Numerical Quadratures for Singular and Hypersingular Integrals

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We present a procedure for the design of high order quadrature rules for the numerical evaluation of singular and hypersingular integrals; such integrals are frequently encountered in solution of integral equations of potential theory in two dimensions. Unlike integrals of both smooth and weakly singular functions, hypersingular integrals are pseudo-differential operators, being limits of certain integrals; as a result, standard quadrature formulae fail for hypersingular integrals. On the other hand, such expressions are often encountered in mathematical physics (see, for example, [11]), and it is desirable to have simple and efficient "quadrature" formulae for them. The algorithm we present constructs high-order "quadratures" for the evaluation of hypersingular integrals. The additional advantage of the scheme is the fact that each of the quadratures it produces can be used *simultaneously* for the efficient evaluation of hypersingular integrals, Hilbert transforms, and integrals involving both smooth and logarithmically singular functions; this results in significantly simplified implementations. The performance of the procedure is illustrated with several numerical examples.

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1 Introduction

Numerical integration is one of most frequently encountered computational procedures. When smooth functions are to be integrated, classical techniques tend to be adequate, especially in one and two dimensions; one of most efficient general-purpose tools consists of various versions of nested Gaussian quadrature rules (see, for example, [20, 18, 3, 6]). In cases where extremely efficient special-purpose quadratures are warranted, Gaussian (and more recently, Generalized Gaussian) quadratures are the approach of choice.

When singular functions are to be integrated, the situation tends to be less satisfactory. Special-purpose Gaussian quadratures can be easily constructed for functions of the form

$$f(x) = s(x) \cdot \phi(x), \tag{1}$$

where s is a fixed singular function, and ϕ is smooth. On the other hand, such situations are relatively rare; much more frequently, one is confronted with integrands of the form

$$f(x) = s(x) \cdot \phi(x) + \psi(x) \tag{2}$$

where s is a fixed singular function, and ϕ and ψ are *two* distinct smooth functions (often, several different singularities are involved). Here, Gaussian quadratures can not be used directly, and during the last several years, Generalized Gaussian quadratures have been developed as a tool (in part) for dealing with such situations.

The situation is further complicated when (as frequently happens in potential theory) the "integrals" to be evaluated are not, strictly speaking, integrals, but involve expressions of the form

$$\int_{-1}^{1} \frac{\phi(t)}{y-x}\, dx, \tag{3}$$

$$\int_{-1}^{1} \frac{\phi(x)}{(y-x)^2}\, dx, \tag{4}$$

$$\int_{-1}^{1} \frac{\phi(x)}{(y-x)^3}\, dx, \tag{5}$$

etc., understood in the appropriate finite part sense (in the engineering literature, (4) is often referred to as the "hypersingular" integral). Normally, "integrals" (3) – (5) (and similar objects) are treated via special-purpose techniques (product integration, interpolatory quadratures, etc.). A drawback of this approach is the need to separate singularities of different types, so that each can be treated via an appropriate procedure. For example, in (2), one would need to have access to each of the functions ϕ, ψ individually, as opposed to being able to evaluate the functions *in toto* (the latter situation is frequently encountered in practice).

In this paper, we design a collection of algorithms for the construction of high-order "quadratures" for the evaluation of hypersingular integrals. The additional advantage of the scheme is the fact that each of the quadratures it produces can be used *simultaneously* for the efficient evaluation of hypersingular integrals, Hilbert transforms, and integrals involving both smooth and logarithmically singular functions; this results in significantly simplified implementations.

Remark 1.1 *Unlike the quadratures for functions of the form (2), the quadratures constructed in this paper are not convergent in the classical sense. Instead, they produce a prescribed accuracy for a prescribed set of functions, such as Legendre polynomials, of all orders no greater than some natural number n, Legendre polynomials multiplied by logarithms, etc. Due to the triangle inequality, it is easy to estimate the precision produced when such quadratures are applied to linear combinations of Legendre polynomials, Legendre polynomials multiplied by logarithms, etc. Finally, we observe that if the chosen accuracy is sufficiently small (such as the machine precision), the behavior of the resulting quadratures is indistinguishable from rapid convergence (as can be seen from, for example, Figures 2 – 3 in this paper).*

Remark 1.2 *During the last two decades, numerical techniques have been developed in the computational potential theory (especially, for the Helmholtz equation and related problems involving time-domain Maxwell's equations) that replace classical integral equations with combined integro-pseudo-differential equations. The reasons for these recent developments are involved, and have to do with so-called "spurious resonances" (see, for example, [4, 15, 16, 19]). Without getting into the analytical details, we observe that the interest in the numerical solution of such integro-pseudo-differential equations is growing rapidly, and one of principal motivations behind this work is the design of appropriate rapidly convergent discretization schemes.*

The paper is organized as follows: In Section 2, the necessary mathematical and numerical preliminaries are introduced. In Section 3, we develop numerical quadratures for integrands that are algebraic combinations of smooth functions and functions with singularities of the form $\log|x|$, $\frac{1}{x}$, $\frac{1}{x^2}$. In Section 4, we describe a numerical procedure for the construction of the quadratures from Section 3.2. Section 5 contains numerical examples of some of the quadratures developed in this paper. Finally, in Section 6 we briefly discuss extensions of results of this paper to singularities other than $\log|x|$, $\frac{1}{x}$, $\frac{1}{x^2}$, and to two-dimensional singular and hypersingular integrals.

2 Mathematical and Numerical Preliminaries

In this section, we summarize several results from classical and numerical analysis to be used in the remainder of this paper. Detailed references are given in the text.

2.1 Principal Value Integrals

Integrals of the form

$$\int_a^b \frac{\varphi(x)}{x-y}\,dx\,, \tag{6}$$

where $y \in (a,b)$, do not exist in the classical sense, and are often referred to as *singular integrals.*

Definition 2.1 *Suppose that φ is a function $[a,b] \to \mathbb{R}$, $y \in (a,b)$, and the limit*

$$\lim_{\epsilon \to 0} \left(\int_a^{y-\epsilon} \frac{\varphi(x)}{x-y}\, dx + \int_{y+\epsilon}^b \frac{\varphi(x)}{x-y}\, dx \right) \tag{7}$$

exists and is finite. Then we will denote the limit (7) by

$$\text{p.v.} \int_a^b \frac{\varphi(x)}{x-y}\, dx\,, \tag{8}$$

and refer to it as a principal value integral.

Theorem 2.1 *Suppose that the function $\varphi : [a,b] \to \mathbb{R}$ is continuously differentiable in a neighborhood of $y \in (a,b)$. Then the principal value integral (8) exists.*

2.2 Finite Part Integrals

In this paper, we will be dealing with integrals of the form

$$\int_a^b \frac{\varphi(x)}{(x-y)^2}\, dx\,, \tag{9}$$

where $y \in (a,b)$, which are divergent in the classical sense. This type of integrals are often referred to as *hypersingular* or *strongly singular.*

Definition 2.2 *Suppose that φ is a function $[a,b] \to \mathbb{R}$, $y \in (a,b)$, and the limit*

$$\lim_{\epsilon \to 0} \left(\int_a^{y-\epsilon} \frac{\varphi(x)}{(x-y)^2}\, dx + \int_{y+\epsilon}^b \frac{\varphi(x)}{(x-y)^2}\, dx - \frac{2\varphi(y)}{\epsilon} \right) \tag{10}$$

exists and is finite. Then we will denote the limit (10) by

$$\text{f.p.} \int_a^b \frac{\varphi(x)}{(x-y)^2}\, dx\,, \tag{11}$$

and refer to it as a finite part integral (see, for example, [9]).

The following obvious theorem provides sufficient conditions for the existence of the finite part integral (10), and establishes a connection between finite part and principal value integrals.

Theorem 2.2 *Suppose that the function $\varphi : [a,b] \to \mathbb{R}$ is twice continuously differentiable in a neighborhood of $y \in (a,b)$. Then the finite part integral (11) exists, and*

$$\text{f.p.} \int_a^b \frac{\varphi(x)}{(x-y)^2}\, dx = \frac{d}{dy}\, \text{p.v.} \int_a^b \frac{\varphi(x)}{x-y}\, dx\,. \tag{12}$$

2.3 Legendre Polynomials and Legendre Expansions

For any natural number n, the Legendre differential equation is

$$(1-x^2)\cdot\frac{d^2u}{dx^2} - 2\,x\cdot\frac{du}{dx} + n\,(n+1)\cdot u = 0\,. \tag{13}$$

One solution of the Legendre differential equation (13) is the Legendre polynomial $P_n(x)$: $[-1,1] \to \mathbb{R}$, defined by the three-term recursion formula

$$P_{n+1}(x) = \frac{2\,n+1}{n+1}\cdot x\cdot P_n(x) - \frac{n}{n+1}\cdot P_{n-1}(x)\,, \tag{14}$$

with

$$P_0(x) \;=\; 1\,, \tag{15}$$

$$P_1(x) \;=\; x\,. \tag{16}$$

As is well-known, the Legendre polynomials have an explicit expression given by the formula

$$P_n(x) = \frac{1}{2^n\,n!}\frac{d^n}{dx^n}(x^2-1)^n\,. \tag{17}$$

Furthermore, they are orthogonal with respect to the inner product

$$(f,g) = \int_{-1}^{1} f(x)\,g(x)\,dx\,. \tag{18}$$

Suppose that $x_1, x_2, \ldots, x_N$ denote the zeros of the N-th Legendre polynomial $P_N : [-1,1]$ $\to \mathbb{R}$. Then we will refer to the points $\widetilde{x}_1, \widetilde{x}_2, \ldots, \widetilde{x}_N$ on the interval $[a,b]$, defined by the formula

$$\widetilde{x}_i = \frac{b-a}{2}\cdot x_i + \frac{a+b}{2}\,, \tag{19}$$

for all $i = 1,2,\ldots,N$, as the N Legendre nodes on $[a,b]$.

For any sufficiently smooth function $\varphi : [-1,1] \to \mathbb{R}$ we will be denoting by a_n the n-th Legendre coefficient of φ, defined by the formula,

$$a_n = \frac{2\,n+1}{2}\int_{-1}^{1}\varphi(x)\,P_n(x)\,dx\,, \tag{20}$$

so that for all $x \in [-1,1]$

$$\varphi(x) = \sum_{n=0}^{\infty} a_n\,P_n(x)\,. \tag{21}$$

The series (21) is referred to as the Legendre expansion of φ. Given any natural number N, for computational purposes we will be approximating the Legendre expansion (21) by its truncated series of degree $N-1$

$$\varphi(x) \approx \sum_{n=0}^{N-1} a_n\,P_n(x)\,. \tag{22}$$

The following lemma states that the truncated Legendre expansion of degree $N-1$ (22) converges rapidly for sufficiently smooth functions, and is proved, for example, in [7].

Lemma 2.3 *Suppose that $\varphi : [-1,1] \to \mathbb{R}$ is k times continuously differentiable and that $\sum_{n=0}^{\infty} a_n P_n(x)$ denotes its Legendre expansion. Then, for any point $x \in [-1,1]$,*

$$\left\| \varphi(x) - \sum_{n=0}^{N-1} a_n P_n(x) \right\|_2 = O\left(\frac{1}{N^k}\right) . \tag{23}$$

The following theorem relates the coefficients in a Legendre expansion to the coefficients in the Legendre expansion of its derivative and integral, respectively. Its proof follows from a combination of results in [21, 1, 7, 8].

Theorem 2.4 *Given a natural number N, suppose that the polynomial $p : [-1,1] \to \mathbb{R}$ is defined by the formula*

$$p(x) = \sum_{n=0}^{N-1} a_n P_n(x) . \tag{24}$$

Then,

$$p'(x) = \sum_{n=0}^{N-2} b_n P_n(x) , \tag{25}$$

with the coefficients b_n given by the formula

$$b_n = (2n+1) \sum_{k=n}^{[\frac{N+n-3}{2}]} a_{2k+1-n} , \quad n = 0, \ldots, N-2 , \tag{26}$$

and with $[\frac{N+n-3}{2}]$ denoting the integer part of $\frac{N+n-3}{2}$. Furthermore,

$$\int_{-1}^{x} p(y)\, dy = \sum_{n=0}^{N} c_n P_n(x) , \tag{27}$$

with the coefficients c_n given by the formulae

$$c_0 = \sum_{n=1}^{N} (-1)^{n+1} c_n , \tag{28}$$

$$c_n = \frac{a_{n-1}}{2(n-1)+1} - \frac{a_{n+1}}{2(n+1)+1} , \quad n = 1, \ldots, N-2 , \tag{29}$$

$$c_{N-1} = \frac{a_{N-2}}{2(N-2)+1} , \tag{30}$$

$$c_N = \frac{a_{N-1}}{2(N-1)+1} . \tag{31}$$

Remark 2.5 *It is well-know that if* $\varphi : [-1,1] \to \mathbb{R}$ *is* k *times continuously differentiable and that* $\sum_{n=0}^{\infty} a_n\, P_n(x)$ *denotes its Legendre expansion, then*

$$\left\| \varphi'(x) - \sum_{n=0}^{N-2} b_n\, P_n(x) \right\|_2 = O\left(\frac{1}{N^{k-1}}\right), \tag{32}$$

and

$$\left\| \int_{-1}^{x} \varphi(y)\, dy - \sum_{n=0}^{N} c_n\, P_n(x) \right\|_2 = O\left(\frac{1}{N^{k}}\right), \tag{33}$$

where the coefficients b_n *and* c_n *are defined by (26), (28) – (31), respectively.*

2.4 Legendre Functions of the Second Kind

The Legendre polynomial P_n (see (17)) is a solution of the Legendre differential equation (13). The other solution is the Legendre function of the second kind $Q_n : \mathbb{C} \setminus [-1,1] \to \mathbb{C}$, defined by the three-term recursion formula

$$Q_{n+1}(z) = \frac{2n+1}{n+1} \cdot z \cdot Q_n(z) - \frac{n}{n+1} \cdot Q_{n-1}(z), \tag{34}$$

with

$$Q_0(z) = \frac{1}{2} \cdot \log\left(\frac{z+1}{z-1}\right), \tag{35}$$

$$Q_1(z) = \frac{z}{2} \cdot \log\left(\frac{z+1}{z-1}\right) - 1. \tag{36}$$

Clearly, $Q_n(z)$ has a branch cut in the complex z-plane on the real axis from -1 to 1. In agreement with standard practice, on the branch cut we define $Q_n : [-1,1] \to \mathbb{R}$ by the formula

$$Q_n(x) = \frac{1}{2} \lim_{h \to 0} \Big(Q_n(x + i\,h) + Q_n(x - i\,h) \Big). \tag{37}$$

The following theorem is known as Neumann's integral representation (see, for example, [8]).

Theorem 2.6 *Suppose that* $P_n : [-1,1] \to \mathbb{R}$ *denotes the n-th Legendre polynomial, and* $Q_n : [-1,1] \to \mathbb{R}$ *the n-th Legendre function of the second kind defined by formula (37). Then, for any point* $y \in (-1,1)$

$$\text{p.v.} \int_{-1}^{1} \frac{P_n(x)}{y - x}\, dx = 2\, Q_n(y). \tag{38}$$

The following theorem follows immediately from Neumann's integral representation (38) and provides two formulae that will be subsequently used in this paper.

Theorem 2.7 *Suppose that* $P_n : [-1,1] \to \mathbb{R}$ *denotes the n-th Legendre polynomial, and* $\widetilde{P}_n : [-1,1] \to \mathbb{R}$ *its primitive function defined by the formula*

$$\widetilde{P}_n(x) = \int_{-1}^{x} P_n(y)\, dy\,. \tag{39}$$

Furthermore, suppose that $Q_n : [-1,1] \to \mathbb{R}$ *denotes the n-th Legendre function of the second kind defined by (37). Then, for any point* $y \in (-1,1)$

$$\int_{-1}^{1} \frac{1}{2} \cdot \log\left((y-x)^2\right) \cdot P_n(x)\, dx = \log\left((y-1)^2\right) + \text{p.v.} \int_{-1}^{1} \frac{\widetilde{P}_n(x)}{y-x}\, dx\,, \tag{40}$$

$$\text{f.p.} \int_{-1}^{1} \frac{P_n(x)}{(y-x)^2}\, dx = \text{p.v.} \int_{-1}^{1} \frac{P_n'(x)}{x-y}\, dx + \frac{1}{y-1} - \frac{(-1)^n}{y+1}\,. \tag{41}$$

2.5 Chebyshev Systems

Definition 2.3 *A set of continuous functions* $\varphi_1, \ldots, \varphi_N$ *is referred to as a Chebyshev system on the interval* $[a,b]$ *if the determinant*

$$\left| \begin{pmatrix} \varphi_1(x_1) & \cdots & \varphi_1(x_N) \\ \vdots & \ddots & \vdots \\ \varphi_N(x_1) & \cdots & \varphi_N(x_N) \end{pmatrix} \right| \tag{42}$$

is nonzero for any set of points $x_1, \ldots, x_N$ *such that* $a \le x_1 < x_2 < \ldots < x_N \le b$.

Definition 2.4 *Given a set of real numbers* $x_1 \le x_2 \le \ldots \le x_N$, *suppose that* $m_1, m_2, \ldots, m_N$ *denotes the natural numbers defined by the formulae*

$$m_1 = 0\,, \tag{43}$$

$$m_j = \begin{cases} 0\,, & \text{for } j > 1 \text{ and } x_j \ne x_{j-1}\,, \\ j-1\,, & \text{for } j > 1 \text{ and } x_j = x_{j-1} = \ldots = x_1\,, \\ k\,, & \text{for } j > k+1 \text{ and } x_j = x_{j-1} = \ldots = x_{j-k} \ne x_{j-k-1}\,. \end{cases} \tag{44}$$

A set of continuously differentiable functions $\varphi_1, \ldots, \varphi_N$ *is referred to as an extended Chebyshev system on the interval* $[a,b]$ *if the determinant*

$$\left| \begin{pmatrix} \frac{d^{m_1}}{dx^{m_1}}\varphi_1(x_1) & \cdots & \frac{d^{m_N}}{dx^{m_N}}\varphi_1(x_N) \\ \vdots & \ddots & \vdots \\ \frac{d^{m_1}}{dx^{m_1}}\varphi_N(x_1) & \cdots & \frac{d^{m_N}}{dx^{m_N}}\varphi_N(x_N) \end{pmatrix} \right|, \tag{45}$$

in which $\frac{d^0}{dx^0}\varphi_i(x_j) \equiv \varphi_i(x_j)$, *is nonzero for any set of points* $x_1, \ldots, x_N$ *such that* $a \le x_1 \le x_2 \le \ldots \le x_N \le b$.

Remark 2.8 *Obviously, an extended Chebyshev system also forms a Chebyshev system. The additional constraint is that the points $x_1, x_2, \ldots, x_N$ at which the functions are evaluated may be identical. In that case, for each duplicated point, the first corresponding column contains the function values, the second column contains the first derivatives of the functions, the third column contains the second derivatives of the functions, and so forth.*

In the following examples several important cases of Chebyshev and extended Chebyshev systems are presented (additional examples can be found in [10]).

Example 2.1 *The monomials $1, x, x^2, \ldots, x^n$ form an extended Chebyshev system on any interval $[a, b] \subset (-\infty, \infty)$.*

Example 2.2 *The exponentials $e^{-\lambda_1 x}, e^{-\lambda_2 x}, \ldots, e^{-\lambda_n x}$ form an extended Chebyshev system for any $\lambda_1, \lambda_2, \ldots, \lambda_n > 0$ on the interval $[0, \infty)$.*

Example 2.3 *The functions 1, $\cos(x)$, $\sin(x)$, $\cos(2\,x)$, $\sin(2\,x)$, ..., $\cos(n\,x)$, $\sin(n\,x)$ form a Chebyshev system on the interval $[0, 2\,\pi)$.*

2.6 Quadrature Formulae

A quadrature rule on the interval $[-1, 1]$ is an expression of the form

$$I_N(\varphi) = \sum_{n=1}^{N} w_n \cdot \varphi(x_n)\,, \tag{46}$$

where the points $x_n \in [-1, 1]$ and the coefficients $w_n \in \mathbb{R}$ are referred to as the nodes and the weights of the quadrature, respectively. The quadrature rule $I_N(\varphi)$ serves as an approximation to integrals of the form

$$I(\varphi) = \int_{-1}^{1} w(x) \cdot \varphi(x)\, dx\,, \tag{47}$$

where $\varphi : [-1, 1] \to \mathbb{R}$ is a sufficiently smooth function and $w : [-1, 1] \to \mathbb{R}$ is some fixed weight function. Since we will permit the function w to be strongly singular, the integral (47) has to be evaluated in the appropriate sense. In particular, for $w(x)$ we will consider, *inter alia*, the singular functions

$$\frac{1}{2} \cdot \log\left((y - x)^2\right), \tag{48}$$

$$\frac{1}{y - x}, \tag{49}$$

$$\frac{1}{(y - x)^2}, \tag{50}$$

where $y \in (-1, 1)$. For the latter two functions, the integral (47) is interpreted as a principal value integral (see (7)) and finite part integral (see (10)), respectively.

Definition 2.5 *A quadrature formula (46) for the integral (47) is said to be of the degree $M \geq 1$, if it integrates all polynomials up to degree M exactly.*

Normally, the degree of a quadrature formula (46) can not exceed $2N-1$ (see, for example, [20]). Quadrature rules (46) of degree $2N-1$ are commonly referred to as *Gaussian quadrature rules.* The following theorem is well-known and can be found in most elementary textbooks on numerical analysis (see, for example, [20]).

Theorem 2.9 *(Gaussian quadrature) Suppose that $w(x) \equiv 1$ for all $x \in [-1,1]$. Then there exists a unique quadrature rule (46) which has the degree $2N-1$. Furthermore, the nodes $x_1, x_2, \ldots, x_N$ are the zeros of the N-th Legendre polynomial $P_N(x)$ (see, (17)), and the weights $w_1, w_2, \ldots, w_N$ are all positive and given by the formula*

$$w_n = \int_{-1}^{1} \prod_{\substack{j=1 \\ j\neq n}}^{N} \left(\frac{x - x_j}{x_n - x_j} \right)^2 dx, \quad n = 1, 2, \ldots, N. \tag{51}$$

2.7 Generalized Gaussian Quadrature

Numerical quadratures are normally constructed such that the quadrature rule (46) is *exactly* equal to the integral (47) for some set of functions. Classical N-point Gaussian quadratures (see, Theorem 2.9) integrate polynomials of order $2N-1$ exactly. In [14], the notion of Gaussian quadrature was generalized as follows.

Definition 2.6 *Suppose that $w : [-1,1] \to \mathbb{R}$ is a non-negative integrable function. A quadrature rule (46) will be referred to as Gaussian with the respect to a set of $2N$ functions $\varphi_1, \varphi_2, \ldots, \varphi_{2N} : [-1,1] \to \mathbb{R}$ and a weight function w, if it consists of N weights and nodes, and integrates the functions $w \circ \varphi_i$ on $[-1,1]$ exactly for all $i = 1, 2, \ldots, 2N$. The weights and the nodes of a Gaussian quadrature will be referred to as Gaussian weights and nodes, respectively.*

The following theorem states that the Gaussian quadrature with respect to a set of functions $\varphi_1, \varphi_2, \ldots, \varphi_{2N}$ exists and is unique if the set $\varphi_1, \varphi_2, \ldots, \varphi_{2N}$ forms a Chebyshev system (see Definition 2.3). It is proved (in a slightly different form) in [10, 13].

Theorem 2.10 *Suppose that the functions $\varphi_1, \varphi_2, \ldots, \varphi_{2N} : [-1,1] \to \mathbb{R}$ form a Chebyshev system (see Definition 2.3) on the interval $[-1,1]$, and that the weight function $w : [-1,1] \to \mathbb{R}$ is non-negative and integrable. Then there exists a unique Gaussian quadrature with respect to the set $\varphi_1, \varphi_2, \ldots, \varphi_{2N}$ and the weight function w. Furthermore, the weights of this quadrature are all positive.*

From Definition 2.6 it immediately follows that the Gaussian quadrature with respect to the functions $\varphi_1, \varphi_2, \ldots, \varphi_{2N} : [-1,1] \to \mathbb{R}$ and the weight function $w : [-1,1] \to \mathbb{R}$ is defined by the system of equations

$$
\begin{aligned}
\sum_{n=1}^{N} w_n \cdot \varphi_1(x_n) &= \int_{-1}^{1} w(x) \cdot \varphi_1(x)\,dx\,, \\
\sum_{n=1}^{N} w_n \cdot \varphi_2(x_n) &= \int_{-1}^{1} w(x) \cdot \varphi_2(x)\,dx\,, \\
&\vdots \\
\sum_{n=1}^{N} w_n \cdot \varphi_{2N}(x_n) &= \int_{-1}^{1} w(x) \cdot \varphi_{2N}(x)\,dx\,.
\end{aligned} \tag{52}
$$

We denote the left hand sides of these equations by $f_1, f_2, \ldots, f_{2N}$; each of the f_i's being a function $[-1,1]^N \times \mathbb{R}^N \to \mathbb{R}$ of the nodes $x_1, x_2, \ldots, x_N$ and weights $w_1, w_2, \ldots, w_N$, respectively. Their partial derivatives are given by the formulae

$$\frac{\partial f_i}{\partial w_n} = \varphi_i(x_n)\,, \tag{53}$$

$$\frac{\partial f_i}{\partial x_n} = w_n\,\varphi_i'(x_n)\,, \tag{54}$$

so that the Jacobian of the system (52) takes the form

$$
J(x_1,\ldots,x_N,w_1,\ldots,w_N) =
\begin{pmatrix}
\varphi_1(x_1) & \cdots & \varphi_1(x_N) & w_1\,\varphi_1'(x_1) & \cdots & w_N\,\varphi_1'(x_N) \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
\varphi_{2N}(x_1) & \cdots & \varphi_{2N}(x_N) & w_1\,\varphi_{2N}'(x_1) & \cdots & w_N\,\varphi_{2N}'(x_N)
\end{pmatrix}. \tag{55}
$$

In practice, the system (52) is solved via Newton's method (see, for example, [5]). The following theorem states that when the functions to be integrated constitute an extended Chebyshev system, Newton's method for this system is always quadratically convergent, provided the starting point for the iteration is within a sufficiently small neighborhood of the solution. A proof can be found in, for example, [5].

Theorem 2.11 *Suppose that the functions $\varphi_1, \varphi_2, \ldots, \varphi_{2N}$ form an extended Chebyshev system (see Definition 2.4). Suppose further that the Gaussian quadrature nodes and weights for these functions are denoted by $\widehat{x}_1, \widehat{x}_2, \ldots, \widehat{x}_N$ and $\widehat{w}_1, \widehat{w}_2, \ldots, \widehat{w}_N$, respectively. Then the determinant of the Jacobian matrix (55) is nonzero at the point $(\widehat{x}_1, \ldots, \widehat{x}_N, \widehat{w}_1, \ldots, \widehat{w}_N)$, i.e.*

$$|J(\widehat{x}_1, \ldots, \widehat{x}_N, \widehat{w}_1, \ldots, \widehat{w}_N)| \neq 0\,. \tag{56}$$

Furthermore, the nodes $\widehat{x}_1, \widehat{x}_2, \ldots, \widehat{x}_N$ and the weights $\widehat{w}_1, \widehat{w}_2, \ldots, \widehat{w}_N$ depend continuously on the weight function w.

Remark 2.12 *In order for Newton's method to converge, the starting point must be within a sufficiently small neighborhood of the solution. In [5] the continuation method (sometimes also referred to as the homotopy method) is used to generate such starting points.*

2.8 Singular Value Decomposition of a Set of Functions

The following theorem generalizes the standard singular value decomposition of a matrix to a set of functions. A proof can be found (in a more general form), for example, in [17].

Theorem 2.13 *Suppose that the functions* φ_1, φ_2, ..., $\varphi_N : [a,b] \to \mathbb{R}$ *are square integrable. Then for some integer* M *there exist an orthonormal set of functions* $u_1, u_2, \ldots, u_M : [a,b] \to \mathbb{R}$, *an* $N \times M$ *matrix* $V = [v_{ij}]$ *with orthonormal columns, and a set of real numbers* $s_1 \geq s_2 \geq \ldots \geq s_M > 0$, *such that*

$$\varphi_j(x) = \sum_{i=1}^{M} u_i(x)\, s_i\, v_{ij}\,, \tag{57}$$

for all $x \in [a,b]$ *and all* $n = 1, 2, \ldots, N$.

By analogy to the well-known singular value decomposition of matrices, we will refer to the factorization (57) as the singular value decomposition of the set of functions φ_1, φ_2, ..., φ_N, the functions $u_1, u_2, \ldots, u_M$ as the singular functions, the columns of the matrix V as singular vectors, and the numbers $s_1 \geq s_2 \geq \ldots \geq s_M$ as the singular values, respectively.

The following theorem from [5] states that the accuracy of a quadrature formula with positive weights for the functions $\varphi_1, \varphi_2, \ldots, \varphi_N$ is determined by its accuracy for the singular functions u_i, corresponding to non-trivial singular values.

Theorem 2.14 *Suppose that under the conditions of Theorem 2.13 there exist a positive real number* ϵ *and an integer* $1 < M_0 < M$, *such that*

$$\sum_{i=M_0+1}^{M} s_i^2 < \frac{\epsilon^2}{4}\,. \tag{58}$$

Suppose further that the L-point quadrature rule with nodes x_1, $x_2, \ldots, x_L$ *and weights* $w_1, w_2, \ldots, w_L$ *integrates the functions* u_i *exactly on the interval* $[a,b]$, *i.e.*

$$\sum_{j=1}^{L} w_j \cdot u_i(x_j) = \int_a^b u_i(x)\, dx \tag{59}$$

for all $i = 1, 2, \ldots, M_0$, *and that the weights* $w_1, w_2, \ldots, w_L$ *are all positive. Then for each* $i = 1, 2, \ldots, N$,

$$\left| \sum_{j=1}^{L} w_j \cdot \varphi_i(x_j) - \int_a^b \varphi_i(x)\, dx \right| < \epsilon \cdot \|\varphi_i\|_2\,. \tag{60}$$

3 Analytical Apparatus

The principal purpose of this paper is to construct quadrature formulae for functions $f : [-1,1] \to \mathbb{R}$ of the form

$$f(x) = \varphi(x) + \psi(x) \cdot \log|x| + \frac{\eta(x)}{x} + \frac{\theta(x)}{x^2}\,, \tag{61}$$

where $\varphi, \psi, \eta, \theta : [-1,1] \to \mathbb{R}$ are smooth. In Section 3.1, we construct separate quadrature formulae for each of the functions of the form

$$\varphi(x)\,, \quad \psi(x)\cdot\log|x|\,, \quad \frac{\eta(x)}{x}\,, \quad \frac{\theta(x)}{x^2}\,, \tag{62}$$

in Section 3.2, we present a scheme were each quadrature it produces can be used *simultaneously* for the efficient numerical integration of functions of the form (61).

Obviously, integrals of the form

$$\int_{-1}^{1} \Big(\varphi(x) + \psi(x)\cdot\log(|y-x|) + \frac{\eta(x)}{y-x} + \frac{\theta(x)}{(y-x)^2}\Big)\, dx \tag{63}$$

with y *outside* the interval of integration $[-1,1]$ and the functions $\varphi, \psi, \eta, \theta$ smooth, can be evaluated with standard Gaussian quadrature formulae. However, when y is sufficiently close to the interval of integration $[-1,1]$, the number of Gaussian nodes needed to achieve acceptable accuracy is often very high. Therefore, more specialized quadratures are desirable in this case; Section 3.3 is devoted to the design of generalized Gaussian quadratures for this environment.

3.1 Quadrature Formulae for Individual Singularities $\log|x|$, $\frac{1}{x}$, $\frac{1}{x^2}$

The following theorem is one of principal analytical tools used in this paper.

Theorem 3.1 *Suppose that $x_1, x_2, \ldots, x_N$ and $w_1, w_2, \ldots, w_N$ denote the N nodes and weights of the Gaussian quadrature on the interval $[-1,1]$, respectively (see, Theorem 2.9). Suppose further that $P_j(x)$ denotes the j-th Legendre polynomial (see, (17)), and that $w(x)\cdot P_j(x)$ is integrable on $[-1,1]$ for all $j = 0, 1, \ldots, N-1$. Then the quadrature rule*

$$\int_{-1}^{1} w(x)\cdot\varphi(x)\, dx \approx \sum_{n=1}^{N} \tilde{w}_n \cdot \varphi(x_n) \tag{64}$$

with the weights $\tilde{w}_n$ defined by the formula

$$\tilde{w}_n = w_n \cdot \sum_{j=0}^{N-1} \Big(\frac{2j+1}{2}\, P_j(x_n)\cdot\Big(\int_{-1}^{1} w(x)\, P_j(x)\, dx\Big)\Big) \tag{65}$$

has the degree $N-1$.

Proof. Suppose that $\varphi : [-1,1] \to \mathbb{R}$ is a polynomial of order $N-1$ given by its Legendre series (21) so that

$$\varphi(x) = \sum_{j=0}^{N-1} a_j\, P_j(x)\,. \tag{66}$$

Substituting (66) into (47), we obtain

$$I(\varphi) = \int_{-1}^{1} w(x) \cdot \varphi(x)\, dx \;=\; \int_{-1}^{1} w(x) \cdot \Big(\sum_{j=0}^{N-1} a_j\, P_j(x) \Big)\, dx$$
$$= \sum_{j=0}^{N-1} a_j \cdot \Big(\int_{-1}^{1} w(x)\, P_j(x)\, dx \Big)\,. \tag{67}$$

The coefficients a_j are given by (20). Evaluating the integral (20) via N-point Gaussian quadrature (see Theorem 2.9), we obtain the identity

$$a_j = \frac{2j+1}{2} \int_{-1}^{1} \varphi(x)\, P_j(x)\, dx = \frac{2j+1}{2} \sum_{n=1}^{N} w_n \cdot \varphi(x_n) \cdot P_j(x_n)\,, \tag{68}$$

for all $j = 0, 1, \ldots, N-1$. Finally, substituting (68) into (67) we obtain

$$\int_{-1}^{1} w(x) \cdot \varphi(x)\, dx \;=\; \sum_{n=1}^{N} \varphi(x_n) \cdot w_n \cdot \sum_{j=0}^{N-1} \Big(\frac{2j+1}{2} P_j(x_n) \cdot \Big(\int_{-1}^{1} w(x)\, P_j(x)\, dx \Big) \Big)\,, \tag{69}$$

from which (64) and (65) immediately follow. □

Remark 3.2 *If the function φ is k times continuously differentiable, it immediately follows from the Cauchy-Schwartz inequality and (23) in Lemma 2.3 that*

$$\left| \int_{-1}^{1} w(x) \cdot \varphi(x)\, dx - \sum_{n=1}^{N} \tilde{w}_n \cdot \varphi(x_n) \right| = O\left(\frac{1}{N^k} \right)\,. \tag{70}$$

The following theorem extends Theorem 3.1 to the case when the function $w : [-1,1] \to \mathbb{R}$ is defined by one of the formulae (48) – (50). The latter two functions are not integrable in the classical sense, and the integral (47) is interpreted as a principal value integral (see (7)) and finite part integral (see (10)), respectively. The theorem follows immediately from the combination of Theorems 2.4, 2.7, 3.1.

Theorem 3.3 *Suppose that $x_1, x_2, \ldots, x_N$ and $w_1, w_2, \ldots, w_N$ denote the N nodes and weights of the Gaussian quadrature on the interval $[-1,1]$ (see, Theorem 2.9). Suppose further that $\varphi : [-1,1] \to \mathbb{R}$ is a sufficiently smooth function, and $P_j(x)$, $Q_j(x)$ denote the j-th Legendre polynomial and Legendre function of the second kind (see, (17), (37)), respectively. Finally, suppose that the coefficients $w_{1,1}, w_{1,2}, \ldots, w_{1,N},\ w_{2,1}, w_{2,2}, \ldots, w_{2,N}$, $w_{3,1}, w_{3,2}, \ldots, w_{3,N}$, are defined by the formulae*

$$w_{1,n} \;=\; w_n \cdot \sum_{j=0}^{N-1} (2j+1) \cdot P_j(x_n) \cdot Q_j(y)\,, \tag{71}$$

$$w_{2,n} \;=\; w_n \cdot \Big(\Big(P_0(x_n) - P_1(x_n)\Big) \cdot R_0(y) + \sum_{j=1}^{N-2} \Big(P_{j-1}(x_n) - P_{j+1}(x_n)\Big) \cdot R_j(y)$$

$$+P_{N-2}(x_n)\cdot R_{N-1}(y)+P_{N-1}(x_n)\cdot R_N(y)\Big), \tag{72}$$

$$w_{3,n} = w_n\cdot\Bigg(-\sum_{j=0}^{N-2}\sum_{k=j}^{[\frac{N+j-3}{2}]}(2j+1)\cdot(4k+3-2n)\cdot Q_j(y)\cdot P_{2k+1-n}(x_n)$$

$$+\sum_{j=0}^{N-1}\frac{2j+1}{2}P_j(x_n)\cdot\left(\frac{1}{y-1}-\frac{(-1)^j}{y+1}\right)\Bigg), \tag{73}$$

for all $n=1,2,\ldots,N$, *with* $[\frac{N+j-3}{2}]$ *denoting the integer part of* $\frac{N+j-3}{2}$, *and the mappings* $R_j:(-1,1)\to\mathbb{R}$ *defined by the formula*

$$R_j(y)=Q_j(y)+\frac{1}{4}\cdot\log\left((y-1)^2\right). \tag{74}$$

Then, for any point $y\in(-1,1)$, *the quadrature rules*

$$\text{p.v.}\int_{-1}^{1}\frac{\varphi(x)}{y-x}\,dx\approx\sum_{n=1}^{N}w_{1,n}\cdot\varphi(x_n), \tag{75}$$

$$\int_{-1}^{1}\frac{1}{2}\cdot\log\left((y-x)^2\right)\cdot\varphi(x)\,dx\approx\sum_{n=1}^{N}w_{2,n}\cdot\varphi(x_n), \tag{76}$$

$$\text{f.p.}\int_{-1}^{1}\frac{\varphi(x)}{(y-x)^2}\,dx\approx\sum_{n=1}^{N}w_{3,n}\cdot\varphi(x_n), \tag{77}$$

have the degree $N-1$, $N-2$, *and* $N-1$, *respectively.*

3.2 Quadrature Formulae for Functions of the Form $\varphi(x)+\psi(x)\cdot\log|x|$ $+\dfrac{\eta(x)}{x}+\dfrac{\theta(x)}{x^2}$

Theorem 3.3 provides a tool for the numerical integration of functions of the form

$$\psi(x)\cdot\log|x|, \tag{78}$$

$$\frac{\eta(x)}{x}, \tag{79}$$

$$\frac{\theta(x)}{x^2}. \tag{80}$$

However, integrands are frequently encountered of the form

$$f(x)=\varphi(x)+\psi(x)\cdot\log|x|+\frac{\eta(x)}{x}+\frac{\theta(x)}{x^2}, \tag{81}$$

where the functions φ,ψ,η,θ are known to be smooth but are not available individually. Specifically, in the numerical solution of scattering problems, one is frequently confronted with the need to evaluate integrals of the form

$$
\begin{aligned}
&\text{f.p.}\int_{-1}^{1} K(x,y)\cdot\sigma(x)\,dx = \\
&= \text{f.p.}\int_{-1}^{1}\left(K_1(x,y)+K_2(x,y)\cdot\log(|x-y|)+\frac{K_3(x,y)}{y-x}+\frac{K_4(x,y)}{(y-x)^2}\right)\cdot\sigma(x)\,dx\,, \qquad (82)
\end{aligned}
$$

where $\sigma : [-1,1] \to \mathbb{R}$ and $K_1(x,y), K_2(x,y), K_3(x,y), K_4(x,y) : [-1,1]\times[-1,1] \to \mathbb{R}$ are smooth functions, and $y \in (-1,1)$. Normally, the functions K_1, K_2, K_3, K_4 are not available separately, so that only the kernel K *in toto* can be evaluated. In such cases, a single quadrature rule integrating functions of the composite form (81) is clearly preferable. Even when each of the functions φ, ψ, η, θ is available separately, the numerical implementation is simplified when a single quadrature formula can be used.

Given a real number $y \in (-1,1)$, we denote by $\psi_1, \psi_2, \ldots, \psi_{4M}$ the functions $[-1,1] \to \mathbb{R}$ defined by the formulae

$$
\psi_i(x) = \begin{cases}
P_{i-1}(x)\,, & \text{for } i = 1,\ldots,M\,,\\
P_{i-M-1}(x)\cdot\log(|y-x|)\,, & \text{for } i = M+1,\ldots,2M\,,\\
P_{i-2M-1}(x)\cdot\dfrac{1}{y-x}\,, & \text{for } i = 2M+1,\ldots,3M\,,\\
P_{i-3M-1}(x)\cdot\dfrac{1}{(y-x)^2}\,, & \text{for } i = 3M+1,\ldots,4M\,.
\end{cases} \qquad (83)
$$

In a minor generalization of the standard terminology, we define the generalized moments $m_1(y)$, $m_2(y)$, …, $m_{4M}(y)$ by the formulae

$$
m_i(y) = \begin{cases}
\displaystyle\int_{-1}^{1} P_{i-1}(x)\,dx\,, & \text{for } i = 1,\ldots,M\,,\\
\displaystyle\int_{-1}^{1} P_{i-M-1}(x)\cdot\log(|y-x|)\,dx\,, & \text{for } i = M+1,\ldots,2M\,,\\
\text{p.v.}\displaystyle\int_{-1}^{1} \frac{P_{i-2M-1}(x)}{y-x}\,dx\,, & \text{for } i = 2M+1,\ldots,3M\,,\\
\text{f.p.}\displaystyle\int_{-1}^{1} \frac{P_{i-3M-1}(x)}{(y-x)^2}\,dx\,, & \text{for } i = 3M+1,\ldots,4M\,.
\end{cases} \qquad (84)
$$

Now, suppose that $x_1, x_2, \ldots, x_N$ denotes the N Legendre nodes on $[-1,1]$ (see (19)). Then we define the weights $w_1, w_2, \ldots, w_N$ of the quadrature formula

$$
\int_{-1}^{1} f(x)\,dx \approx \sum_{n=1}^{N} w_n\cdot f(x_n) \qquad (85)
$$

as the solution of the system of the $4M$ linear algebraic equations

$$
\sum_{n=1}^{N} w_n\cdot\psi_1(x_n) \;=\; m_1(y)\,,
$$

$$\sum_{n=1}^{N} w_n \cdot \psi_2(x_n) = m_2(y)\,, \tag{86}$$

$$\vdots$$

$$\sum_{n=1}^{N} w_n \cdot \psi_{4M}(x_n) = m_{4M}(y)\,.$$

Obviously, the matrix of the system (86) might be square, or it might be over- or under-determined, depending on the values of the parameters M, N. On the other hand, given a solution $w_1, w_2, \ldots, w_n$ of (86), we can be sure that the quadrature formula (85) will integrate exactly all functions f of the form (81), as long as the functions φ, ψ, η, θ are polynomials of order not greater than $M - 1$. Due to Theorem A.6 in Appendix A below, for sufficiently large N, there always exist multiple solutions of (86), and a solution $\tilde{w}_1, \tilde{w}_2, \ldots, \tilde{w}_n$ can be found such that

$$\sum_{n=1}^{N} \tilde{w}_n^2 \leq C \cdot \sum_{n=1}^{N} w_n^2\,, \tag{87}$$

where $w_1, w_2, \ldots, w_N$ are the weights of the N-point Gaussian quadrature and C is a positive real constant. In practice, least squares are used to find $w_1, w_2, \ldots, w_n$ satisfying the bound (87) (see Section 4 below). Denoting the $N \times 4M$ matrix of system (86) by A and its right-hand side by b, we rewrite (86) in the form

$$Aw = b\,. \tag{88}$$

3.3 Generalized Gaussian Quadrature Formulae for Functions of the Form $\varphi(x) + \psi(x) \cdot \log|x| + \frac{\eta(x)}{x} + \frac{\theta(x)}{x^2}$

In Section 3.2 we described the quadrature formula (85) for integrals of the form (82) where the point of evaluation y is *inside* the interval of integration. While standard numerical quadratures (eg. Newton-Cotes or Gaussian quadratures) can be used for integrals of the form (82) when the point of evaluation y is *outside and sufficiently far away* from the interval of integration, more specialized quadratures are desirable when y is *outside but close* to the interval of integration.

Given two positive real numbers d and R such that $d < R$, we will denote by $D_{R,d}$ the set $[-R, -1-d] \cup [1+d, R]$ (see Figure 1). We define the functions ψ_1, ψ_2, $\ldots$, $\psi_{4M} : [-1,1] \times D_{R,d} \to \mathbb{R}$ by the formulae

$$\psi_i(x,y) = \begin{cases} P_{i-1}(x)\,, & \text{for } i = 1, \ldots, M\,, \\ P_{i-M-1}(x) \cdot \log(|y-x|)\,, & \text{for } i = M+1, \ldots, 2M\,, \\ P_{i-2M-1}(x) \cdot \dfrac{1}{y-x}\,, & \text{for } i = 2M+1, \ldots, 3M\,, \\ P_{i-3M-1}(x) \cdot \dfrac{1}{(y-x)^2}\,, & \text{for } i = 3M+1, \ldots, 4M\,, \end{cases} \tag{89}$$

where P_j denotes the j-th Legendre polynomial (17).

Now, suppose that $y_1, y_2, \ldots, y_K$ are points in $D_{R,d}$. We will denote by $\eta_{ij} : [-1,1] \to \mathbb{R}$ the $4 \cdot K \cdot M$ functions defined by the formula

$$\eta_{ij}(x) = \psi_i(x, y_j) \tag{90}$$

where $i = 1, 2, \ldots, 4M$ and $j = 1, 2, \ldots, K$. Since it will be convenient to view the functions η_{ij} as a finite sequence of functions $[-1,1] \to \mathbb{R}$, we introduce the notation

$$k = 4(j-1)M + i, \tag{91}$$

so that

$$i = k - 4(j-1)M, \tag{92}$$

$$j = \frac{k-i}{4M} + 1. \tag{93}$$

In a mild abuse of notation, we will use η_k and η_{ij} interchangeably.

Due to Theorem 2.13, there exist orthonormal functions $u_1, u_2, \ldots, u_L : [-1,1] \to \mathbb{R}$, a matrix $V \in \mathbb{R}^{4 \cdot K \cdot M \times L}$ with orthonormal columns, and real numbers $s_1 \geq s_2 \geq \cdots \geq s_L > 0$, for some integer $L \leq 4 \cdot K \cdot M$, such that

$$\eta_k(x) = \sum_{i=1}^{L} u_i(x)\, s_i\, v_{ik} \tag{94}$$

for all $k = 1, 2, \ldots, 4 \cdot K \cdot M$.

Remark 3.4 *For an arbitrary positive real number ϵ, we will denote by $n(\epsilon)$ the number of coefficients s_i in the decomposition (94) such that $s_i > \epsilon$. It turns out that for fixed d and R, $n(\epsilon)$ is proportional to $\log(\frac{1}{\epsilon})$, and is virtually independent of K. For a fixed ϵ, $n(\epsilon)$ is proportional to $\log(\frac{R}{d})$, and is virtually independent of K. The behavior of $n(\epsilon)$ as a function ϵ, d, R is investigated in detail in [22].*

The following theorem is an immediate consequence of Theorems 2.11, 2.14.

Theorem 3.5 *Suppose that for a sufficiently large integer number K, $y_1, y_2, \ldots, y_K$ are points in $D_{R,d}$ such that $y_i \neq y_j$ for all $i \neq j$. Suppose further that the functions η_1, η_2, ..., $\eta_{4KM} : [-1,1] \to \mathbb{R}$, the real positive numbers $s_1, s_2, \ldots, s_L$, and the functions $u_1, u_2, \ldots, u_L : [-1,1] \to \mathbb{R}$ are defined by the formulae (90), (94), respectively. Given a positive real number ϵ, we denote by L_0 the smallest even integer such that $1 < L_0 < L$ and*

$$\sum_{i=L_0+1}^{L} s_i^2 < \frac{\epsilon^2}{4}. \tag{95}$$

Then there exists a unique solution $(w_1, \ldots w_{\frac{L_0}{2}}, x_1, \ldots x_{\frac{L_0}{2}})$ *of the non-linear system*

$$\begin{aligned} \sum_{n=1}^{\frac{L_0}{2}} w_n \cdot u_1(x_n) &= \int_{-1}^{1} u_1(x)\, dx\,, \\ \sum_{n=1}^{\frac{L_0}{2}} w_n \cdot u_2(x_n) &= \int_{-1}^{1} u_2(x)\, dx\,, \\ &\vdots \\ \sum_{n=1}^{\frac{L_0}{2}} w_n \cdot u_{L_0}(x_n) &= \int_{-1}^{1} u_{L_0}(x)\, dx\,, \end{aligned} \tag{96}$$

where all w_n, $n = 1, 2, \ldots, \frac{L_0}{2}$, *are positive. Furthermore, for each* $k = 1, 2, \ldots, 4 \cdot K \cdot M$, *the* $\frac{L_0}{2}$*-point quadrature rule*

$$\sum_{n=1}^{\frac{L_0}{2}} w_n \cdot \eta_k(x_n) \approx \int_{-1}^{1} \eta_k(x)\, dx\,, \tag{97}$$

has relative accuracy ϵ*; that is*

$$\left| \sum_{n=1}^{\frac{L_0}{2}} w_n \cdot \eta_k(x_n) - \int_{-1}^{1} \eta_k(x)\, dx \right| < \epsilon \cdot \|\eta_k\|_2\,. \tag{98}$$

Remark 3.6 *The solution of the system of non-linear equations (96) can be found by Newton's method. For a detailed discussion of a Newton method for non-linear systems arising in the construction of generalized Gaussian quadratures, the reader is referred to [5].*

4 Numerical Algorithm

In Sections 3.1, 3.2 we have described quadratures rules for integrands of the form (78) – (81). While the numerical evaluation of the weights of the quadratures (75) – (77) in Section 3.1 via the formulae (72) – (73) is straightforward, the evaluation of the weights $w_1, w_2, \ldots, w_N$ of the quadrature (85) is more involved; we summarize the computational procedure below.

The input to the algorithm is a real number $y \in (-1, 1)$, a natural number N where N is the number of Legendre nodes (19) on the interval $[-1, 1]$, and a natural number M where $M - 1$ is the degree of the quadrature rule. The algorithm will then compute quadrature weights $w_1, w_2, \ldots, w_N$, such that

$$\sum_{n=1}^{N} w_n \cdot \varphi(x_n) \approx \int_{-1}^{1} w(x) \cdot \varphi(x)\, dx\,, \tag{99}$$

where $\varphi : [-1,1] \to \mathbb{R}$ is smooth and $w : [-1,1] \to \mathbb{R}$ is a linear combination of smooth functions and functions of the form (48) – (50), respectively. It consists of the following steps:

1. Construct the N-point Gaussian nodes $x_1, x_2, \ldots, x_N$ and weights $w_1, w_2, \ldots w_N$ on the interval $[-1,1]$ (see Theorem 2.9).
2. Evaluate the Legendre polynomials $P_0, P_1, \ldots, P_{M-1}$ at the nodes $x_1, x_2, \ldots, x_N$ via the three-term recursion (14).
3. Evaluate all the functions $\psi_1, \psi_2, \ldots, \psi_{4M}$ (see (83)) at the nodes $x_1, x_2, \ldots, x_N$.
4. Construct the moments $m_1(y), m_2(y), \ldots, m_{4M}(y)$ (see (84)) exactly, using Gaussian quadrature for m_1, m_2, ..., m_M and quadrature rules (75) – (77) for $m_{M+1}(y)$, $m_{M+2}(y)$, ..., $m_{4M}(y)$, respectively.
5. Solve the linear algebraic system (88) in the least squares sense with any standard routine (available, for example, in LAPACK [2]).

5 Numerical Examples

FORTRAN codes have been written constructing the quadratures described in Sections 3.1, 3.2, 3.3; in this section, their performance is illustrated with several numerical examples. In all examples below the quadrature nodes and weights are first computed in extended precision arithmetic (`REAL *16`) to assure full double precision accuracy. The quadrature rules are then used in double precision (`REAL *8`) to numerically integrate a number of functions with singularities $\log|x|$, $\frac{1}{x}$, $\frac{1}{x^2}$.

Example 5.1 In the first example, we use the quadrature rules (75) – (77) to evaluate integrals of the form (47) for each of the singularities (48) – (50) with the function φ : $[-1,1] \to \mathbb{R}$ defined by the formula

$$\varphi(x) = \sin(2\,x) + \cos(3\,x)\,, \tag{100}$$

so that the actual functions to be integrated are of the form

$$\log(|x-y|) \cdot \Big(\sin(2\,x) + \cos(3\,x)\Big)\,, \tag{101}$$

$$\frac{1}{y-x} \cdot \Big(\sin(2\,x) + \cos(3\,x)\Big)\,, \tag{102}$$

$$\frac{1}{(y-x)^2} \cdot \Big(\sin(2\,x) + \cos(3\,x)\Big)\,. \tag{103}$$

We denote by $y_1, y_2, \ldots, y_{14}$ the 14 Legendre nodes on the interval $[-1,1]$ (see (19)). The integrals of (101) – (103) were evaluated at $y_1, y_2, \ldots, y_{14}$, and the relative errors in the l^2

norm were obtained via the formula

$$E_2^{rel} = \frac{\sqrt{\sum_i E^{abs}(y_i)^2}}{\sqrt{\sum_i I(\varphi)(y_i)^2}}, \tag{104}$$

where $E^{abs}(y_i)$ and $I(\varphi)(y_i)$ denote the absolute error and the exact integral (47) evaluated at the point y_i, respectively. The integrals $I(\varphi)(y_i)$ were computed analytically using MATHEMATICA.

In Figure 2, the relative errors of the integrals of (101) – (103) are presented for $N = 6, 8, \ldots, 26$. For comparison, the relative errors of the N-point Gaussian rules (see Theorem 2.9) with $N = 6, 8, \ldots, 26$ applied to the function (100) are shown as well.

Remark 5.1 *The weights (see (72) – (73)) of the quadrature rules (75) – (77) used in Example 5.1 above, depend upon the point of evaluation y. Therefore, for the evaluation of each of the integrals (101) – (103) at each of the points $y_1, y_2, \ldots, y_{14}$, a different set of quadrature weights is used. As an example, in Table 1 we list the quadrature nodes x_n and weights $w_{1,n}$, $w_{2,n}$, $w_{3,n}$ of the 14-node version of the quadratures (75) – (77) for the integration of functions with singularities $\log(|x - y_1|)$, $\frac{1}{y_1 - x}$, $\frac{1}{(y_1-x)^2}$, with $y_1 = -0.9862838086968123$ (the smallest of the 14 Legendre nodes on $[-1, 1]$).*

Example 5.2 In this example, we compute the same integrals as in Example 5.1. However, this time we use the quadrature rule (85) that integrates functions of the combined form (81). Specifically, the quadrature weights were constructed via the numerical algorithm described in Section 4 for integrands of the form

$$\sum_{i=1}^{M} \left(a_i + b_i \cdot \log(|y_k - x|) + \frac{c_i}{y_k - x} + \frac{d_i}{(y_k - x)^2} \right) \cdot P_{i-1}(x), \tag{105}$$

for each Legendre node y_k, $k = 1, 2, \ldots, 14$, on the interval $[-1, 1]$ (see (19)). In our computations, we chose the number of weights N equal to $6M$.

In Figure 3 the relative errors (see (104)) are presented for $N = 36, 48, \ldots, 144$.

Example 5.3 In this example, we use the generalized Gaussian quadrature described in Section 3.3 to integrate the functions (101) – (103) where y is a point *outside* but *close* to the interval $[-1, 1]$. Specifically, 36 and 42-node versions of the quadrature formula (97) were constructed for integrands of the form

$$\sum_{i=1}^{M} \left(a_i + b_i \cdot \log(|y - x|) + \frac{c_i}{y - x} + \frac{d_i}{(y - x)^2} \right) \cdot P_{i-1}(x), \tag{106}$$

where $y \in [-10, -1.0016] \cup [1.0016, 10]$. The 36 and 42-node versions were constructed with $M = 11$ and $M = 21$, respectively. In order to test the accuracy of the resulting quadratures, the integrals (101) – (103) were evaluated at 202 equispaced points $y_1, y_2, \ldots, y_{202} \in$

$[-2.002, -1.002] \cup [1.002, 2.002]$, defined by the formula

$$y_k = \begin{cases} -2.002 + 0.01 \cdot (k-1)\,, & \text{for } k = 1, \ldots, 101\,, \\ 1.002 + 0.01 \cdot (k-102)\,, & \text{for } k = 102, \ldots, 202\,. \end{cases} \tag{107}$$

In Table 2, the relative errors (see (104)) of the N-point generalized Gaussian quadratures with $N = 36, 42$ applied to the the functions (100), (101) – (103) are presented. For comparison, the relative errors of the N-point Gaussian rules (see Theorem 2.9) with $N = 36, 42, 100, 150, \ldots, 300$ applied to the same functions are shown in Table 3. In Tables 4, 5 we list the quadrature nodes x_n and weights w_n of the 36 and 42-node versions of the quadrature (97).

Example 5.4 In this example, we use a compound quadrature formula based on the combination of the singular quadrature (85), generalized Gaussian quadrature (97), and Gaussian quadrature (see Theorem 2.9) to evaluate the integral

$$F(y) = \text{f.p.} \int_{-1}^{1} \Big(1 + \log(|y-x|) + \frac{1}{y-x} + \frac{1}{(y-x)^2}\Big) \cdot \Big(\sin(200x) + \cos(300x)\Big)\, dx\,, \tag{108}$$

at several points $y \in (-1, 1)$. Specifically, we subdivide the interval of integration $[-1, 1]$ into K subintervals $I_1, \ldots, I_K$ where

$$I_i = \Big[-1 + \frac{2}{K} \cdot (i-1), -1 + \frac{2}{K} \cdot i\Big]\,, \tag{109}$$

for all $i = 1, 2, \ldots, K$, and then apply a specific quadrature rule on each subinterval to evaluate (108). The quadrature rule used on subinterval I_i is determined by one of the following criteria:

- if $y \in I_i$, then the combined singular quadrature rule (85) is used;
- if $y \notin I_i$ and $y \in I_{i-1} \cup I_{i+1}$, then generalized Gaussian quadrature (97) is used;
- if $y \notin I_i$ and $y \notin I_{i-1} \cup I_{i+1}$, then Gaussian quadrature (see Theorem 2.9) is used.

We denote by

$$y_1^i, y_2^i, \ldots, y_M^i \tag{110}$$

the M Legendre nodes (see (19)) on subinterval I_i. Furthermore, we denote by y_1, y_2, ..., y_{MK} the set of all points (110) from all subintervals I_i, $i = 1, 2, \ldots, K$. In other words,

$$y_j^i = y_{M(i-1)+j}\,, \tag{111}$$

where $i = 1, 2, \ldots, K$ and $j = 1, \ldots, M$. Obviously, by evaluating the integral (108) at the points $y_1, y_2, \ldots, y_{MK}$ via the procedure described above, we obtain approximations to $F(y_1), F(y_2), \ldots, F(y_{MK})$. We perform the calculations with $M = 4, 6, 10, 12, 16$ and $K = 2, 4, 8, \ldots, 8192$; and in order to compare the accuracy for two different choices of

K, we interpolate the obtained values with an M order interpolation scheme to the 100 equispaced points $t_1, t_2, \ldots, t_{100}$ on the interval $(-1, 1)$ defined by the formula

$$t_i = -1 + \frac{2}{101} \cdot i, \tag{112}$$

for all $i = 1, \ldots, 100$.

In Table 6, the relative errors (see (104)) of the scheme described above of degrees $M = 4, 6, 10, 12, 16$ and the number of subintervals $K = 2, 4, 8, \ldots, 8192$, applied to the integral (108) are presented.

The following observations can be made from the examples of this section, and from the more detailed numerical experiments performed by the authors.

1. The quadrature formulae (85), (97) are not convergent in the classical sense; they are only convergent to a prescribed precision ϵ. Needless to say, the two are indistinguishable, as long as the prescribed precision is less than machine precision.

2. The schemes producing the quadrature formulae (75) – (77), (97) do not lose many digits compared to machine precision; constructing the quadratures in double precision arithmetic results in 11 – 12 correct digits; constructing them in extended precision arithmetic results in full double precision accuracy. Needless to say, the nodes and weights of the quadrature formulae (75) – (77), (97) can be (and have been) precomputed and stored, so that the need for extended precision during the *construction* of the quadrature is not a serious limitation.

3. The quadrature formula (85) experiences some loss of precision, not only during the precomputation of the nodes and weights, but also when the formula is applied to specific functions of the form (81). A fairly detailed investigation has led us to the conclusion that the loss of precision is associated with the evaluation of the "hypersingular" function (80), and is unavoidable; the phenomenon is very similar to the loss of precision associated with numerical differentiation, both in character and severity.

4. When the quadrature formulae of this paper are applied to oscillatory functions (of the form (108), or similar), they achieve their full precision at $10 - 15$ nodes per wavelength (for the formulae (75) – (77), (97)), and $20 - 45$ nodes per wavelength (for the formula (85)), respectively.

6 Generalizations and Conclusions

A set of quadratures has been constructed for functions $f : [-1, 1] \to \mathbb{R}$ of the form

$$f(x) = \varphi(x) + \psi(x) \cdot \log|x| + \frac{\eta(x)}{x} + \frac{\theta(x)}{x^2}, \tag{113}$$

where $\varphi, \psi, \eta, \theta : [-1,1] \to \mathbb{R}$ are smooth functions. The term "quadratures" in this case is somewhat of a misnomer, as functions of the form (113) are not integrable in the classical sense, and their integrals are to be interpreted in the appropriate "finite part" sense. One of anticipated applications for such quadratures is the evaluation of integro-pseudo-differential operators (eg. Hilbert transform and derivative of Hilbert transform) arising from the solution of integral equations of potential theory in two dimensions (see, for example, [11, 12]).

The work presented here admits several straightforward extensions:

1. The quadratures in this paper can easily be modified for functions with singularities other than $\log|x|$, $\frac{1}{x}$, $\frac{1}{x^2}$. For example, using Chebyshev polynomials, quadrature formulae similar to (75) – (77), (85) for functions with singularities of the form

$$\frac{\log|x|}{\sqrt{1-x^2}}, \tag{114}$$

$$\frac{1}{x\sqrt{1-x^2}}, \tag{115}$$

$$\frac{1}{x^2\sqrt{1-x^2}}, \tag{116}$$

etc. are easily constructed.

2. A straightforward generalization of the quadratures of this paper in two dimensions leads to quadrature formulae on the square, integrating functions $f : [-1,1]\times[-1,1] \to \mathbb{R}$ of the form

$$f(x_1,x_2) = \varphi(x_1,x_2) + \frac{\psi(x_1,x_2)}{(x_1^2+x_2^2)^{\frac{1}{2}}} + \frac{\eta(x_1,x_2)}{x_1^2+x_2^2} + \frac{\theta(x_1,x_2)}{(x_1^2+x_2^2)^{\frac{3}{2}}}, \tag{117}$$

where $\varphi, \psi, \eta, \theta : [-1,1]\times[-1,1] \to \mathbb{R}$ are smooth functions. Quadrature formulae of this type have been constructed, and the paper reporting them is in preparation.

A Existence of Quadrature Formulae for Functions of the Form $\varphi(x) + \psi(x) \cdot \log|x| + \frac{\eta(x)}{x} + \frac{\theta(x)}{x^2}$

In Section 3.2, we numerically construct quadrature formulae on the interval $[-1,1]$ for functions of the form

$$f(x) = \varphi(x) + \psi(x) \cdot \log|x| + \frac{\eta(x)}{x} + \frac{\theta(x)}{x^2}. \tag{118}$$

The nodes of the quadratures we construct are Gaussian nodes $x_1, x_2, \ldots, x_N$ with a sufficiently large N, and their weights are determined via a least squares procedure. The purpose of this Appendix is to prove that the least squares process of Section 3.2 can be used to obtain quadratures of arbitrary accuracy. We do so by constructing a procedure that, given a real $\epsilon > 0$ and a sufficiently large integer N, produces a set of weights $w_1, w_2, \ldots, w_N$ such that, in combination with the Gaussian nodes $x_1, x_2, \ldots, x_N$ evaluates the integral (82) to precision ϵ.

Remark A.1 *The procedure of this Appendix is quite inefficient, in the sense that it requires a very large number of nodes to obtain acceptable levels of accuracy; its purpose is to prove that such quadratures exist. The procedure for the actual evaluation of coefficients is described in Section 3.2, and results in schemes whose precision is satisfactory at moderate values of N (see Section 5).*

The following lemma follows immediately from the definition of the integral, and the fact that a logarithmic singularity is integrable.

Lemma A.2 *Suppose that $j \geq 0$ is an integer number, and that P_j denotes the j-th Legendre polynomial (see (17)). Then for any positive real number ϵ, there exists an integer $N_0 \geq 1$ such that for any $N \geq N_0$*

$$\left| \int_{-1}^{1} P_j(x) \cdot \log|x| \, dx - \sum_{\substack{i=1 \\ x_i \neq 0}}^{N} w_i \cdot P_j(x_i) \cdot \log|x_i| \right| \leq \epsilon, \tag{119}$$

with $x_1, x_2, \ldots, x_N$ and $w_1, w_2, \ldots, w_N$ the nodes and the weights of the N-point Gaussian quadrature (see Theorem 2.9).

The following lemma is an immediate consequence of Lemma A.2.

Lemma A.3 *Suppose that P_j denotes the j-th Legendre polynomial (see (17)). Then for any positive real number ϵ and integer $M \geq 0$, there exists an integer $N_0 \geq 1$ such that for any $N \geq N_0$ and each $j = 0, 1, \ldots, M$*

$$\left| \int_{-1}^{1} P_j(x) \, dx - \sum_{\substack{i=1 \\ x_i \neq 0}}^{N} w_i \cdot P_j(x_i) \right| \leq \epsilon, \tag{120}$$

and

$$\left| \int_{-1}^{1} P_j(x) \cdot \log|x| \, dx - \sum_{\substack{i=1 \\ x_i \neq 0}}^{N} w_i \cdot P_j(x_i) \cdot \log|x_i| \right| \leq \epsilon, \tag{121}$$

with $x_1, x_2, \ldots, x_N$ and $w_1, w_2, \ldots, w_N$ the nodes and the weights of the N-point Gaussian quadrature (see Theorem 2.9). Furthermore, for any function $F : [-1, 1] \to \mathbb{R}$ of the form

$$F(x) = \sum_{j=0}^{M} \Big(a_j + b_j \cdot \log|x| \Big) \cdot P_j(x), \tag{122}$$

with a_j, b_j arbitrary real coefficients,

$$\left| \int_{-1}^{1} F(x)\,dx - \sum_{\substack{i=1 \\ x_i \neq 0}}^{N} w_i \cdot F(x_i) \right| \leq \epsilon \cdot \sum_{j=0}^{M} \left(|a_j| + |b_j| \right). \tag{123}$$

The following lemma provides a formula for the evaluation of the integrals of functions that are linear combinations of polynomials, and polynomials composed with the singular function $\frac{1}{x^2}$.

Lemma A.4 *Suppose that $n \geq 1$ is an integer number, and that the function $F : [-1,1] \to \mathbb{R}$ is defined by the formula*

$$F(x) = P_n(x) + \frac{S_n(x)}{x^2}, \tag{124}$$

with $P_n, S_n : [-1,1] \to \mathbb{R}$ arbitrary polynomials of degree n. Furthermore, suppose that the function $f : [-1,1] \to \mathbb{R}$ is defined by the formula

$$f(x) = x^2 \cdot F(x). \tag{125}$$

Then

$$\text{f.p.} \int_{-1}^{1} F(x)\,dx = \sum_{\substack{i=1 \\ x_i \neq 0}}^{n} w_i \cdot \left(F(x_i) - \frac{f(0)}{x_i^2} \right) - 2\,f(0), \tag{126}$$

where $w_1, w_2, \ldots, w_n$ and $x_1, x_2, \ldots, x_n$ are the weights and nodes of the n-point Gaussian quadrature, respectively (see Theorem 2.9).

Proof. Defining the function $G : [-1,1] \to \mathbb{R}$ by the formula

$$G(x) = F(x) - \frac{f(0)}{x^2} - \frac{f'(0)}{x}, \tag{127}$$

we observe that G is a polynomial of order n, and therefore

$$\int_{-1}^{1} G(x)\,dx = \sum_{\substack{i=1 \\ x_i \neq 0}}^{n} w_i \cdot \left(F(x_i) - \frac{f(0)}{x_i^2} - \frac{f'(0)}{x_i} \right). \tag{128}$$

Now, observing that

$$\sum_{\substack{i=1 \\ x_i \neq 0}}^{n} \frac{w_i}{x_i} = 0, \tag{129}$$

(due to the symmetry of the Gaussian nodes and weights about zero), and substituting (129) into (128), we have

$$\int_{-1}^{1} G(x)\,dx = \sum_{\substack{i=1 \\ x_i \neq 0}}^{n} w_i \cdot \left(F(x_i) - \frac{f(0)}{x_i^2} \right). \tag{130}$$

It immediately follows from (10) that

$$\text{f.p.} \int_{-1}^{1} \frac{f(0) + f'(0) \cdot x}{x^2} \, dx = -2\, f(0)\,, \tag{131}$$

and, combining (127), (130), (131), we obtain

$$\begin{aligned} \text{f.p.} \int_{-1}^{1} F(x)\, dx &= \int_{-1}^{1} G(x)\, dx + \text{f.p.} \int_{-1}^{1} \frac{f(0) + f'(0) \cdot x}{x^2} \, dx & (132) \\ &= \sum_{\substack{i=1 \\ x_i \neq 0}}^{n} w_i \cdot \left(F(x_i) - \frac{f(0)}{x_i^2} \right) - 2\, f(0)\,. & (133) \end{aligned}$$

□

Lemma A.5 *Suppose that $F : [-1,1] \to \mathbb{R}$ and $f : [-1,1] \to \mathbb{R}$ are two functions defined by (124) and (125), respectively. Then there exists a positive real C_1 such that for any sufficiently small h,*

$$\left| f(0) - \Big(F(h) + F(-h) \Big) \cdot \frac{h^2}{2} \right| \leq C_1 \cdot h^2\,. \tag{134}$$

Furthermore, for any real $\gamma \notin \{-1, 0, 1\}$, there exists a positive real number C_2 such that for any sufficiently small h,

$$\left| f(0) - \Big(F(h) + F(-h) - F(\gamma\, h) - F(-\gamma\, h) \Big) \cdot \frac{\gamma^2 \cdot h^2}{2\,(\gamma^2 - 1)} \right| \leq C_2 \cdot h^4\,. \tag{135}$$

Proof. We start with observing that for any $F : [-1,1] \to \mathbb{R}$ defined by (124), there exist such real numbers $a_{-2}, a_{-1}, a_0, a_1, \ldots, a_n$ that

$$F(x) = \frac{a_{-2}}{x^2} + \frac{a_{-1}}{x} + a_0 + a_1\, x + \ldots + a_n\, x^n\,, \tag{136}$$

and due to (125),

$$a_{-2} = f(0)\,. \tag{137}$$

It immediately follows from (136) that for small h,

$$\begin{aligned} F(h) &= \frac{a_{-2}}{h^2} + \frac{a_{-1}}{h} + a_0 + a_1\, h + a_2\, h^2 + O(h^3)\,, & (138) \\ F(-h) &= \frac{a_{-2}}{h^2} - \frac{a_{-1}}{h} + a_0 - a_1\, h + a_2\, h^2 + O(h^3)\,. & (139) \end{aligned}$$

Adding (138) to (139), we obtain

$$F(h) + F(-h) = \frac{2\, a_{-2}}{h^2} + 2\, a_0 + 2\, a_2\, h^2 + O(h^4)\,, \tag{140}$$

and (134) immediately follows from the combination of (137) and (140).

In order to prove (135), we replace h with $\gamma \cdot h$ in (140) above, obtaining

$$F(\gamma h) + F(-\gamma h) = \frac{2\, a_{-2}}{\gamma^2 h^2} + 2\, a_0 + 2\, a_2\, \gamma^2 h^2 + O(h^4)\,. \tag{141}$$

Subtracting (141) from (140), we have

$$F(h) + F(-h) - \Big(F(\gamma h) + F(-\gamma h) \Big) = \frac{2\, a_{-2}(\gamma^2 - 1)}{\gamma^2 h^2} + 2\, a_2\, h^2 (1 - \gamma^2) + O(h^4)\,, \tag{142}$$

and (135) immediately follows from the combination of (137) and (142). □

The following theorem now immediately follows from the combination of Lemmas A.3 - A.5.

Theorem A.6 *Suppose that P_j denotes the j-th Legendre polynomial (see (17)). Then for any positive real number ϵ and integer $M \geq 0$, there exists an integer $N_0 \geq 1$, real coefficients $\tilde{w}_1, \tilde{w}_2, \ldots, \tilde{w}_N$, and a positive constant C such that for any $N \geq N_0$ and each $j = 0, 1, \ldots, M$*

$$\left| \int_{-1}^{1} P_j(x)\, dx - \sum_{\substack{i=1 \\ x_i \neq 0}}^{N} \tilde{w}_i \cdot P_j(x_i) \right| \leq \epsilon\,, \tag{143}$$

$$\left| \int_{-1}^{1} P_j(x) \cdot \log|x|\, dx - \sum_{\substack{i=1 \\ x_i \neq 0}}^{N} \tilde{w}_i \cdot P_j(x_i) \cdot \log|x_i| \right| \leq \epsilon\,, \tag{144}$$

$$\left| \int_{-1}^{1} \frac{P_j(x)}{x^2}\, dx - \sum_{\substack{i=1 \\ x_i \neq 0}}^{N} \tilde{w}_i \cdot \frac{P_j(x_i)}{x_i^2} \right| \leq \epsilon\,, \tag{145}$$

and

$$\sum_{i=1}^{N} \tilde{w}_i^2 \leq C \cdot \sum_{i=1}^{N} w_i^2\,, \tag{146}$$

with $x_1, x_2, \ldots, x_N$ and $w_1, w_2, \ldots, w_N$ the nodes and the weights of the N-point Gaussian quadrature (see Theorem 2.9). Furthermore, for any function $F : [-1, 1] \to \mathbb{R}$ of the form

$$F(x) = \sum_{j=0}^{M} \left(a_j + b_j \cdot \log|x| + \frac{c_j}{x^2} \right) \cdot P_j(x)\,, \tag{147}$$

with a_j, b_j, c_j arbitrary real coefficients,

$$\left| \int_{-1}^{1} F(x)\, dx - \sum_{\substack{i=1 \\ x_i \neq 0}}^{N} \tilde{w}_i \cdot F(x_i) \right| \leq \epsilon \cdot \sum_{j=0}^{M} \Big(|a_j| + |b_j| + |c_j| \Big)\,. \tag{148}$$

x_n	$w_{1,n}$	$w_{2,n}$	$w_{3,n}$
-.9862838086968123E+00	0.6158759029892887E+00	-.1749507584908717E+00	-.1130556007318105E+03
-.9284348836635735E+00	-.3449922634155065E+01	-.2439832523477966E+00	0.2343635742304627E+02
-.8272013150697650E+00	0.6341017949494823E+00	-.2035606965679834E+00	0.2052970256686051E+02
-.6872929048116855E+00	-.1619416300699971E+01	-.2159934769461259E+00	-.1376240462154258E+02
-.5152486363581541E+00	0.4959237125495822E+00	-.1075251867819710E+00	0.1455155616946274E+02
-.3191123689278897E+00	-.1038139679411058E+01	-.1196358314284132E+00	-.1125576720477356E+02
-.1080549487073437E+00	0.3511876142040904E+00	0.1088206509124769E-01	0.1005717417020061E+02
0.1080549487073437E+00	-.6752486832724772E+00	-.1913486054919796E-01	-.7774959517403008E+01
0.3191123689278897E+00	0.2161950693504096E+00	0.9038214134065220E-01	0.6382331406035814E+01
0.5152486363581541E+00	-.4027047889340547E+00	0.4482568706166883E-01	-.4626948764626759E+01
0.6872929048116855E+00	0.1014500308386035E+00	0.1047670461892695E+00	0.3365725647246004E+01
0.8272013150697650E+00	-.1896412777930365E+00	0.5616254115094882E-01	-.2045992407816295E+01
0.9284348836635735E+00	0.2050334687326519E-01	0.6074345322744063E-01	0.1083005671766590E+01
0.9862838086968123E+00	-.3560786461470516E-01	0.2130791084865406E-01	-.2941688960408355E+00

Table 1: 14-node quadratures of the form (75) – (77) for $y = -0.9862838086968123$ (see Example 5.1 and Remark 5.1).

N	1	$(y-x)^{-1}$	$\log(\|x-y\|)$	$(y-x)^{-2}$
36	0.560E-12	0.250E-13	0.420E-13	0.885E-15
42	0.257E-15	0.119E-14	0.225E-15	0.147E-13

Table 2: Relative errors of the quadrature formula (97) applied to the integrands (100), (101) – (103) (see Example 5.3).

N	1	$(y-x)^{-1}$	$\log(\|x-y\|)$	$(y-x)^{-2}$
36	0.114E-14	0.581E-02	0.108E-04	0.121E+00
42	0.700E-15	0.277E-02	0.427E-05	0.680E-01
100	0.775E-15	0.192E-05	0.112E-08	0.114E-03
150	0.333E-15	0.350E-08	0.133E-11	0.310E-06
200	0.196E-14	0.631E-11	0.188E-14	0.746E-09
250	0.262E-14	0.106E-13	0.551E-15	0.167E-11
300	0.269E-14	0.967E-15	0.568E-15	0.525E-14

Table 3: Relative errors of the standard Gaussian quadrature (see Theorem 2.9) applied to the integrands (100), (101) – (103) (see Example 5.3).

$\pm x_n$	w_n
0.1065589476527457E+00	0.2116935969670785E+00
0.3113548847160309E+00	0.1954154182193890E+00
0.4932817445063880E+00	0.1668941295018453E+00
0.6431876254991823E+00	0.1325004013421312E+00
0.7584402200373317E+00	0.9850855499442945E-01
0.8418072582807350E+00	0.6923612105413195E-01
0.8991123360358894E+00	0.4649700037042145E-01
0.9369451420922662E+00	0.3015693021568984E-01
0.9611808158857813E+00	0.1907410671190122E-01
0.9763813583671749E+00	0.1186194584542522E-01
0.9857845370872045E+00	0.7299783922072470E-02
0.9915537349540954E+00	0.4465717196444791E-02
0.9950772406715330E+00	0.2722792056317777E-02
0.9972224562334544E+00	0.1654307961017307E-02
0.9985216206191467E+00	0.9963611678876147E-03
0.9992964931862838E+00	0.5843631686022078E-03
0.9997376213125204E+00	0.3153728101867406E-03
0.9999525789657767E+00	0.1230964950065995E-03

Table 4: 36-node generalized Gaussian quadrature (97) for functions of the form (106) with $M = 11$, and precision 10^{-15} (see Example 5.3).

$\pm x_n$	w_n
0.7824400816570354E-01	0.1559838796617961E+00
0.2317400514932991E+00	0.1500543303602524E+00
0.3765817141635966E+00	0.1388302709124357E+00
0.5080234535636137E+00	0.1234870921831402E+00
0.6226938088738944E+00	0.1055618635285824E+00
0.7188418253624399E+00	0.8671614170628514E-01
0.7963343649196293E+00	0.6848351985661966E-01
0.8564163016327517E+00	0.5205731921370713E-01
0.9013001486524265E+00	0.3816842653276627E-01
0.9336896680922276E+00	0.2707608184111357E-01
0.9563457975135937E+00	0.1865610690150748E-01
0.9717714213532305E+00	0.1254153267525754E-01
0.9820411592483684E+00	0.8264234965377917E-02
0.9887573995032291E+00	0.5361830655763248E-02
0.9930900683346067E+00	0.3438177342595994E-02
0.9958561171201172E+00	0.2184437514815405E-02
0.9976063686147585E+00	0.1375256690097983E-02
0.9987019026654443E+00	0.8535706349265051E-03
0.9993734804740140E+00	0.5129451502696074E-03
0.9997640500479557E+00	0.2818251084208615E-03
0.9999571252163234E+00	0.1111565642688685E-03

Table 5: 42-node generalized Gaussian quadrature (97) for functions of the form (106) with $M = 21$, and precision 10^{-15} (see Example 5.3).

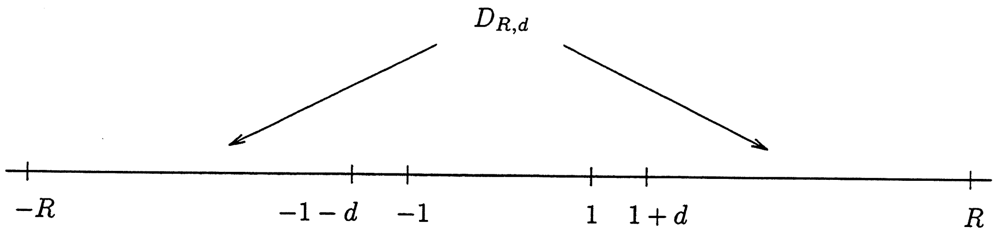

Figure 1: The set $D_{R,d}$.

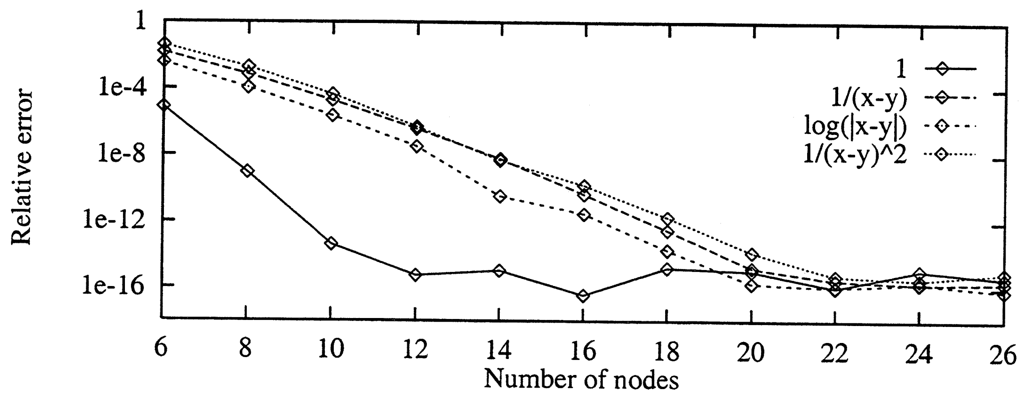

Figure 2: Relative errors of the quadrature formulae (75) – (77) with $N = 6, 8, \ldots, 26$ applied to the integrands (101) – (103) (see Example 5.1). The relative error of the N-point Gaussian quadratures with $N = 6, 8, \ldots, 26$ applied to the function (100) are presented for comparison.

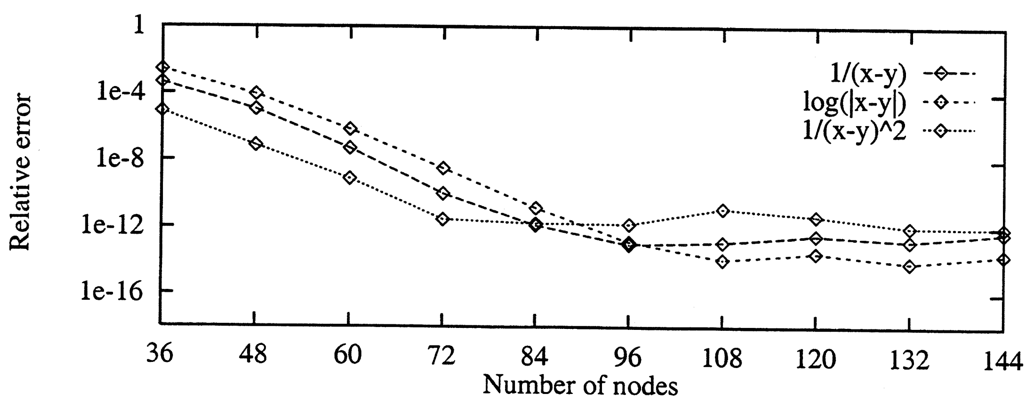

Figure 3: Relative errors of the quadrature formula (85) with $M = 6, 8, \ldots, 24$ and $N = 6 \cdot M$, applied to the integrands (101) – (103) (see Example 5.2).

K	degree 4	degree 6	degree 10	degree 12	degree 16
2	0.976E+00	0.105E+01	0.904E+01	0.372E+01	0.799E+01
4	0.109E+01	0.178E+01	0.998E+01	0.622E+01	0.325E+01
8	0.157E+01	0.226E+01	0.429E+01	0.239E+01	0.188E+01
16	0.215E+01	0.149E+01	0.212E+01	0.103E+01	0.788E+00
32	0.131E+01	0.103E+01	0.219E+00	0.483E-01	0.184E-02
64	0.556E+00	0.115E+00	0.194E-02	0.166E-02	0.368E-03
128	0.614E-01	0.285E-02	0.115E-05	0.126E-07	0.364E-09
256	0.442E-02	0.498E-04	0.133E-08	0.270E-09	0.693E-09
512	0.280E-03	0.778E-06	0.837E-09	0.476E-08	0.384E-08
1024	0.165E-04	0.125E-07	0.150E-08	0.149E-07	0.147E-07
2048	0.102E-05	0.271E-08	0.171E-07	0.293E-07	0.532E-07
4096	0.635E-07	0.231E-07	0.613E-07	0.921E-07	0.128E-06
8192	0.110E-07	0.113E-06	0.300E-06	0.134E-05	0.705E-06

Table 6: Relative errors of the compound quadrature formula of degrees $M = 4, 6, 10, 12, 16$ and the number of subintervals $K = 2, 4, \ldots, 8192$ applied to the integral (108) (see Example 5.4).

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