [1.,-105.000003614,4488.75031948,-101745.0112407,1335403.328746,
     -10416146.43445,47740673.47245,-122761738.1863, 161124790.4129,
     -89513777.86579,13427067.5557] ;
x = real(z) ;
y = imag(z) ;
ay = abs(y) ;
az = abs(z) ;
p = abs(x) + i*ay ;
if az > 6
   q = p.*p ;
   w =  0.4613135279626./(q-0.1901635091935) +
        0.09999216171032./(q-1.784492748543) +
        0.002883893874874./(q-5.525343742263) ;
   w = i*p.*w ;
elseif  2.3*ay + az.*(az-4.4) < 0
   q = p.*p ;
   w = ratnal(a1,b1,q) ;
   w = exp(-q) + i*p.*w ;
else
   pinv = 1./p ;
   q = pinv.*pinv ;
   w = i*pinv.*ratnal(a2,b2,q) ;
end
if x.*y < 0
   w = conj(w) ;
   p = -conj(p) ;
end
if y == 0 & x < 0
   w = conj(w) ;
end
if y < 0
   q = -p.*p ;
```

```
   x = real(q) ;
   w = -w ;
   w = w + 2*exp(q) ;
end
clear ay az p pinv q x y z

function y = ratnal(a,b,z)
% Where m1 = length(a), m2 = length(b),
% y = (a(1) + a(2)*z + ... + a(m1)*z^(m1-1))/
%     (b(1) + b(2)*z + ... + b(m2)*z^(m2-1))
%
af = fliplr(a) ;
NUMER = polyval(af,z) ;
bf = fliplr(b);
DENOM = polyval(bf,z) ;
y = NUMER./DENOM ;
clear NUMER DENOM z
```

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