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HYBRID GAUSS-TRAPEZOIDAL QUADRATURE RULES*

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Abstract. A new class of quadrature rules for the integration of both regular and singular functions is constructed and analyzed. For each rule the quadrature weights are positive and the class includes rules of arbitrarily high-order convergence. The quadratures result from alterations to the trapezoidal rule, in which a small number of nodes and weights at the ends of the integration interval are replaced. The new nodes and weights are determined so that the asymptotic expansion of the resulting rule, provided by a generalization of the Euler–Maclaurin summation formula, has a prescribed number of vanishing terms. The superior performance of the rules is demonstrated with numerical examples and application to several problems is discussed.

Key words. Euler–Maclaurin formula, Gaussian quadrature, high-order convergence, numerical integration, positive weights, singularity

AMS subject classifications. 41A55, 41A60, 65B15, 65D32

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1. Introduction.

Recent advances in algorithms for the numerical solution of integral equations have stimulated renewed interest in integral equation formulations of problems in potential theory, wave propagation, and other application areas. Fast algorithms, including those by Rokhlin [1], [2], Greengard and Rokhlin [3], Hackbusch and Nowak [4], Beylkin, Coifman, and Rokhlin [5], Alpert, Beylkin, Coifman, and Rokhlin [6], and Kelley [7], have generally reduced the computational complexity to $O(n)$ or $O(n \log n)$ operations, with n unknowns, for the application of an integral operator or its inverse.

The appearance of these fast algorithms has increased the urgency of developing accurate quadratures for the discretization of integral operators. Such quadratures must effectively treat the kernel singularities of the operators and the varying location of the singularities with a fixed set of density nodes, and must allow the application of the fast algorithms. In this paper, we develop quadrature rules, based on alterations to the trapezoidal rule, that obey these constraints.

The well-known Euler–Maclaurin summation formula provides an asymptotic expansion for the trapezoidal rule applied to regular functions. While the constant term of the expansion is an integral, the other terms depend on the integrand's derivatives at the endpoints of the interval of integration. This expansion is often used to "correct" the trapezoidal rule to a quadrature with high-order convergence, through the use of either known derivative values or their finite-difference approximations. A generalization of the Euler–Maclaurin formula by Navot [8], for integrable functions with singularities of the form x^γ, can also be used to correct the trapezoidal rule to achieve high-order convergence (provided the exponent γ is known).

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We derive new quadratures, based on the Euler–Maclaurin formula and its generalization, of arbitrarily high-order convergence, for regular or singular functions with power or logarithm singularity. Each quadrature is constructed by changing the trapezoidal rule: a few of the nodes and weights at the interval endpoints are replaced with new nodes and weights determined so as to annihilate several terms in the asymptotic expansion. The nodes always lie within the interval of integration and the weights are always positive.

For a regular function $f : [0,1] \to \mathbb{R}$, we approximate $\int_0^1 f(x)\,dx$ with the quadrature

$$\begin{aligned}\tilde{T}_n(f) = h\Big[&w_1\, f(x_1 h) + w_2\, f(x_2 h) + \cdots + w_j\, f(x_j h)\\ &+ f(ah) + f(ah+h) + \cdots + f(1-ah)\\ &+ w_j\, f(1-x_j h) + \cdots + w_1\, f(1-x_1 h)\Big].\end{aligned} \tag{1}$$

There are n "internal" nodes with spacing $h = 1/(n+2a-1)$ and j "endpoint" nodes at each end, with the endpoint nodes $x_1, \ldots, x_j$ and weights $w_1, \ldots, w_j$ chosen so that the asymptotic expansion of $\tilde{T}_n$ as $n \to \infty$ has $2j$ vanishing terms and

$$\tilde{T}_n(f) = \int_0^1 f(x)\,dx + O(h^{2j+1}) \tag{2}$$

(Theorem 3.1 and Corollary 3.2). The parameters a and j, and the nodes $x_1, \ldots, x_j$ and weights $w_1, \ldots, w_j$, are independent of n. The nodes and weights are determined by $2j$ nonlinear equations, which have a unique solution, with

$$0 < x_i < a, \quad w_i > 0, \qquad i = 1, \ldots, j, \tag{3}$$

provided a is sufficiently large (Theorem 4.7). For integrands that are singular at one endpoint, $\tilde{T}_n$ is altered so that the nodes and weights at that end differ from those at the other end and depend on the singularity (Theorem 3.4 and Corollary 3.6; Theorem 3.7 and Corollary 3.8). For improper integrals in which the integrand is oscillatory and slowly decaying, $\tilde{T}_n$ is combined with Gauss–Laguerre quadrature to give rules with high-order convergence (Theorem 3.9 and Corollary 3.10).

Several authors have studied the problems treated here. It has been observed that endpoint corrections can be derived for singular integrands; Rokhlin [9] implemented such a scheme for integrands with a known singularity at an interval endpoint. He derived corrections to the trapezoidal rule by placing additional quadrature nodes near the endpoint, with the corresponding weights determined so that low-order polynomials and the singularity times low-order polynomials were integrated exactly. He showed that under fairly general conditions, these weights had limiting values (up to scale) as the number of nodes in the trapezoidal rule increased without bound and that these limiting weights could be used to form quadrature rules with good convergence. Unfortunately, the order of convergence of these rules is restricted in practice by the fact that the weights increase in magnitude rapidly as the order increases. Efforts by Starr [10] and subsequently by Alpert [11] reduced the growth in size of the weights with order, primarily by using more weights than the number of equations satisfied and minimizing their sum of squares. In another approach, Kress [12] uses all quadrature weights in the quadrature rule, rather than a few near the endpoints, to handle the singularity. More recently, Kapur and Rokhlin [13] successfully constructed rules of arbitrary order by separating the integrand's regular and singular parts and allowing some quadrature nodes to lie outside the interval of integration.

The present approach does not suffer from limitations on order of convergence, separation of the integrand into parts, or quadrature nodes outside the interval of convergence. On the other hand, the quadrature nodes near the interval endpoints are not equispaced. Also, the equations for the nodes $x_1, \ldots, x_j$ and weights $w_1, \ldots, w_j$, in addition to being nonlinear, are poorly conditioned; the conditioning deteriorates rapidly with increasing order. Nevertheless, we are able to use an algorithm developed recently by Ma, Rokhlin, and Wandzura [14] for computing generalized Gaussian quadratures to obtain accurate quadrature nodes and weights. The author would also like to credit that paper for inspiring the present work.

The paper is organized around section 3, where the new asymptotic expansions are derived and the quadratures defined, and section 4, where it is shown that the equations defining the quadratures actually have solutions, which are unique. These sections are preceded by mathematical preliminaries and followed by a discussion of the computation of the quadrature nodes and weights. Numerical examples are presented in section 6 and we conclude with some applications and a summary.

2. Mathematical preliminaries. The material in this section, which is found in standard references, is used in the subsequent development.

2.1. Bernoulli polynomials. The Bernoulli polynomials are defined by generating function (see, for example, [15, (23.1.1)])

$$\frac{t\,e^{xt}}{e^t - 1} = \sum_{n=0}^{\infty} B_n(x)\,\frac{t^n}{n!}$$

from which

$$B_0(x) = 1, \quad B_1(x) = x - \frac{1}{2}, \quad B_2(x) = x^2 - x + \frac{1}{6}, \quad B_3(x) = x^3 - \frac{3}{2}x^2 + \frac{1}{2}x.$$

The Bernoulli polynomials satisfy the difference formula

$$\frac{B_n(x+k) - B_n(x)}{n} = \sum_{i=0}^{k-1} (x+i)^{n-1}, \qquad n = 1, 2, \ldots, \tag{4}$$

the differentiation formula

$$B_n'(x) = n\,B_{n-1}(x), \qquad n = 1, 2, \ldots, \tag{5}$$

and the expansion formula

$$B_n(x+h) = \sum_{r=0}^{n} \binom{n}{r} B_r(x)\,h^{n-r}, \qquad n = 0, 1, \ldots. \tag{6}$$

2.2. Euler–Maclaurin summation formula. For a function $f \in C^p(\mathbb{R})$, $p \geq 1$, the Euler–Maclaurin summation formula (see, for example, [15, (23.1.30)]) can be derived by repeated integration by parts. We first consider the interval $[c, c+h]$ and apply (5) to obtain

$$\begin{aligned}
(7)\qquad \int_c^{c+h} f(x)\,dx &= h\int_0^1 B_0(1-x)\,f(c+xh)\,dx \\
&= -h\frac{B_1(1-x)}{1!}\,f(c+xh)\Big|_0^1 + h^2\int_0^1 \frac{B_1(1-x)}{1!}\,f'(c+xh)\,dx \\
&\quad\vdots \\
&= -\sum_{r=0}^{p-1} \frac{h^{r+1}\,B_{r+1}(1-x)}{(r+1)!}\,f^{(r)}(c+xh)\Big|_0^1 \\
&\qquad + h^{p+1}\int_0^1 \frac{B_p(1-x)}{p!}\,f^{(p)}(c+xh)\,dx \\
&= h\,\frac{f(c)+f(c+h)}{2} - \sum_{r=1}^{p-1}\frac{h^{r+1}\,B_{r+1}}{(r+1)!}\left[f^{(r)}(c+h)-f^{(r)}(c)\right] \\
&\qquad + h^{p+1}\int_0^1 \frac{B_p(1-x)}{p!}\,f^{(p)}(c+xh)\,dx,
\end{aligned}$$

where we have used

$$\begin{aligned}
-B_1(0) = B_1(1) &= \frac{1}{2}, \\
B_n(0) = B_n(1) &= B_n, \qquad n \neq 1.
\end{aligned}$$

To derive the Euler–Maclaurin formula for the interval $[a,b]$, we let $h = (b-a)/n$ and $c = a + ih$ in (7), sum over $i = 0, 1, \ldots, n-1$, and rearrange terms to obtain

$$\begin{aligned}
(8)\qquad & h\left[\frac{f(a)}{2} + f(a+h) + \cdots + f(b-h) + \frac{f(b)}{2}\right] \\
&= \int_a^b f(x)\,dx + \sum_{r=1}^{p-1}\frac{h^{r+1}B_{r+1}}{(r+1)!}\left[f^{(r)}(b)-f^{(r)}(a)\right] \\
&\qquad - h^{p+1}\int_0^1 \frac{B_p(1-x)}{p!}\left\{\sum_{i=0}^{n-1} f^{(p)}(a+ih+xh)\right\}dx.
\end{aligned}$$

The expression on the left-hand side of (8) is the well-known trapezoidal rule. Evaluation of the expression on the right-hand side of (8) is simplified by the fact that $B_{2r+1} = 0$ for $r \geq 1$.

2.3. Generalized Riemann zeta-function. The generalized Riemann zeta-function is defined by the formula

$$\zeta(s,v) = \sum_{n=0}^{\infty} \frac{1}{(v+n)^s}, \qquad \mathrm{Re}(s) > 1, \quad v \neq 0, -1, \ldots.$$

This function has a continuation that is analytic in the entire complex s-plane, with the exception of $s = 1$, where it has a simple pole. In what follows, we shall be concerned primarily with real s and v, with $s < 1$ and $v > 0$. We will use the following representation derived from Plana's summation formula (see, for example, [16, section 1.10 (7)]):

$$\zeta(s,v) = \frac{v^{1-s}}{s-1} + \frac{v^{-s}}{2} + 2v^{1-s}\int_0^\infty \frac{\sin(s\arctan t)}{(1+t^2)^{s/2}}\frac{dt}{e^{2\pi vt}-1}, \qquad \mathrm{Re}(v) > 0. \tag{9}$$

Equation (9) can be used to derive the asymptotic expansion of ζ as $v \to \infty$. We treat the integral as a sum of Laplace integrals, each with an asymptotic expansion given by Watson's lemma (see, for example, [17, p. 263]), and obtain

$$\zeta(s,v) = \frac{v^{1-s}}{s-1} + \frac{v^{-s}}{2} + \frac{1}{s-1}\sum_{r=1}^{p}\binom{s+2r-2}{2r}\frac{B_{2r}}{v^{s+2r-1}} + O(v^{-s-2p-1}), \tag{10}$$

as $v \to \infty$, with $s \in \mathbb{C}$, $s \neq 1$, and p an arbitrary positive integer. Equation (10) is a slight generalization of [16, section 1.18 (9)]. There is a direct connection between the Bernoulli polynomials and ζ,

$$\frac{B_n(x)}{n} = -\zeta(1-n,x), \qquad n = 1,2,\dots,$$

and generalizations of the difference and differentiation formulae hold:

$$\zeta(s,v) - \zeta(s,v+k) = \sum_{i=0}^{k-1}\frac{1}{(v+i)^s}, \tag{11}$$

$$\frac{\partial\zeta(s,v)}{\partial v} = -s\,\zeta(s+1,v). \tag{12}$$

2.4. Orthogonal polynomials and Gaussian quadrature. Suppose that ω is a positive continuous function on the interval (a,b) and ω is integrable on $[a,b]$. We define the inner product with respect to ω of real-valued functions f and g by the integral

$$(f,g) = \int_a^b f(x)\,g(x)\,\omega(x)\,dx.$$

There exist polynomials $p_0, p_1, \dots,$ of degree $0, 1, \dots,$ respectively, such that $(p_n, p_m) = 0$ for $n \neq m$ (orthogonality); they are unique up to the choice of leading coefficients. With leading coefficients one, they can be obtained recursively by the formulae (see, for example, [18, p. 143])

$$p_0(x) = 1, \tag{13}$$

$$p_{n+1}(x) = (x - \delta_{n+1})\,p_n(x) - {\gamma_{n+1}}^2\,p_{n-1}(x), \qquad n \geq 0, \tag{14}$$

where $p_{-1}(x) = 0$ and δ_n, γ_n are defined by the formulae

$$\delta_{n+1} = (xp_n, p_n)/(p_n, p_n), \qquad n \geq 0,$$

$${\gamma_{n+1}}^2 = \begin{cases} 0, & n = 0, \\ (p_n,p_n)/(p_{n-1},p_{n-1}), & n \geq 1. \end{cases}$$

The zeros $x_1^n, \dots, x_n^n$ of p_n are distinct and lie in the interval (a,b). There exist positive numbers $\omega_1^n, \dots, \omega_n^n$ such that

$$\int_a^b f(x)\,\omega(x)\,dx = \sum_{i=1}^{n}\omega_i^n\,f(x_i^n) \tag{15}$$

whenever f is a polynomial of degree less than $2n$. These *Christoffel numbers* are given by the formula (see, for example, [19, p. 48])

$$\omega_i^n = \frac{(p_{n-1}, p_{n-1})}{p_{n-1}(x_i^n)\, p_n'(x_i^n)}, \qquad i = 1, \dots, n. \tag{16}$$

Moreover, if $\omega(x) = (b - x)\,\tau(x)$ with τ integrable on $[a, b]$, then, with the definition $x_{n+1}^n = b$, there exist positive numbers $\tau_1^n, \dots, \tau_{n+1}^n$ such that

$$\int_a^b f(x)\,\tau(x)\,dx = \sum_{i=1}^{n+1} \tau_i^n\, f(x_i^n) \tag{17}$$

whenever f is a polynomial of degree less than or equal to $2n$. These modified Christoffel numbers are given by the formula

$$\tau_i^n = \begin{cases} \dfrac{\omega_i^n}{b - x_i^n}, & i = 1, \dots, n, \\ \displaystyle\int_a^b \frac{p_n(x)}{p_n(b)}\,\tau(x)\,dx, & i = n+1, \end{cases} \tag{18}$$

where ω_i^n is given by (16).

The summation in (15) is the n-node Gaussian quadrature with respect to ω, while that in (17) is an $(n + 1)$-node Gauss–Radau quadrature with respect to τ.

3. Hybrid Gauss-trapezoidal quadrature rules. In this section we introduce new quadrature rules for regular integrands, singular integrands with a power or logarithmic singularity, and improper integrals and determine their rate of convergence as the number of quadrature nodes increases.

For notational convenience we generally consider quadratures on canonical intervals, primarily $[0, 1]$. It is understood that these are readily transformed to quadratures on any finite interval $[a, b]$ by the appropriate linear transformation of the nodes and weights.

3.1. Regular integrands. For j, n positive integers and $a \in \mathbb{R}^+ = \{x \in \mathbb{R} | \, x > 0\}$, we define a linear operator T_n^{ja} on $C([0, 1])$, depending on nodes $x_1, \dots, x_j$ and weights $w_1, \dots, w_j$, by the formula

$$T_n^{ja}(f) = h \sum_{i=1}^{j} w_i\, f(x_i h) + h \sum_{i=0}^{n-1} f(ah + ih) + h \sum_{i=1}^{j} w_i\, f(1 - x_i h), \tag{19}$$

where $h = (n + 2a - 1)^{-1}$ is chosen so that $ah + (n - 1)h = 1 - ah$.

THEOREM 3.1. *Suppose $f \in C^p([0, 1])$. The asymptotic expansion of $T_n^{ja}(f)$ as $n \to \infty$ is given by the formula*

$$T_n^{ja}(f) = \int_0^1 f(x)\,dx + \sum_{r=0}^{p-1} h^{r+1} \frac{f^{(r)}(0) + (-1)^r f^{(r)}(1)}{r!} \left\{ \sum_{i=1}^{j} w_i\, {x_i}^r - \frac{B_{r+1}(a)}{r+1} \right\} + O(h^{p+1}). \tag{20}$$

Proof. We apply the Euler–Maclaurin formula (8) on the interval $[ah, 1-ah]$ to obtain

$$h\sum_{i=0}^{n-1} f(ah+ih) = h\,\frac{f(ah)+f(1-ah)}{2} + \int_{ah}^{1-ah} f(x)\,dx + \sum_{r=1}^{p-1} \frac{h^{r+1}B_{r+1}}{(r+1)!}\left[f^{(r)}(1-ah) - f^{(r)}(ah)\right] + O(h^{p+1}). \tag{21}$$

We now combine (19) and (21), the equality

$$\int_{ah}^{1-ah} f(x)\,dx = \int_0^1 f(x)\,dx - \int_0^{ah} f(x)\,dx - \int_{1-ah}^{1} f(x)\,dx,$$

Taylor expansion of all quantities about $h=0$, the Bernoulli polynomial expansion formula (6), and difference formula (4) to obtain (20). ∎

COROLLARY 3.2. *Suppose the nodes $x_1,\ldots,x_j$ and weights $w_1,\ldots,w_j$ satisfy the equations*

$$\sum_{i=1}^{j} w_i\, {x_i}^r = \frac{B_{r+1}(a)}{r+1}, \qquad r = 0,1,\ldots,2j-1. \tag{22}$$

Then T_n^{ja} is a quadrature rule with convergence of order $2j+1$ for $f \in C^p([0,1])$ with $p \geq 2j$. Moreover,

$$T_n^{ja}(f) - \int_0^1 f(x)\,dx \sim h^{2j+1}\frac{f^{(2j)}(0)+f^{(2j)}(1)}{(2j)!}\left\{\sum_{i=1}^{j} w_i\,{x_i}^{2j} - \frac{B_{2j+1}(a)}{2j+1}\right\} \tag{23}$$

as $n\to\infty$, provided $f^{(2j)}(0)+f^{(2j)}(1) \neq 0$.

COROLLARY 3.3. *Suppose $x_j = a-1$ and the remaining nodes $x_1,\ldots,x_{j-1}$ and weights $w_1,\ldots,w_j$ satisfy the equations*

$$\sum_{i=1}^{j} w_i\, {x_i}^r = \frac{B_{r+1}(a)}{r+1}, \qquad r = 0,1,\ldots,2j-2. \tag{24}$$

Then T_n^{ja} is a quadrature rule with convergence of order $2j$ for $f \in C^p([0,1])$ with $p \geq 2j-1$. Moreover,

$$T_n^{ja}(f) - \int_0^1 f(x)\,dx \sim h^{2j}\frac{f^{(2j-1)}(0)-f^{(2j-1)}(1)}{(2j-1)!}\left\{\sum_{i=1}^{j} w_i\,{x_i}^{2j-1} - \frac{B_{2j}(a)}{2j}\right\} \tag{25}$$

as $n\to\infty$, provided $f^{(2j-1)}(0)-f^{(2j-1)}(1) \neq 0$.

We shall see below that (22) has a solution with the nodes and weights all positive if a is sufficiently large and that numerical solution of (22) is equivalent to computing the roots of a particular polynomial. This statement holds for (24) as well.

3.2. Singular integrands. For j,k,n positive integers and $a,b\in\mathbb{R}^+$, we define a linear operator S_n^{jkab} on $C((0,1])$, depending on nodes $v_1,\ldots,v_j,x_1,\ldots,x_k$ and weights $u_1,\ldots,u_j,w_1,\ldots,w_k$, by the formula

$$S_n^{jkab}(g) = h\sum_{i=1}^{j} u_i\,g(v_ih) + h\sum_{i=0}^{n-1} g(ah+ih) + h\sum_{i=1}^{k} w_i\,g(1-x_ih), \tag{26}$$

where $h = (n + a + b - 1)^{-1}$ is chosen so that $ah + (n - 1)h = 1 - bh$. The following theorem, which follows from a generalization of the Euler–Maclaurin formula due to Navot [8] or a further generalization due to Lyness [20], presents a somewhat different proof than the earlier ones.

THEOREM 3.4. *Suppose $g(x) = x^\gamma f(x)$, where $\gamma > -1$ and $f \in C^p([0, 1])$. The asymptotic expansion of $S_n^{jkab}(g)$ as $n \to \infty$ is given by the formula*

$$\begin{aligned} S_n^{jkab}(g) = \int_0^1 g(x)\,dx &+ \sum_{r=0}^{p-1} h^{\gamma+r+1} \frac{f^{(r)}(0)}{r!} \left\{ \sum_{i=1}^{j} u_i\, {v_i}^{\gamma+r} + \zeta(-\gamma - r, a) \right\} \\ &+ \sum_{r=0}^{p-1} h^{r+1} \frac{(-1)^r\, g^{(r)}(1)}{r!} \left\{ \sum_{i=1}^{k} w_i\, {x_i}^r - \frac{B_{r+1}(b)}{r + 1} \right\} + O(h^{p+1+\min\{0,\gamma\}}). \end{aligned} \tag{27}$$

Proof. For $c \in \mathbb{R}^+$, we define polynomials $p_0^c, p_1^c, \ldots,$ in analogy with the Bernoulli polynomials, by the formula

$$p_n^c(x) = \sum_{r=0}^{n} \binom{n}{r} \zeta(-\gamma - r, c)\, (1 - c - x)^{n-r}. \tag{28}$$

Differentiating, we verify that

$$\frac{d}{dx} p_n^c(x) = -n\, p_{n-1}^c(x), \qquad n = 1, 2, \ldots$$

and, combining the ζ difference formula (11) with (28), we obtain

$$p_n^c(1) - p_n^{c+1}(0) = \begin{cases} c^\gamma, & n = 0, \\ 0, & n \geq 1. \end{cases}$$

Additionally, we define functions $q_0^c, q_1^c, \ldots$ by the formula

$$q_n^c(x) = \begin{cases} (x + c)^\gamma, & n = 0, \\ \dfrac{(-1)^n (x + c)^{\gamma+n}}{(\gamma + 1) \cdots (\gamma + n)} - \dfrac{p_{n-1}^{c+1}(x)}{(n - 1)!}, & n = 1, 2, \ldots\,, \end{cases} \tag{29}$$

and observe that

$$\frac{d}{dx} q_n^c(x) = -q_{n-1}^c(x), \qquad n = 1, 2, \ldots\,.$$

With these definitions, the proof follows that of the Euler–Maclaurin formula:

$$
\begin{aligned}
(30)\qquad \int_{ah}^{1-bh} x^\gamma f(x)\,dx &= \sum_{i=0}^{n-2} h^{1+\gamma}\int_0^1 q_0^{a+i}(x)\, f(ah+ih+xh)\,dx \\
&= \sum_{i=0}^{n-2}\Bigg\{ -\sum_{r=0}^{p-1} h^{\gamma+r+1} q_{r+1}^{a+i}(x)\, f^{(r)}(ah+ih+xh)\Bigg|_0^1 \\
&\qquad + h^{\gamma+p+1}\int_0^1 q_p^{a+i}(x)\, f^{(p)}(ah+ih+xh)\,dx\Bigg\} \\
&= h\sum_{i=1}^{n-2}(ah+ih)^\gamma f(ah+ih) \\
&\quad - \sum_{r=0}^{p-1} h^{\gamma+r+1}\left[q_{r+1}^{a+n-2}(1) f^{(r)}(1-bh) - q_{r+1}^{a}(0) f^{(r)}(ah)\right] \\
&\quad + h^{\gamma+p+1}\int_0^1 \left\{\sum_{i=0}^{n-2} q_p^{a+i}(x) f^{(p)}(ah+ih+xh)\right\}dx.
\end{aligned}
$$

Taylor expansion of $f^{(r)}(ah)$ about $h=0$, the definitions (28) and (29) for p_n^c and q_n^c, and the binomial theorem combine to yield

$$
\begin{aligned}
(31)\qquad &\sum_{r=0}^{p-1} h^{\gamma+r+1} q_{r+1}^{a}(0)\, f^{(r)}(ah) \\
&\quad = -\sum_{k=0}^{p-1}\frac{h^{\gamma+k+1} f^{(k)}(0)}{k!}\left[\frac{a^{\gamma+k+1}}{\gamma+k+1} + \zeta(-\gamma-k, a+1)\right] + O(h^{\gamma+p+1}).
\end{aligned}
$$

Likewise, Taylor expansion of $f^{(r)}(1-bh)$ about $h=0$, the definitions for p_n^c and q_n^c, the asymptotic expansion (10) for ζ, the Bernoulli polynomial expansion formula (6), and the binomial theorem combine to yield

$$
\begin{aligned}
(32)\qquad &\sum_{r=0}^{p-1} h^{\gamma+r+1} q_{r+1}^{a+n-2}(1)\, f^{(r)}(1-bh) \\
&\quad = \sum_{k=0}^{p-1}\frac{h^{k+1}(-1)^k g^{(k)}(1)}{k!}\left[\frac{b^{k+1}}{k+1} - \frac{B_{k+1}(b+1)}{k+1}\right] + O(h^{p+1}).
\end{aligned}
$$

We now combine (26) and (30)–(32), the equality

$$
\int_{ah}^{1-bh} g(x)\,dx = \int_0^1 g(x)\,dx - \int_0^{ah} g(x)\,dx - \int_{1-bh}^1 g(x)\,dx,
$$

expansion of the latter two integrals about $h=0$, and the difference formula (4) for the Bernoulli polynomials and (11) for ζ to obtain (27). ∎

COROLLARY 3.5. *Suppose the nodes $u_1,\dots,u_j$ and weights $v_1,\dots,v_j$ satisfy the equations*

$$
(33)\qquad \sum_{i=1}^{j} u_i\, {v_i}^{\gamma+r} = -\zeta(-\gamma-r, a), \qquad r = 0,1,\dots,2j-1,
$$

and the nodes $x_1, \dots, x_j$ and weights $w_1, \dots, w_j$ satisfy the equations

$$\sum_{i=1}^{j} w_i\, {x_i}^r = \frac{B_{r+1}(b)}{r+1}, \qquad r = 0, 1, \dots, 2j-1. \tag{34}$$

Then S_n^{jjab} is a quadrature rule with convergence of order $2j+1+\min\{0,\gamma\}$ for g, where $g(x) = x^\gamma f(x)$, with $f \in C^p([0,1])$ and $p \ge 2j$. Moreover,

$$S_n^{jjab}(g) - \int_0^1 g(x)\,dx \sim \begin{cases} h^{\gamma+2j+1} \dfrac{f^{(2j)}(0)}{(2j)!} \left\{ \displaystyle\sum_{i=1}^{j} u_i\, {v_i}^{\gamma+2j} + \zeta(-\gamma-2j, a) \right\}, & \gamma < 0,\ f^{(2j)}(0) \ne 0, \\ h^{2j+1} \dfrac{g^{(2j)}(1)}{(2j)!} \left\{ \displaystyle\sum_{i=1}^{j} w_i\, {x_i}^{2j} - \frac{B_{2j+1}(b)}{2j+1} \right\}, & \gamma > 0,\ g^{(2j)}(1) \ne 0, \end{cases} \tag{35}$$

as $n \to \infty$.

Corollary 3.6. *Suppose the nodes $u_1, \dots, u_j$ and weights $v_1, \dots, v_j$ satisfy the equations*

$$\begin{aligned} \sum_{i=1}^{j} u_i\, {v_i}^{\gamma+r} &= -\zeta(-\gamma-r, a), \qquad r = 0, 1, \dots, j-1, \\ \sum_{i=1}^{j} u_i\, {v_i}^{r} &= \frac{B_{r+1}(a)}{r+1}, \qquad r = 0, 1, \dots, j-1, \end{aligned} \tag{36}$$

and the nodes $x_1, \dots, x_k$ and weights $w_1, \dots, w_k$ satisfy the equations

$$\sum_{i=1}^{k} w_i\, {x_i}^r = \frac{B_{r+1}(b)}{r+1}, \qquad r = 0, 1, \dots, 2k-1. \tag{37}$$

Then S_n^{jkab} is a quadrature rule with convergence of order $\min\{j+1, \gamma+j+1, 2k+1\}$ for g, where $g(x) = x^\gamma \phi(x) + \psi(x)$, with $\phi, \psi \in C^p([0,1])$ and $p \ge \min\{j, 2k\}$.

In Corollaries 3.5 and 3.6, an even number of constraints on the nodes and weights at both ends of the interval are considered. Clearly, there are analogous quadrature rules arising from an odd number of constraints at one or both ends; these are similar, and explicit presentation of them is omitted. We now consider a different type of singularity.

Theorem 3.7. *Suppose $g(x) = f(x)\log x$, where $f \in C^p([0,1])$. The asymptotic expansion of $S_n^{jkab}(g)$ as $n \to \infty$ is given by the formula*

$$\begin{aligned} S_n^{jkab}(g) &= \int_0^1 g(x)\,dx \\ &+ \sum_{r=0}^{p-1} h^{r+1} \frac{f^{(r)}(0)}{r!} \left\{ \sum_{i=1}^{j} u_i\, {v_i}^r \log(v_j h) - \zeta'(-r, a) - \frac{B_{r+1}(a)}{r+1} \log h \right\} \\ &+ \sum_{r=0}^{p-1} h^{r+1} \frac{(-1)^r g^{(r)}(1)}{r!} \left\{ \sum_{i=1}^{k} w_i\, {x_i}^r - \frac{B_{r+1}(b)}{r+1} \right\} + O(h^{p+1}\log h), \end{aligned} \tag{38}$$

where ζ' denotes the derivative of ζ with respect to its first argument.

Proof. This asymptotic expansion is derived from that of Theorem 3.4 by differentiating (27) with respect to γ and evaluating the result at $\gamma = 0$. ∎

COROLLARY 3.8. *Suppose the nodes $u_1, \dots, u_j$ and weights $v_1, \dots, v_j$ satisfy the equations*

$$\sum_{i=1}^{j} u_i\, {v_i}^r \log v_i = \zeta'(-r, a), \qquad r = 0, 1, \dots, j-1,$$
$$\sum_{i=1}^{j} u_i\, {v_i}^r = \frac{B_{r+1}(a)}{r+1}, \qquad r = 0, 1, \dots, j-1, \tag{39}$$

and the nodes $x_1, \dots, x_k$ and weights $w_1, \dots, w_k$ satisfy the equations

$$\sum_{i=1}^{k} w_i\, {x_i}^r = \frac{B_{r+1}(b)}{r+1}, \qquad r = 0, 1, \dots, 2k-1. \tag{40}$$

Then S_n^{jkab} is a quadrature rule with error of order $O(\min\{h^{j+1}\log h, h^{2k+1}\})$ for g, where $g(x) = \phi(x)\log x + \psi(x)$, with $\phi, \psi \in C^p([0,1])$ and $p \geq \min\{j, 2k\}$.

3.3. Improper integrals. For j, n positive integers, we define a linear operator R_n^j on $C([n,\infty))$, depending on nodes $x_1, \dots, x_j$ and weights $w_1, \dots, w_j$, by the formula

$$R_n^j(g) = \sum_{k=1}^{j} w_k\, g(n + x_k). \tag{41}$$

THEOREM 3.9. *Suppose $g(x) = e^{i\gamma x} f(x)$, where $\gamma \in \mathbb{R}, \gamma \neq 0$, and $f \in C^p([1,\infty))$, and that there exist positive constants β, $\alpha_0, \dots, \alpha_p$, such that*

$$\left|f^{(r)}(x)\right| < \frac{\alpha_r}{x^{\beta+r}} \quad \text{for } x > 1, \qquad r = 0, \dots, p. \tag{42}$$

The asymptotic expansion of $R_n^j(g)$ as $n \to \infty$ is given by the formula

$$R_n^j(g) = \int_n^\infty g(x)\,dx + e^{i\gamma n}\sum_{r=0}^{p-1}\frac{f^{(r)}(n)}{r!}\left\{\sum_{k=1}^{j} w_k\, {x_k}^r\, e^{i\gamma x_k} - r!\left(\frac{i}{\gamma}\right)^{r+1}\right\} + O(n^{-p}). \tag{43}$$

Proof. We integrate by parts repeatedly to obtain

$$\int_n^\infty e^{i\gamma x} f(x)\,dx = e^{i\gamma n}\sum_{r=0}^{p-1}\left(\frac{i}{\gamma}\right)^{r+1} f^{(r)}(n) + \int_n^\infty e^{i\gamma x}\left(\frac{i}{\gamma}\right)^p f^{(p)}(x)\,dx, \tag{44}$$

and in (41) we compute the Taylor expansion of f about $x_k = 0$ to get

$$R_n^j(g) = e^{i\gamma n}\sum_{k=1}^{j} e^{i\gamma x_k} w_k \left\{\sum_{r=0}^{p-1}\frac{f^{(r)}(n)}{r!}{x_k}^r + \frac{f^{(p)}(n+\xi_i k)}{p!}{x_k}^p\right\}, \tag{45}$$

where ξ_k lies between 0 and x_k for $k = 1, \dots, j$. Now combining (42), (44), and (45), we obtain (43). □

Example. The function f defined by the formula

$$f(x) = \sum_{r=0}^{\infty} \frac{a_r}{x^{\beta+r}}, \tag{46}$$

with $\sum |a_r| < \infty$, satisfies the assumptions of Theorem 3.9 for every positive integer p. We remark that Theorem 3.9 can, in some instances, be generalized to $\gamma = 0$, but the corresponding asymptotic expansion depends on a more detailed knowledge of f. For f given by (46), for example, the quadrature nodes and weights for $\gamma = 0$ depend on β.

COROLLARY 3.10. *Suppose $f \in C^p([1, \infty))$, f satisfies* (42) *for $x \in \mathbb{R}$, and f is analytic in the half-plane* $\mathrm{Re}(x) > a$ *for some $a \in \mathbb{R}$. Suppose further that $v_1, \dots, v_j$ are the roots of the Laguerre polynomial L_j of degree j, that coefficients $u_1, \dots, u_j$ satisfy the equations*

$$\sum_{k=1}^{j} u_k {v_k}^r e^{-v_k} = r!, \qquad r = 0, 1, \dots, j-1, \tag{47}$$

and that the operator R_n^j is defined with nodes $x_k = (i/\gamma)v_k$ and weights $w_k = (i/\gamma)u_k$ for $k = 1, \dots, j$. Suppose finally that $\hat{T}_m^{ja}$ is defined to be the quadrature rule T_m^{ja} with nodes and weights satisfying (22) *but translated and scaled to the interval* $[1, n]$. *Then for $p \geq 2j$, the expression $\hat{T}_{(n-1)n}^{ja}(g) + R_n^j(g)$ is an approximation for the integral $\int_1^\infty g(x)\,dx$, where $g(x) = e^{i\gamma x} f(x)$, with error of order $O(n^{-2j})$ as $n \to \infty$.*

Proof. This result is just a combination of the quadrature rule of Corollary 3.2, for the interval $[1, n]$, with the asymptotic expansion of Theorem 3.9, for the interval $[n, \infty)$, provided

$$\sum_{k=1}^{j} u_k {v_k}^r e^{-v_k} = r!, \qquad r = 0, 1, \dots, 2j-1. \tag{48}$$

But (48) follows from (47), the equations

$$r! = \int_0^\infty x^r e^{-x}\,dx, \qquad r = 0, 1, \dots,$$

$$\int_0^\infty L_j(x)\, L_k(x)\, e^{-x}\,dx = 0 \quad \text{for } j \neq k,$$

(see, for example, [15, (6.1.1) and (22.2.13)]), and the fact that Gaussian quadratures, which are exact for polynomials of degree less than twice the number of nodes, have nodes that coincide with the roots of the corresponding orthogonal polynomials (see section 2.4). □

We have completed the *definition* of the new quadratures, along with the demonstration of their asymptotic performance. We shall see that the *existence* of these rules, which depends on the solvability of the nonlinear systems of equations that define the nodes and weights, is assured by the theory of Chebyshev systems. The *uniqueness* of the rules is similarly assured. These issues of existence and uniqueness are treated next.

4. Existence and uniqueness.

4.1. Chebyshev systems. Material of this subsection is taken, with minor alterations, from Karlin and Studden [21]. Suppose I is an interval of $\mathbb{R}$, possibly infinite. A collection of n real-valued continuous functions $f_1, \dots, f_n$ defined on I is a *Chebyshev system* if any linear combination

$$f(x) = \sum_{i=1}^{n} a_i f_i(x),$$

with a_i not all zero, has at most $n-1$ zeros on I. This condition is equivalent to the statement that for distinct $x_1, \dots, x_n$ in I,

$$\det \begin{pmatrix} f_1(x_1) & \cdots & f_n(x_1) \\ \vdots & \ddots & \vdots \\ f_1(x_n) & \cdots & f_n(x_n) \end{pmatrix} \neq 0. \tag{49}$$

The Chebyshev property is a characteristic of the space, rather than the basis: if $f_1, \dots, f_n$ is a Chebyshev system, then so is any other basis of $\operatorname{span}\{f_1, \dots, f_n\}$. If u is a continuous, positive function on I, then scaling by u preserves a Chebyshev system. Finally, if u is strictly increasing and continuous on interval J with range I, then $f_1 \circ u, \dots, f_n \circ u$ is a Chebyshev system on J if and only if $f_1, \dots, f_n$ is on I. (Here $f_i \circ u$ denotes the composition u followed by f_i.)

The best-known example of a Chebyshev system is the set of polynomials

$$1, x, \dots, x^{n-1}$$

on any interval $I \subset \mathbb{R}$. We shall be concerned also with the Chebyshev systems

$$1, x^{\gamma}, x, x^{\gamma+1}, \dots, x^{(n-1)/2}, x^{\gamma+(n-1)/2},$$
$$1, \log x, x, x \log x, \dots, x^{(n-1)/2}, x^{(n-1)/2} \log x$$

on $I = (0, a]$, where $\gamma \in \mathbb{R} \backslash \mathbb{Z}$ and $a > 0$. These systems are special cases of the system of *Müntz functions* (see, for example, [22, p. 133])

$$M = \left\{ x^{\gamma_i} \log^k x \,\middle|\, k = 0, \dots, n_i - 1,\ i = 1, \dots, j \right\} \tag{50}$$

on $I = (0, \infty)$, where $\gamma_1, \dots, \gamma_j$ are distinct real numbers and $n_1, \dots, n_j$ are positive integers with $\sum n_i = n$. To see this is a Chebyshev system, suppose $f \in \operatorname{span} M$ and use induction in n on $(d/d \log x)[f(x)\, x^{-\gamma_j}]$, in combination with Rolle's theorem. Another Chebyshev system that will arise is the system

$$L = \left\{ (x + \gamma_i)^{-k} \,\middle|\, k = 1, \dots, n_i,\ i = 1, \dots, j \right\} \tag{51}$$

on $I = [0, \infty)$, where $\gamma_1, \dots, \gamma_j$ are distinct positive real numbers and $n_1, \dots, n_j$ are positive integers with $\sum n_i = n$. This is indeed a Chebyshev system, for if $f \in \operatorname{span} L$, then the function $f(x) \prod_{i=1}^{j} (x + \gamma_i)^{n_i}$ is a polynomial in x of degree $n-1$.

Suppose $f_1, \dots, f_n$ is a Chebyshev system on the interval I. The *moment space* $\mathcal{M}_n$ with respect to $f_1, \dots, f_n$ is the set

$$\mathcal{M}_n = \left\{ \mathbf{c} = (c_1, \dots, c_n) \in \mathbb{R}^n \,\middle|\, c_i = \int_I f_i(x)\, d\sigma(x),\ i = 1, \dots, n \right\}, \tag{52}$$

where the *measure* σ ranges over the set of nondecreasing right-continuous functions of bounded variation on I. It can be shown that $\mathcal{M}_n$ is the convex cone associated with points in the curve C, where

$$C = \big\{ \big(f_1(x), \dots, f_n(x)\big) \big|\, x \in I \big\}.$$

In other words, $\mathcal{M}_n$ can be represented as

$$\mathcal{M}_n = \Big\{ \mathbf{c} = \sum_{j=1}^{p} \alpha_j\, y_j \Big|\, \alpha_j > 0, y_j \in C,\ j = 1, \dots, p,\ p \geq 1 \Big\}.$$

The *index* $\mathcal{I}(\mathbf{c})$ of a point $\mathbf{c}$ of $\mathcal{M}_n$ is the minimum number of points of C that can be used in the representation of $\mathbf{c}$, under the convention that a point $(f_1(x), \dots, f_n(x))$ is counted as a half point if x is from the boundary of I and receives a full count otherwise. The index of a quadrature involving $x_1, \dots, x_p$ is determined by counting likewise.

Proofs of the next three theorems are somewhat elaborate and are omitted here; they can be found in Karlin and Studden [21].

THEOREM 4.1. (See [21, p. 42].) *Suppose $I = [a, b]$ is a closed interval. A point $\mathbf{c} \in \mathcal{M}_n$, $\mathbf{c} \neq \mathbf{0}$, is a boundary point of $\mathcal{M}_n$ if and only if $\mathcal{I}(\mathbf{c}) < n/2$. Moreover, if σ is a measure corresponding to a boundary point $\mathbf{c} \in \mathcal{M}_n$, then there is a unique quadrature*

$$\sum_{i=1}^{p} w_i\, f_r(x_i) = \int_I f_r(x)\, d\sigma(x), \qquad r = 1, \dots, n, \tag{53}$$

where $p \leq (n+1)/2$, $a \leq x_1 < x_2 < \cdots < x_p \leq b$, and $w_i > 0$, $i = 1, \dots, p$.

THEOREM 4.2. (See [21, p. 47].) *Suppose $I = [a, b]$ is a closed interval. Any point $\mathbf{c}$ in the interior of $\mathcal{M}_n$ satisfies $\mathcal{I}(\mathbf{c}) = n/2$. Moreover, if σ is a measure corresponding to $\mathbf{c}$, then there are exactly two quadratures*

$$\sum_{i=1}^{p} w_i\, f_r(x_i) = \int_I f_r(x)\, d\sigma(x), \qquad r = 1, \dots, n, \tag{54}$$

of index $n/2$, where $w_i > 0$, $i = 1, \dots, p$. In particular, if $n = 2m$, then $p = m$ or $p = m + 1$ and

$$a < x_1 < x_2 < \cdots < x_m < b \quad \text{or} \tag{55}$$

$$a = x_1 < x_2 < \cdots < x_{m+1} = b; \tag{56}$$

if $n = 2m + 1$, then $p = m + 1$ and

$$a = x_1 < x_2 < \cdots < x_{m+1} < b \quad \text{or} \tag{57}$$

$$a < x_1 < x_2 < \cdots < x_{m+1} = b. \tag{58}$$

THEOREM 4.3. (See [21, p. 65].) *Let $\mathcal{P}_n$ denote the nonnegative linear combinations of functions $f_1, \dots, f_n$,*

$$\mathcal{P}_n = \left\{ f \,\middle|\, f(x) = \sum_{i=1}^{n} a_i\, f_i(x) \text{ and } f(x) \geq 0 \text{ for all } x \in I \right\}. \tag{59}$$

The point $\mathbf{c} = (c_1, \ldots, c_n)$ *is an element of* $\mathcal{M}_n$ *if and only if*

$$\sum_{i=1}^{n} a_i\, f_i \in \mathcal{P}_n \quad \textit{implies} \quad \sum_{i=1}^{n} a_i\, c_i \geq 0. \tag{60}$$

Moreover, $\mathbf{c}$ *is in the interior of* $\mathcal{M}_n$ *if and only if*

$$\sum_{i=1}^{n} a_i\, f_i \in \mathcal{P}_n \quad \textit{and} \quad \sum_{i=1}^{n} {a_i}^2 > 0 \quad \textit{imply} \quad \sum_{i=1}^{n} a_i\, c_i > 0. \tag{61}$$

THEOREM 4.4. (See [21, p. 106].) *Suppose* $f_i(x) = x^{i-1}$ *for* $i = 1, \ldots, n$, *and* $I = [a, b]$. *If* $n = 2m$, *then* $\mathbf{c} = (c_1, \ldots, c_n)$ *is an element of* $\mathcal{M}_n$ *if and only if the two quadratic forms*

$$\sum_{i,j=1}^{m} [c_{i+j} - a\, c_{i+j-1}]\, \alpha_i \alpha_j \quad \textit{and} \quad \sum_{i,j=1}^{m} [b\, c_{i+j-1} - c_{i+j}]\, \beta_i \beta_j \tag{62}$$

are nonnegative definite. If $n = 2m+1$, *then* $\mathbf{c} \in \mathcal{M}_n$ *if and only if the two quadratic forms*

$$\sum_{i,j=1}^{m+1} c_{i+j-1} \alpha_i \alpha_j \quad \textit{and} \quad \sum_{i,j=1}^{m} [(a+b)c_{i+j} - a\, b\, c_{i+j-1} - c_{i+j+1}]\, \beta_i \beta_j \tag{63}$$

are nonnegative definite. Moreover, for either parity of n, $\mathbf{c}$ *is in the interior of* $\mathcal{M}_n$ *if and only if the corresponding quadratic forms are both positive definite.*

Proof. A theorem of Lukács (see, for example, [19, p. 4]) states that a polynomial f of degree $n-1$ that is nonnegative on $[a, b]$ can be represented in the form

$$f(x) = \begin{cases} (x-a)p(x)^2 + (b-x)q(x)^2, & n = 2m, \\ p(x)^2 + (b-x)(x-a)q(x)^2, & n = 2m+1, \end{cases} \tag{64}$$

where p and q are polynomials such that the degree of each term in (64) does not exceed $n-1$. The combination of (64) and Theorem 4.3 proves the theorem. ∎

4.2. Müntz system quadratures. The systems of (22), (24), (36), and (39) that define the quadrature rules of section 3 are special cases of the system of equations

$$\sum_{m=1}^{\lceil n/2 \rceil} w_m\, {x_m}^{\gamma_i} \log^k x_m = (-1)^{k+1} \zeta^{(k)}(-\gamma_i, a), \qquad k = 0, \ldots, n_i - 1,\ i = 1, \ldots, j, \tag{65}$$

for distinct real numbers $\gamma_1, \ldots, \gamma_j$ and positive integers $n_1, \ldots, n_j$ with $\sum n_i = n$. Here $\zeta^{(k)}$ denotes the kth derivative of ζ with respect to its first argument. The existence and uniqueness of the solution of (65) follow from the existence and uniqueness of quadratures for Chebyshev systems, once it is established that there is a measure σ_a with

$$\int_0^a x^{\gamma_i} \log^k x\, d\sigma_a(x) = (-1)^{k+1} \zeta^{(k)}(-\gamma_i, a), \qquad k = 0, \ldots, n_i - 1,\ i = 1, \ldots, j, \tag{66}$$

in other words, that the moment space $\mathcal{M}_n$ of the Chebyshev system of Müntz functions

$$M = \left\{ x^{\gamma_i} \log^k x \,\middle|\, k = 0, \ldots, n_i - 1,\ i = 1, \ldots, j \right\} \tag{67}$$

on $(0, a]$ contains the point

$$\mathbf{c} = \big(-\zeta(-\gamma_1, a), \ldots, (-1)^{n_j} \zeta^{(n_j-1)}(-\gamma_j, a) \big). \tag{68}$$

We will show that this condition is satisfied provided that a is sufficiently large. It would be convenient to have tight bounds for a, in particular for systems (22), (24), (36), and (39), but it appears that such bounds are difficult to obtain. Even for the regular cases (22) and (24), where by Theorem 4.4 the existence of σ_a is equivalent to the positive definiteness of two matrices, precise bounds for arbitrary j appear difficult. (Numerical examples below provide evidence that a/j may be chosen as small as 5/6.)

THEOREM 4.5. *Suppose $\gamma_1, \ldots, \gamma_j$ are distinct real numbers, each greater than -1, and $n_1, \ldots, n_j$ are positive integers with $\sum n_i = n$. Then for sufficiently large a, there exists a measure σ_a such that the system of* (66) *is satisfied and* $\mathbf{c}$ *defined by* (68) *is in the interior of the moment space $\mathcal{M}_n$.*

Proof. We construct a continuous weight function σ_a' satisfying (66) and show that for sufficiently large a, $\sigma_a'(x)$ is positive for $x \in [0, a]$.

We linearly combine the equations of (66) to obtain the equivalent system

$$\int_0^a (x/a)^{\gamma_i} \log^k(x/a)\, d\sigma_a(x) = (-1)^{k+1} \sum_{r=0}^{k} \binom{k}{r} \frac{\zeta^{(r)}(-\gamma_i, a)}{a^{\gamma_i}} \log^{k-r} a, \qquad k = 0, \ldots, n_i - 1,\ i = 1, \ldots, j, \tag{69}$$

where we have used the binomial theorem to expand $\log^k(x/a) = (\log x - \log a)^k$. We define the weight σ_a' by the formula

$$\sigma_a'(x) = \sum_{m=0}^{n-1} \alpha_{m,a}\, (x/a)^m \tag{70}$$

and combine (69), (70), and the equalities

$$\int_0^1 x^\gamma \log^k x\, dx = \frac{(-1)^k\, k!}{(1+\gamma)^{k+1}}, \qquad \gamma > -1,\ k = 0, 1, \ldots,$$

to obtain the equations in $\alpha_{0,a}, \ldots, \alpha_{n-1,a}$,

$$\sum_{m=0}^{n-1} \frac{\alpha_{m,a}\, (-1)^k\, k!}{(1+\gamma_i+m)^{k+1}} = (-1)^{k+1} \sum_{r=0}^{k} \binom{k}{r} \frac{\zeta^{(r)}(-\gamma_i, a)}{a^{1+\gamma_i}} \log^{k-r} a, \qquad k = 0, \ldots, n_i - 1,\ i = 1, \ldots, j. \tag{71}$$

This n-dimensional linear system is nonsingular, since the set of functions

$$\left\{ (x+\gamma_i+1)^{-k} \,\middle|\, k = 1, \ldots, n_i,\ i = 1, \ldots, j \right\}$$

forms a Chebyshev system on $[0, \infty)$, as established at (51). Thus (71) possesses a unique solution $\alpha_{0,a}, \ldots, \alpha_{n-1,a}$.

We now determine

$$\alpha_m = \lim_{a\to\infty} \alpha_{m,a}, \qquad m = 0, \dots, n-1. \tag{72}$$

The asymptotic expansion of $\zeta^{(r)}(-\gamma_i, a)$ as $a \to \infty$ can be derived by differentiating (10); the first several terms are given by

$$\zeta^{(r)}(-\gamma_i, a) = a^{1+\gamma_i} \sum_{l=0}^{r} \binom{r}{l} \frac{(-1)^{l+1}\,(r-l)!\,\log^l a}{(1+\gamma_i)^{r-l+1}} + O(a^{\gamma_i} \log^r a). \tag{73}$$

Combining (71) and (73), changing the order of summation, and twice applying the product differentiation rule

$$\frac{d^r}{d\gamma^r}\big(f(\gamma)\,g(\gamma)\big) = \sum_{s=0}^{r} \binom{r}{s} f^{(s)}(\gamma)\,g^{(r-s)}(\gamma),$$

we obtain

$$\sum_{m=0}^{n} \frac{\alpha_m\,(-1)^k\,k!}{(1+\gamma_i+m)^{k+1}} = \frac{(-1)^k\,k!}{(1+\gamma_i)^{k+1}}, \qquad k = 0, \dots, n_i - 1,\ i = 1, \dots, j,$$

which immediately reduces to

$$\alpha_m = \begin{cases} 1, & m = 0, \\ 0, & m = 1, \dots, n-1. \end{cases} \tag{74}$$

The combination of (70), (72), and (74) gives

$$\lim_{a\to\infty} \sigma_a'(ax) = 1, \qquad x \in [0, 1],$$

which implies that for a sufficiently large, $\sigma_a'(x) > 0$ for $x \in [0, a]$. The point $\mathbf{c}$ defined by (68) is in the interior of $\mathcal{M}_n$, since small perturbations of $\mathbf{c}$ will preserve the positivity of σ_a'. ◻

Theorem 4.2 ensures the existence of Gaussian quadratures for a Chebyshev system $f_1, \dots, f_n$ defined on an interval I, under the assumption that I is closed, whereas the system M of (67) is Chebyshev on $I = (0, a]$. As a consequence, we require the following result.

THEOREM 4.6. *Suppose the collection of functions $f_1, \dots, f_n$ forms a Chebyshev system on $I = (a, b]$ and each is integrable on $[a, b]$ with respect to a measure σ corresponding to a point $\mathbf{c}$ in the interior of $\mathcal{M}_n$. Then there exists a unique quadrature*

$$\sum_{i=1}^{p} w_i\, f_r(x_i) = \int_a^b f_r(x)\,d\sigma(x), \qquad r = 1, \dots, n, \tag{75}$$

of index $n/2$, where $w_i > 0$ and $x_i \in I$, $i = 1, \dots, p$. In particular, if $n = 2m$, then $p = m$ and

$$a < x_1 < x_2 < \cdots < x_m < b; \tag{76}$$

if $n = 2m+1$, then $p = m+1$ and

$$a < x_1 < x_2 < \cdots < x_{m+1} = b. \tag{77}$$

Proof. The Chebyshev property implies that there exists δ with $a < \delta < b$ such that f_i is nonzero on $(a, \delta]$, $i = 1, \dots, n$. We define the function u on I by the formula

$$u(x) = \begin{cases} \max\limits_{i=1,\dots,n} |f_i(x)|, & x \in (a, \delta], \\ u(\delta), & x \in (\delta, b], \end{cases}$$

and observe that u is continuous and positive on I and integrable on $[a, b]$ with respect to σ. Now we define functions $g_1, \dots, g_n$ on $[a, b]$ by the formula

$$g_i(x) = \begin{cases} \dfrac{f_i(x)}{u(x)}, & x \in (a, b], \\ \lim\limits_{x \to a} g_i(x), & x = a, \end{cases} \qquad i = 1, \dots, n.$$

The system $g_1, \dots, g_n$ is a Chebyshev system on $[a, b]$ and is integrable with respect to the measure $\int_a^x u(t)\, d\sigma(t)$. Theorem 4.2 therefore is applicable and ensures the existence of exactly two quadratures of index $n/2$ for the interval $[a, b]$, one of which includes the point $x_1 = a$. Our assumption $x_i \in (a, b]$ excludes this case and we are left with the single quadrature presented in (76) and (77). □

The next theorem, which is the principal analytical result of this section, follows directly from Theorems 4.5 and 4.6. The existence and uniqueness of the quadratures defined in section 3 follow from it. It also hints at the existence of somewhat more general quadratures, for singularities of the form $x^\gamma \log^k x$, but we do not evaluate these here.

THEOREM 4.7. *Suppose $\gamma_1, \dots, \gamma_j$ are distinct real numbers, each greater than -1, and $n_1, \dots, n_j$ are positive integers with $\sum n_i = n$. For sufficiently large a, the system of equations*

$$(78) \qquad \sum_{m=1}^{\lceil n/2 \rceil} w_m\, {x_m}^{\gamma_i} \log^k x_m = (-1)^{k+1} \zeta^{(k)}(-\gamma_i, a),$$
$$k = 0, \dots, n_i - 1,\ i = 1, \dots, j,$$

has a unique solution $w_1, \dots, w_{\lceil n/2 \rceil}, x_1, \dots, x_{\lceil n/2 \rceil}$ satisfying $w_i > 0$ for $i = 1, \dots, \lceil n/2 \rceil$ and $0 < x_1 < \cdots < x_{\lceil n/2 \rceil} \le a$, with $x_{\lceil n/2 \rceil} = a$ if n is odd.

5. Computation of the nodes and weights. The nodes and weights of the quadratures defined in section 3 are computed by numerically solving the nonlinear systems (22), (24), (36), and (39). Conventional techniques for this problem either are overly cumbersome or converge too slowly to be practical. Recently, Ma, Rokhlin, and Wandzura [14] addressed this need by developing a practical numerical algorithm that is effective in a fairly general setting. They construct a simplified Newton's method and combine it with a continuation (homotopy) method. We present their method in an abbreviated form in section 5.2; the reader is referred to [14] for more detail.

The systems for regular integrands, however, can be solved even more simply, as we see next.

5.1. Regular integrands. The classical theory of Gaussian quadratures for polynomials, summarized in section 2.4, can be exploited to solve (22) and (24). In particular, suppose that $p_0, \dots, p_j$ are the orthogonal polynomials on $[0, a]$, given by the recurrence (13)–(14), under the assumption that

$$\int_0^a x^r\,\omega(x)\,dx = \frac{B_{r+1}(a)}{r+1}, \qquad r = 0, \dots, 2j-1.$$

Then the roots $x_1, \dots, x_j$ of p_j and the corresponding Christoffel numbers $w_1, \dots, w_j$ satisfy (22). The polynomials $p_1, \dots, p_j$ can be calculated in symbolic form; their coefficients are rational if a is rational. The roots of p_j can be computed by Newton iteration and the Christoffel numbers can be obtained using (16). Similar treatment can be applied to the system (24) containing an odd number of equations, using the interval $[0, a-1]$, under the assumption

$$\int_0^{a-1} x^r\,\tau(x)\,dx = \frac{B_{r+1}(a)}{r+1}, \qquad r = 0, \dots, 2j-2.$$

The Gauss–Radau quadrature is computed using the formula (18) for the modified Christoffel numbers. For these tasks it is convenient to use a software system that can manipulate polynomials with full-precision rational coefficients. The author implemented code for these computations in Pari/GP [23].

It should be noted that the proposed procedure is suitable for relatively small values of j (less than, say, 20). It is neither very efficient nor very stable, but it was quite adequate for our purposes. (Unlike the situation for standard Gaussian quadratures, where the number of nodes depends on the size of the problem, here j depends only on the desired order of convergence.) If it is required to compute the nodes and weights of (22) or (24) for large j, the reader may consider numerical schemes for Gaussian quadrature proposed by other authors, for example, that of Gautschi [24] or Golub and Welsch [25].

5.2. Singular integrands. The systems (36) and (39) for singular integrands cannot be solved using methods for standard Gaussian quadrature, since the nodes to be computed do not coincide with the roots of any closely related orthogonal polynomials. We employ instead the algorithm for such systems developed by Ma, Rokhlin, and Wandzura [14], which we now describe.

A collection of $2n$ real-valued continuously differentiable functions $f_1, \dots, f_{2n}$ defined on an interval $I = [a, b]$ is a *Hermite system* if

$$\det \begin{pmatrix} f_1(x_1) & f_2(x_1) & \cdots & f_{2n}(x_1) \\ f_1'(x_1) & f_2'(x_1) & \cdots & f_{2n}'(x_1) \\ f_1(x_2) & f_2(x_2) & \cdots & f_{2n}(x_2) \\ f_1'(x_2) & f_2'(x_2) & \cdots & f_{2n}'(x_2) \\ \vdots & \vdots & & \vdots \\ f_1(x_n) & f_2(x_n) & \cdots & f_{2n}(x_n) \\ f_1'(x_n) & f_2'(x_n) & \cdots & f_{2n}'(x_n) \end{pmatrix} \neq 0 \tag{79}$$

for any choice of distinct $x_1, \dots, x_n$ on I. A Hermite system that is also a Chebyshev system is an *extended Hermite system*. The following theorem is a direct consequence of the definition; the proofs of the subsequent two theorems are contained in [14].

THEOREM 5.1. *Suppose that the functions $f_1, \dots, f_{2n}$ constitute a Hermite system on the interval $[a, b]$ and $x_1, \dots, x_n$ are n distinct points on $[a, b]$. Then there exist unique coefficients α_{ij}, β_{ij}, $i = 1, \dots, n$, $j = 1, \dots, 2n$, such that*

$$\sigma_i(x_k) = 0, \qquad \eta_i(x_k) = \delta_{ik}, \tag{80}$$

$$\sigma_i'(x_k) = \delta_{ik}, \qquad \eta_i'(x_k) = 0, \tag{81}$$

for $i = 1, k = 1, \ldots, n$, where the functions σ_i, η_i are defined by the formulae

$$\sigma_i(x) = \sum_{j=1}^{2n} \alpha_{ij}\, f_j(x), \tag{82}$$

$$\eta_i(x) = \sum_{j=1}^{2n} \beta_{ij}\, f_j(x), \tag{83}$$

for $i = 1, \ldots, n$.

THEOREM 5.2. (See [14, p. 979].) *Suppose that the functions $f_1, \ldots, f_{2n}$ constitute a Hermite system on $[a, b]$. Suppose further that $S \subset [a, b]^n$ is the set of points with distinct coordinates $x_1, \ldots, x_n$. Suppose finally that the mapping $F : S \to \mathbb{R}^n$ is defined by the formula*

$$F(x_1, \ldots, x_n) = \left(\int_a^b \sigma_1(x)\,\omega(x)\,dx, \ldots, \int_a^b \sigma_n(x)\,\omega(x)\,dx \right) \tag{84}$$

with the functions $\sigma_1, \ldots, \sigma_n$ defined by (80)–(82). Then $x_1, \ldots, x_n$ are the Gaussian nodes for the system of functions $f_1, \ldots, f_{2n}$ with respect to the weight ω if and only if $F(x_1, \ldots, x_n) = \mathbf{0}$.

THEOREM 5.3. (See [14, p. 983].) *Suppose that the functions $f_1, \ldots, f_{2n}$ are an extended Hermite system on $[a, b]$, $S \subset [a, b]^n$ is the set of points with distinct coordinates, and the mapping $G : S \to \mathbb{R}^n$ is defined by the formula*

$$G(x_1, \ldots, x_n) = \left(x_1 + \frac{\int_a^b \sigma_1(x)\,\omega(x)\,dx}{\int_a^b \eta_1(x)\,\omega(x)\,dx}, \ \ldots,\ x_n + \frac{\int_a^b \sigma_n(x)\,\omega(x)\,dx}{\int_a^b \eta_n(x)\,\omega(x)\,dx} \right) \tag{85}$$

with the functions $\sigma_1, \ldots, \sigma_n$ and $\eta_1, \ldots, \eta_n$ defined by (80)–(83). Suppose further that $f_i \in C^3((a, b))$ for $i = 1, \ldots, 2n$ and the function F is defined by (84). Suppose finally that $\mathbf{x}^*$ is the unique zero of F, that $\mathbf{x}_0$ is an arbitrary point of S, and that the sequence $\mathbf{x}_1, \mathbf{x}_2, \ldots$ is defined by the formula

$$\mathbf{x}_{i+1} = G(x_i), \qquad i = 0, 1, \ldots. \tag{86}$$

Then there exists $\epsilon > 0$ and $\alpha > 0$ such that the sequence $\mathbf{x}_1, \mathbf{x}_2, \ldots$ generated by (86) converges to $\mathbf{x}^*$ and

$$\|\mathbf{x}_{i+1} - \mathbf{x}^*\| \le \alpha\, \|\mathbf{x}_i - \mathbf{x}^*\|^2 \tag{87}$$

for any initial point $\mathbf{x}_0$ such that $\|\mathbf{x}_0 - \mathbf{x}^*\| < \epsilon$.

The key feature of this theorem is the quadratic convergence indicated by (87). The solution $\mathbf{x}^*$ is obtained by an iterative procedure; each step consists of computing the coefficients that determine $\sigma_1, \ldots, \sigma_n$ and $\eta_1, \ldots, \eta_n$ by inverting the matrix of (79) then computing the integrals that define G by taking linear combinations, using these coefficients, of integrals of $f_1, \ldots, f_{2n}$. Theorem 5.3 ensures that with appropriate choice of starting value $\mathbf{x}_0$, convergence is rapid and certain.

For quadrature nodes $\mathbf{x}^* = (x_1, \ldots, x_n)$, the quadrature weights are given by the integrals of η_i, namely,

$$(w_1, \ldots, w_n) = \left(\int_a^b \eta_1(x)\,\omega(x)\,dx, \ldots, \int_a^b \eta_n(x)\,\omega(x)\,dx \right). \tag{88}$$

We note that Theorems 5.1–5.3 concern Gaussian quadratures with n nodes and weights to integrate $2n$ functions on the interval $[a, b]$ exactly. For Gauss–Radau quadratures, in which node $x_n = b$ is fixed and $2n-1$ functions are integrated exactly, only a slight change is required. In particular, functions $\sigma_1, \ldots, \sigma_{n-1}$ (without σ_n) and $\eta_1, \ldots, \eta_n$ are defined as before by (80)–(83), except that the summations in (82) and (83) exclude f_{2n}. Their coefficients α_{ij}, $i = 1, \ldots, n-1$, $j = 1, \ldots, 2n-1$, and β_{ij}, $i = 1, \ldots, n$, $j = 1, \ldots, 2n-1$, are obtained by inverting the matrix which results from removing the last row and column from the matrix of (79). The revised mapping $G: S \to \mathbb{R}^{n-1}$ has $n-1$ components defined as the first $n-1$ components in (85). Finally, as before, the quadrature weights are given by (88).

In order to obtain a sufficiently good starting estimate for the solution of $F(\mathbf{x}) = 0$, a continuation procedure can be used, as outlined in the following theorem.

THEOREM 5.4. (See, for example, [14, p. 975].) *Suppose that* $\mathbf{F}: [0,1] \times [a,b]^n \to \mathbb{R}^n$ *is a function with a unique solution* $\mathbf{x}_t$ *to the equation* $\mathbf{F}(t, \mathbf{x}) = \mathbf{0}$ *for all* $t \in [0,1]$, *suppose that* $\mathbf{x}_t$ *is a continuous function of* t, *and suppose that* $\mathbf{F}(1, \mathbf{x}) = F(\mathbf{x})$. *Finally, suppose* $\mathbf{x}_0$ *is given and for some* $\delta > 0$ *there is a procedure* $\mathbf{P}$ *to compute* $\mathbf{x}_t$ *for* $t \in [0,1]$, *given an estimate* $\tilde{\mathbf{x}}_t$ *with* $|\tilde{\mathbf{x}}_t - \mathbf{x}_t| < \delta$. *Then there exists a positive integer* m *such that the following procedure can be used to compute the solution of* $F(\mathbf{x}) = \mathbf{0}$*:*

For $i = 1, \ldots, m$, *use* $\mathbf{P}$ *to compute* $\mathbf{x}_{i/m}$, *given the estimate* $\mathbf{x}_{(i-1)/m}$.

The required solution of $F(\mathbf{x}) = \mathbf{0}$ *is* $\mathbf{x}_1$.

More typically, of course, δ and any bound on $|\mathbf{x}_{t+\epsilon} - \mathbf{x}_t|/\epsilon$ depend on t and in a practical implementation the step size is chosen adaptively.

To compute the solutions of (36) and (39), it is effective to use a continuation procedure with respect to both j and a. Solutions for the first few values of j are readily obtained without requiring good initial estimates. Given a solution of (36) for the interval $[0, a]$ with nodes $u_1, \ldots, u_j$ and weights $v_1, \ldots, v_j$, we choose an initial estimate $\tilde{u}_1, \ldots, \tilde{u}_{j+1}$, $\tilde{v}_1, \ldots, \tilde{v}_{j+1}$ for $j+1$ and the interval $[0, a+1]$ defined by the formulae

$$\tilde{u}_i = \begin{cases} u_i, & i = 1, \ldots, j, \\ a, & i = j+1, \end{cases} \qquad \tilde{v}_i = \begin{cases} v_i, & i = 1, \ldots, j, \\ 1, & i = j+1. \end{cases} \tag{89}$$

This choice exactly satisfies the equations

$$\begin{aligned} \sum_{i=1}^{j+1} \tilde{u}_i \, \tilde{v}_i^{\,\gamma+r} &= -\zeta(-\gamma - r, a+1), \qquad r = 0, 1, \ldots, j-1, \\ \sum_{i=1}^{j+1} \tilde{u}_i \, \tilde{v}_i^{\,r} &= \frac{B_{r+1}(a+1)}{r+1}, \qquad r = 0, 1, \ldots, j-1, \end{aligned} \tag{90}$$

as follows immediately from the difference formula (4) for B_n and (11) for ζ, but the corresponding equations for $r = j$ are not satisfied. Those equations are approximately satisfied, however, and we can start with the actual values of the sums for $r = j$ as the required values. These are then varied continuously, obtaining the corresponding solutions, until they coincide with the intended values $-\zeta(-\gamma - j, a+1)$ and $B_{j+1}(a+1)/(j+1)$. This procedure can be used without alteration for (39).

Once the solution for $j+1$ and the interval $[0, a+1]$ is obtained, a can be continuously varied, in a continuation procedure, to obtain solutions for different intervals.

TABLE 1

The minimum value of a, as a function of j, such that the point $\big(B_1(a)/1, \ldots, B_j(a)/j\big)$ is in the moment space $\mathcal{M}_{2j}$ of the polynomials $1, x, \ldots, x^{2j-1}$ on the interval $[0, a]$. The moment space is defined at (52).

j	$\min a$	j	$\min a$	j	$\min a$	j	$\min a$
1	0.78868	5	3.96696	9	7.21081	13	10.47885
2	1.57085	6	4.77448	10	8.02618	14	11.29815
3	2.36347	7	5.58463	11	8.84274	15	12.11815
4	3.16288	8	6.39687	12	9.66035	16	12.93878

6. Numerical examples. The procedures described in section 5 were implemented in Pari/GP [23] for both the regular cases and the singular cases. The matrix in (79), which must be inverted, is very poorly conditioned for many choices of n, $x_1, \ldots, x_n$, and $f_1, \ldots, f_{2n}$. This difficulty was met by using the extended precision capability of Pari/GP.

6.1. Nodes and weights. The nodes and weights of (22), (24), (36), and (39) that determine the quadratures of section 3 were computed for a range of values of the parameter j. For each choice of j, a was chosen, by experiment, to be the smallest integer leading to positive nodes and weights (see Theorem 4.7). For the regular case (22), the characterization expressed in Theorem 4.4 was used to determine the minimum value of $a \in \mathbb{R}$, for $j = 1, \ldots, 16$, that satisfies $\mathbf{c} = \big(B_1(a)/1, \ldots, B_j(a)/j\big) \in \mathcal{M}_{2j}$. In particular, we obtained the minimum value of a such that the quadratic forms in (62) are nonnegative definite. This determination was made by calculating the determinant of each corresponding matrix symbolically and solving for the largest root of the resulting polynomial in a. These values are given in Table 1. This evidence suggests that $\lim_{j\to\infty} j^{-1} \min a$ exists and is roughly 5/6, meaning that the number of trapezoidal nodes displaced is less than the number of Gaussian nodes replacing them, for quadrature rules of all orders. This relationship also appears to hold, to an even greater extent, for the singular cases.

The values of selected nodes and weights, for the regular cases and for singularities $x^{-1/2}$ and $\log x$, are presented in an appendix. Of particular simplicity are the first two rules for regular integrands,

$$T_n^{1,1}(f) = h\left[\frac{1}{2}f(h/6) + f(h) + \cdots + f(1-h) + \frac{1}{2}f(1-h/6)\right], \tag{91}$$

where $h = 1/(n+1)$, for $n = 0, 1, \ldots$, and

$$\begin{aligned} T_n^{2,2}(f) = h\Bigg[&\frac{25}{48}f(h/5) + \frac{47}{48}f(h) + f(2h) + \cdots \\ &+ f(1-2h) + \frac{47}{48}f(1-h) + \frac{25}{48}f(1-h/5)\Bigg], \end{aligned} \tag{92}$$

where $h = 1/(n+3)$, for $n = 0, 1, \ldots$. These rules are of third- and fourth-order convergence, respectively. The first is noteworthy for having the same weights as, but higher order than, the trapezoidal rule; the second has asymptotic error 1/4 that of Simpson's rule with the same number of nodes.

The lowest-order rule presented for logarithmic singularities,

$$S_n^{1,1,1,1}(g) = h\left[\frac{1}{2}g(h/(2\pi)) + g(h) + \cdots + g(1-h) + \frac{1}{2}g(1)\right], \tag{93}$$

TABLE 2

Relative errors in the computation of the integral in (94), for the regular case $s(x) = 0$. Quadrature rules with convergence of order $2, 4, 8, 16,$ and 32 were used with various numbers $m = n + 2j$ of nodes. Here $f = m/(200/\pi)$ is the oversampling factor.

m	f	2	4	8	16	32
70	1.10	0.622D+00	0.114D−01	0.382D−02	0.170D−05	0.234D−10
80	1.26	0.488D+00	0.938D−02	0.184D−02	0.354D−06	0.115D−11
90	1.41	0.391D+00	0.744D−02	0.934D−03	0.841D−07	0.720D−13
100	1.57	0.321D+00	0.584D−02	0.498D−03	0.223D−07	0.192D−14
115	1.81	0.246D+00	0.408D−02	0.211D−03	0.365D−08	0.331D−14
130	2.04	0.194D+00	0.289D−02	0.964D−04	0.715D−09	0.331D−14
145	2.28	0.157D+00	0.209D−02	0.472D−04	0.162D−09	0.471D−14
160	2.51	0.129D+00	0.154D−02	0.245D−04	0.415D−10	0.262D−14
180	2.83	0.102D+00	0.106D−02	0.110D−04	0.794D−11	0.471D−14
200	3.14	0.832D−01	0.747D−03	0.531D−05	0.177D−11	0.331D−14
230	3.61	0.631D−01	0.465D−03	0.199D−05	0.235D−12	0.523D−15
260	4.08	0.495D−01	0.303D−03	0.828D−06	0.375D−13	0.384D−14

TABLE 3

Relative errors for the singular case $s(x) = x^{-1/2}$, for various numbers $m = n + j + k$ of nodes and orders of convergence.

m	f	2	4	8	16
70	1.10	0.692D−01	0.519D−01	0.850D−02	0.163D−03
80	1.26	0.925D−01	0.258D−01	0.260D−02	0.578D−05
90	1.41	0.921D−01	0.133D−01	0.698D−03	0.667D−06
100	1.57	0.838D−01	0.717D−02	0.146D−03	0.277D−06
115	1.81	0.686D−01	0.307D−02	0.201D−04	0.360D−07
130	2.04	0.550D−01	0.144D−02	0.269D−04	0.437D−08
145	2.28	0.441D−01	0.724D−03	0.171D−04	0.557D−09
160	2.51	0.357D−01	0.389D−03	0.964D−05	0.733D−10
180	2.83	0.273D−01	0.186D−03	0.440D−05	0.408D−11
200	3.14	0.212D−01	0.976D−04	0.207D−05	0.218D−12
230	3.61	0.151D−01	0.427D−04	0.724D−06	0.130D−12
260	4.08	0.110D−01	0.215D−04	0.280D−06	0.201D−13

approximates $\int_0^1 g(x)\,dx$ with error of order $O(h^2 \log h)$ for $g(x) = \phi(x)\,\log x + \psi(x)$, provided ϕ and ψ are regular functions on $[0, 1]$. The corresponding rule for the singularity $x^{-1/2}$ is not quite as simple, for there the quantity 2π in (93) is replaced with $4\zeta(1/2)^2$.

6.2. Quadrature performance. To demonstrate the performance of the quadrature rules, they were used in a Fortran routine (with `real*8` arithmetic) to numerically compute the integrals

$$\int_0^1 \left[\cos(200x)\,s(x) + \cos(200x + .3)\right] dx, \tag{94}$$

for the functions $s(x) = 0$, $s(x) = x^{-1/2}$, and $s(x) = \log x$. These integrals were also obtained analytically and the relative error of the quadratures was computed. The numerical integrations were computed for various orders of quadrature and various numbers of nodes. Minimum sampling was taken to be two points per period of the cosine (i.e., $200/\pi \approx 63.7$ quadrature nodes). The accuracies were then compared for various degrees of oversampling. The quadrature errors are listed in Tables 2–4 and plotted, as a function of oversampling factor, in Figure 1. We note that the graphs are

TABLE 4

Relative errors for the singular case $s(x) = \log x$. Here the error is of order $O(h^l \log h)$, where l is shown.

m	f	2	4	8	16
70	1.10	0.369D+00	0.217D−01	0.354D−01	0.243D−03
80	1.26	0.271D+00	0.238D−02	0.328D−02	0.487D−04
90	1.41	0.206D+00	0.765D−02	0.707D−03	0.394D−05
100	1.57	0.162D+00	0.768D−02	0.687D−03	0.121D−05
115	1.81	0.117D+00	0.576D−02	0.291D−03	0.886D−07
130	2.04	0.882D−01	0.398D−02	0.120D−03	0.903D−08
145	2.28	0.687D−01	0.272D−02	0.548D−04	0.123D−08
160	2.51	0.549D−01	0.188D−02	0.272D−04	0.177D−09
180	2.83	0.421D−01	0.119D−02	0.118D−04	0.965D−11
200	3.14	0.332D−01	0.774D−03	0.550D−05	0.956D−12
230	3.61	0.243D−01	0.433D−03	0.196D−05	0.398D−12
260	4.08	0.185D−01	0.258D−03	0.778D−06	0.106D−12

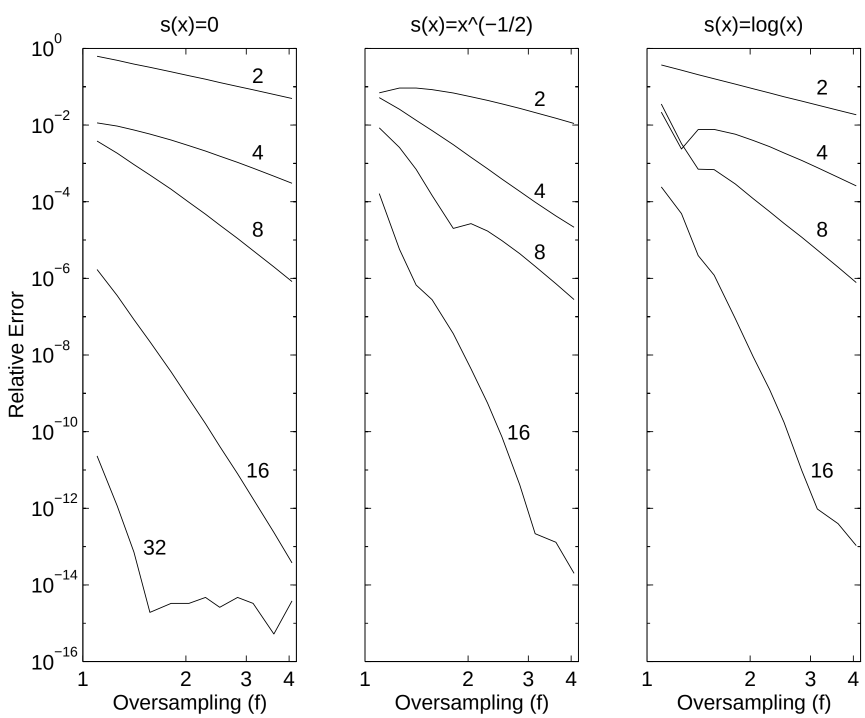

FIG. 1. *The relative errors of the quadratures, shown in Tables* 2–4*, are plotted using logarithmic scaling on both axes.*

nearly straight lines (until the limit of machine precision is reached), as predicted from the theoretical convergence rates. We remark also that excellent accuracy is attained for even quite modest oversampling when quadratures with high-order convergence are employed. For problems where the number of quadrature nodes is the major cost factor, therefore, one may benefit by using the high-order quadratures even for modest accuracy requirements.

TABLE 5

Relative errors in the computation of the integral in (95)*, for* $\xi = 1$*. Quadrature rules defined in Corollary* 3.10 *with* $j = 1, 2, 4, 8,$ *and* 16 *were used with various numbers* m *of nodes.*

m	1	2	4	8	16
70	0.999D+00	0.400D+00	0.305D+00	0.180D+00	0.104D−01
80	0.304D+00	0.200D−01	0.247D−01	0.238D−02	0.474D−03
90	0.113D+00	0.217D−01	0.136D−02	0.383D−03	0.866D−05
100	0.273D−01	0.137D−01	0.137D−02	0.440D−04	0.900D−06
115	0.210D−01	0.247D−02	0.137D−03	0.573D−05	0.331D−07
130	0.228D−01	0.107D−02	0.632D−04	0.423D−06	0.107D−09
145	0.118D−01	0.115D−02	0.305D−04	0.196D−06	0.490D−10
160	0.212D−02	0.521D−03	0.307D−05	0.430D−07	0.216D−09
180	0.625D−02	0.824D−04	0.451D−05	0.101D−07	0.166D−11
200	0.558D−02	0.206D−03	0.184D−05	0.291D−08	0.867D−12
230	0.863D−03	0.676D−04	0.463D−06	0.626D−09	0.586D−13
260	0.266D−02	0.433D−04	0.291D−06	0.596D−10	0.346D−14

We test the quadratures for improper integrals by numerically computing for $\xi = 1$ the integral

$$\int_{-\infty}^{\infty} e^{-ix\xi} \sum_{r=-10}^{10} \frac{r+1}{x+r+i}\, dx = -2\pi i\, H(\xi) \sum_{r=-10}^{10} (r+1)\, e^{ir\xi-\xi}, \tag{95}$$

where H is the Heaviside step function. The integrand is oscillatory and decays like x^{-1} as $x \to \pm\infty$. The quadratures defined in Corollary 3.10 are employed, for which the integral is split into a regular integral on a finite interval, chosen here to be $[-5\sqrt{m}/4, 5\sqrt{m}/4]$, where m is the total number of quadrature nodes, and two improper integrals in the imaginary direction, using Laguerre quadratures. The quadrature errors are shown in Table 5.

7. Applications and summary. The chief motivation for the hybrid Gauss-trapezoidal quadrature rules is the accurate computation of integral operators. We define an integral operator A by the formula

$$(Af)(x) = \int_\Gamma K(x,y)\, f(y)\, dy,$$

where Γ is a regular, simple closed curve in the complex plane, the function f is regular on Γ, and the kernel $K : \mathbb{C} \times \mathbb{C} \to \mathbb{C}$ is a regular function of its arguments, except where they coincide; we assume

$$K(x,y) = \phi(x,y)\, s(|x-y|) + \psi(x,y) \tag{96}$$

with ϕ and ψ regular on $\Gamma \times \Gamma$ and s regular on $(0,\infty)$, with an integrable singularity at 0. A large variety of problems of classical physics can be formulated as integral equations that involve such operators. When the operator occurs in an integral equation

$$f(x) + (Af)(x) = g(x), \qquad x \in \Gamma, \tag{97}$$

some choice of discretization must be used to reduce the problem to a finite-dimensional one for numerical solution. In the *Nyström method* the integrals are replaced by quadratures to yield the finite system of equations

$$f(x_i) + \sum_{j=1}^{m} w_{ij}\, f(x_j) = g(x_i), \qquad i = 1, \ldots, m. \tag{98}$$

This linear system can be solved for $f(x_1), \dots, f(x_m)$ by a variety of techniques. The particular choice of x_i and w_{ij} for $i, j = 1, \dots, m$ determines the order of convergence (and therefore efficiency) of the method.

For a curve parametrization $\nu : [0,1] \to \Gamma$, such as scaled arc length, the operator A becomes

$$(Af)(\nu(t)) = \int_0^1 K(\nu(t), \nu(\tau))\, f(\nu(\tau))\, \nu'(\tau)\, d\tau.$$

It is convenient to use a uniform discretization $1/m, 2/m, \dots, 1$ in t and τ, so $x_i = \nu(i/m)$, $i = 1, \dots, m$. How then is w_{ij} determined? We assume for the moment that f is available at locations other than $x_1, \dots, x_m$. Continuing ν periodically with period 1, and using the Gauss-trapezoidal quadratures, we obtain

$$(99) \quad (Af)(\nu(i/m)) = \int_{i/m}^{1+i/m} K(\nu(i/m), \nu(\tau))\, f(\nu(\tau)\, \nu'(\tau))\, d\tau$$

$$\approx \frac{1}{m} \sum_{k=1}^{j} u_k\, \sigma_{i/m}(v_k/m) + \frac{1}{m} \sum_{k=0}^{n-1} \sigma_{i/m}(a/m + k/m) + \frac{1}{m} \sum_{k=1}^{j} u_k\, \sigma_{i/m}(1 - v_k/m),$$

for $i = 1, \dots, m$, where $\sigma_\alpha : [0,1] \to \mathbb{C}$ is defined by the formula

$$\sigma_\alpha(\tau) = K(\nu(\alpha), \nu(\alpha + \tau))\, f(\alpha + \tau)\, \nu'(\alpha + \tau) \tag{100}$$

and $m = n + 2a - 1$ and $u_1, \dots, u_j$, $v_1, \dots, v_j$ are determined for the singularity s of K. Provided that the periodic continuation of ν is sufficiently regular, the quadrature will converge to the integral with order greater than j as $m \to \infty$, for $i = 1, \dots, m$. We relax the restriction that f be available outside $x_1, \dots, x_m$ by using local Lagrange interpolation of order $j + 1$ for equispaced nodes,

$$f(\nu(\tau)) \approx \sum_{r=0}^{j} f(\nu(i/m + r/m))\, l_r(m\tau - i), \tag{101}$$

where $i = \lfloor m\tau - (j-1)/2 \rfloor$ and

$$l_r(x) = \prod_{s=0, s\neq r}^{j} \frac{x - s}{r - s}, \qquad r = 0, \dots, j.$$

Now w_{ij} for $i, j = 1, \dots, m$ is determined by combining (97)–(101). The computation of all m^2 coefficients requires $m(m + 2j - 2a + 1)$ evaluations of the kernel K and therefore order $O(m^2)$ operations. This cost can often be substantially reduced using techniques that exploit kernel smoothness (see, for example, [6], [5]).

A slightly different application of the quadratures is the computation of Fourier transforms of functions that fail to satisfy the assumptions usually made when using the discrete Fourier transform. In particular, if a function decays slowly for large argument or is compactly supported and singular at the ends of the support interval, these quadratures can be used to compute its Fourier transform. One example of such a function is that in (95). Since most of the nodes in these quadratures are equispaced, with function values given equal weight, the fast Fourier transform can be used to do the bulk of the computations; the overall complexity is $O(n \log n)$, where n is the number of Fourier coefficients to be computed. Other applications may include the representation of functions for solving ordinary or partial differential equations, when high-order methods are required. In addition, an extension of these quadratures to integrals on surfaces is under study.

In summary, the characteristics of the hybrid Gauss-trapezoidal quadrature rules include

- arbitrary order convergence for regular functions or functions with known singularities of power or logarithmic type,
- positive weights,
- most nodes equispaced and most weights constant, and
- invariant nodes and weights (aside from scaling) as the problem size increases.

The primary disadvantage of the quadrature rules, shared with other Gaussian quadratures but exacerbated here by poor conditioning, is that the computation of the nodes and weights is not trivial. Nevertheless, tabulation of nodes and weights for a given order of convergence allows this issue to be avoided in the construction of high-order, general-purpose quadrature routines.

Appendix. Tables of quadrature nodes and weights.

Quadrature nodes and weights may also be obtained electronically from the author.

TABLE 6

The nodes and weights for the quadrature rule $T_n^{ja}(f) = h\sum_{i=1}^{j} w_i\, f(x_i h) + h\sum_{i=0}^{n-1} f(ah + ih) + h\sum_{i=1}^{j} w_i\, f(1 - x_i h)$, *with* $h = (n + 2a - 1)^{-1}$, *for several choices of* j *and corresponding minimum integer* a. *For* f *a regular function,* $T_n^{ja}(f)$ *converges to* $\int_0^1 f(x)\,dx$ *as* $n \to \infty$ *with convergence of order* O.

O	a	x_i	w_i
3	1	1.66666 66666 66667D−01	5.00000 00000 00000D−01
4	2	2.00000 00000 00000D−01	5.20833 33333 33333D−01
		1.00000 00000 00000D+00	9.79166 66666 66667D−01
5	2	2.24578 49798 12614D−01	5.54078 16436 06372D−01
		1.01371 93743 59164D+00	9.45921 83563 93628D−01
6	3	2.25099 10426 10971D−01	5.54972 43271 64180D−01
		1.01426 90609 87992D+00	9.45131 74118 45473D−01
		2.00000 00000 00000D+00	9.99895 82609 90347D−01
7	3	2.18054 06725 43505D−01	5.40808 89672 08193D−01
		1.00118 18730 31216D+00	9.51661 50458 23566D−01
		1.99758 05264 18033D+00	1.00752 95986 96824D+00
8	4	2.08764 74220 32129D−01	5.20798 82772 46498D−01
		9.78608 73737 14483D−01	9.53503 80185 55888D−01
		1.98954 13865 79751D+00	1.02487 16264 02471D+00
		3.00000 00000 00000D+00	1.00082 57440 17291D+00
12	5	7.02395 54616 21939D−02	1.92231 59778 43698D−01
		4.31229 78572 27970D−01	5.34839 95305 14687D−01
		1.11775 27345 18115D+00	8.17020 94424 88760D−01
		2.01734 37245 72518D+00	9.59211 15214 45966D−01
		3.00083 78428 47590D+00	9.96714 34080 44999D−01
		4.00000 00000 00000D+00	9.99982 01196 61890D−01
16	7	9.91933 78414 51028D−02	2.52819 89287 66921D−01
		5.07659 26696 45529D−01	5.55015 82301 59486D−01
		1.18497 29258 27278D+00	7.85232 14536 15224D−01
		2.04749 34671 34072D+00	9.24591 56738 76714D−01
		3.00716 89118 69310D+00	9.83935 02004 45296D−01
		4.00047 49967 76184D+00	9.98446 34484 13151D−01
		5.00000 78790 22339D+00	9.99959 23784 64547D−01
		6.00000 00000 00000D+00	9.99999 96862 58662D−01
20	9	9.20920 04462 33291D−02	2.35183 61446 43984D−01
		4.75202 19477 58861D−01	5.24882 05090 85946D−01
		1.12468 79458 44539D+00	7.63402 64098 69887D−01
		1.97738 73856 42367D+00	9.28471 13366 58351D−01
		2.95384 89578 22108D+00	1.01096 98865 87741D+00
		3.97613 67860 48776D+00	1.02495 97253 11073D+00
		4.99435 42819 79877D+00	1.01051 75346 39652D+00
		5.99946 95393 35291D+00	1.00155 15957 97932D+00
		6.99998 67048 74333D+00	1.00006 16817 94188D+00
		8.00000 00000 00000D+00	1.00000 01358 43597D+00

Table 6
(*Continued*)

O	a	x_i	w_i
24	10	6.00106 47314 74805D−02	1.53893 21045 18340D−01
		3.14968 50162 29433D−01	3.55105 81285 59424D−01
		7.66450 82405 18316D−01	5.44920 00362 80007D−01
		1.39668 57813 42510D+00	7.10407 84977 15549D−01
		2.17519 59032 06602D+00	8.39878 09402 53654D−01
		3.06232 05758 80355D+00	9.27276 79508 90611D−01
		4.01644 09887 92476D+00	9.75060 56973 71132D−01
		5.00287 20642 75734D+00	9.94262 96508 23470D−01
		6.00028 54533 10164D+00	9.99242 17784 21898D−01
		7.00001 29649 62529D+00	9.99953 43707 86161D−01
		8.00000 01755 54469D+00	9.99999 08549 12925D−01
		9.00000 00000 00000D+00	9.99999 99894 66828D−01
28	12	6.23436 05331 94102D−02	1.59597 52797 34157D−01
		3.25028 67217 02614D−01	3.63704 60281 93864D−01
		7.83735 07942 82182D−01	5.49875 31772 97441D−01
		1.41567 31126 16924D+00	7.08798 67920 86956D−01
		2.18989 42500 61313D+00	8.33517 22755 01195D−01
		3.07005 38774 83040D+00	9.20444 65106 08518D−01
		4.01861 37562 18047D+00	9.71088 17765 52090D−01
		5.00270 59020 35397D+00	9.93329 65785 55239D−01
		5.99992 97418 10400D+00	9.99475 90879 10050D−01
		6.99990 47208 46024D+00	1.00013 30302 54421D+00
		7.99998 68948 43540D+00	1.00003 29150 11460D+00
		8.99999 93733 80393D+00	1.00000 22616 53775D+00
		9.99999 99920 02911D+00	1.00000 00423 93520D+00
		1.10000 00000 00000D+01	1.00000 00000 42872D+00
32	14	5.89955 06143 25259D−02	1.51107 60238 74179D−01
		3.08275 70622 27814D−01	3.45939 59211 69090D−01
		7.46370 72530 79130D−01	5.27350 28051 46873D−01
		1.35599 37264 94664D+00	6.87844 40945 43021D−01
		2.11294 32173 46336D+00	8.21031 91400 34114D−01
		2.98724 14965 45946D+00	9.21838 28755 15803D−01
		3.94479 89209 61176D+00	9.87302 74875 53060D−01
		4.95026 92028 42798D+00	1.01825 19134 41155D+00
		5.97212 30431 17706D+00	1.02193 34303 49293D+00
		6.98978 35581 37742D+00	1.01256 79834 13513D+00
		7.99767 30195 12965D+00	1.00405 22895 54521D+00
		8.99969 49327 47039D+00	1.00071 34133 44501D+00
		9.99997 92252 11805D+00	1.00006 36183 02950D+00
		1.09999 99382 66130D+01	1.00000 24863 85216D+00
		1.19999 99994 62073D+01	1.00000 00304 04477D+00
		1.30000 00000 00000D+01	1.00000 00000 20760D+00

TABLE 7

The nodes $v_1, \ldots, v_j$ *and weights* $u_1, \ldots, u_j$ *for the quadrature rule* $S_n^{jkab}(g) = h\sum_{i=1}^{j} u_i\, g(v_i h) + h\sum_{i=0}^{n-1} g(ah+ih) + h\sum_{i=1}^{k} w_i\, g(1-x_i h)$, *with* $h = (n+a+b-1)^{-1}$, *for* $g(x) = x^{-1/2}\phi(x) + \psi(x)$, *with* ϕ *and* ψ *regular functions. The nodes* $x_1, \ldots, x_k$ *and weights* $w_1, \ldots, w_k$ *are found in Table* 6.

O	a	v_i	u_i
1.5	1	1.17225 85713 93266D−01	5.00000 00000 00000D−01
2.0	2	9.25211 27154 21378D−02	4.19807 96252 66162D−01
		1.00000 00000 00000D−00	1.08019 20374 73384D+00
2.5	2	6.02387 37964 08450D−02	2.85843 99904 20468D−01
		8.78070 40506 76215D−01	1.21415 60009 57953D+00
3.0	2	7.26297 84134 70474D−03	3.90763 87675 31813D−02
		2.24632 55125 21893D−01	4.87348 40566 46474D−01
		1.00000 00000 00000D+00	9.73575 20666 00344D−01
3.5	2	1.28236 89094 58828D−02	6.36399 66631 05925D−02
		2.69428 63467 92474D−01	5.07743 45780 43636D−01
		1.01841 45237 86358D+00	9.28616 57556 45772D−01
4.0	3	1.18924 24340 21285D−02	5.92721 50356 16424D−02
		2.57822 04347 38662D−01	4.95598 17403 06228D−01
		1.00775 00645 85281D+00	9.42713 12906 28058D−01
		2.00000 00000 00000D+00	1.00241 65465 50407D+00
6.0	4	3.31792 59426 99451D−03	1.68178 09298 83469D−02
		8.28301 97052 96352D−02	1.75524 44045 44475D−01
		4.13609 49257 26231D−01	5.03935 05038 58001D−01
		1.08874 43736 88402D+00	8.26624 13396 80867D−01
		2.00648 21018 52379D+00	9.77306 58489 81277D−01
		3.00000 00000 00000D+00	9.99791 98099 47032D−01
8.0	5	1.21413 06065 23435D−03	6.19984 48842 97793D−03
		3.22395 27000 27058D−02	7.10628 67917 20044D−02
		1.79093 53836 49920D−01	2.40893 01044 10471D−01
		5.43766 38052 44631D−01	4.97592 92636 68960D−01
		1.17611 66283 96759D+00	7.59244 65404 41226D−01
		2.03184 82107 16014D+00	9.32244 63996 14420D−01
		3.00196 12256 90812D+00	9.92817 14381 60095D−01
		4.00000 00000 00000D+00	9.99944 91256 89846D−01
10.0	6	1.74586 29891 63252D−04	1.01695 09859 48944D−03
		8.61367 05404 57314D−03	2.29467 06865 17670D−02
		6.73338 50887 03690D−02	1.07665 79680 22888D−01
		2.51448 87747 33840D−01	2.73457 76624 65576D−01
		6.34184 55737 37690D−01	4.97881 55919 24992D−01
		1.24840 40550 83152D+00	7.25620 89195 65360D−01
		2.06568 80319 53401D+00	8.95263 86903 20078D−01
		3.00919 93586 62542D+00	9.77815 74653 81624D−01
		4.00041 62696 90208D+00	9.98339 07813 99277D−01
		5.00000 00000 00000D+00	9.99991 63424 08948D−01

TABLE 7
(*Continued*)

O	a	v_i	u_i
12.0	8	5.71021 84272 06990D−04	2.92101 89269 12141D−03
		1.54042 43511 15548D−02	3.43113 06112 56885D−02
		8.83424 84071 96555D−02	1.22466 94956 38615D−01
		2.82446 20545 09770D−01	2.76110 82420 22520D−01
		6.57486 98923 05580D−01	4.79780 96430 10337D−01
		1.24654 10609 77993D+00	6.96655 56772 71379D−01
		2.03921 84951 30811D+00	8.79007 79419 72658D−01
		2.97933 34870 49800D+00	9.86862 24492 94327D−01
		3.98577 25953 93049D+00	1.01514 23896 88201D+00
		4.99724 08043 11428D+00	1.00620 97126 32210D+00
		5.99986 87939 51190D+00	1.00052 88299 22287D+00
		7.00000 00000 00000D+00	1.00000 23977 96838D+00
14.0	9	3.41982 14602 49725D−04	1.75095 72432 02047D−03
		9.29659 34301 87960D−03	2.08072 65842 87380D−02
		5.40621 47717 55252D−02	7.58683 06164 33430D−02
		1.76394 50965 08648D−01	1.76602 05266 71851D−01
		4.21848 66056 53738D−01	3.20662 43620 72232D−01
		8.27402 28958 84040D−01	4.93440 52905 53812D−01
		1.41028 75856 37014D+00	6.70749 70306 98472D−01
		2.16099 75052 38153D+00	8.24495 90253 66557D−01
		3.04350 47493 58223D+00	9.31464 67421 62802D−01
		4.00569 25790 69439D+00	9.84576 84431 63154D−01
		4.99973 27079 05968D+00	9.99285 27691 54770D−01
		5.99987 51919 71098D+00	1.00027 31129 57723D+00
		6.99999 45605 68667D+00	1.00002 28574 02321D+00
		8.00000 00000 00000D+00	1.00000 00814 05180D+00
16.0	10	2.15843 89882 80793D−04	1.10580 48735 01181D−03
		5.89843 27437 09196D−03	1.32449 99447 07956D−02
		3.46279 59568 96131D−02	4.89984 23075 92144D−02
		1.14558 64950 70213D−01	1.16532 61928 68815D−01
		2.79034 42188 56415D−01	2.17858 66931 94957D−01
		5.60011 37986 53321D−01	3.48176 60169 45031D−01
		9.81409 12428 83119D−01	4.96402 79159 11545D−01
		1.55359 48539 74655D+00	6.46902 61896 23831D−01
		2.27017 91140 36658D+00	7.82368 89717 83889D−01
		3.10823 46017 15371D+00	8.87777 24458 93361D−01
		4.03293 08939 96553D+00	9.55166 50770 35583D−01
		5.00680 32702 28157D+00	9.87628 55797 41800D−01
		6.00081 54667 35179D+00	9.97992 91838 63017D−01
		7.00004 50350 79542D+00	9.99847 06206 34641D−01
		8.00000 07389 23901D+00	9.99996 28916 45340D−01
		9.00000 00000 00000D+00	9.99999 99468 93169D−01

Table 8

The nodes $v_1, \ldots, v_j$ and weights $u_1, \ldots, u_j$ for the quadrature rule $S_n^{jkab}(g) = h\sum_{i=1}^{j} u_i\, g(v_i h) + h\sum_{i=0}^{n-1} g(ah+ih) + h\sum_{i=1}^{k} w_i\, g(1-x_i h)$, with $h = (n+a+b-1)^{-1}$, for $g(x) = \phi(x)\log x + \psi(x)$, with ϕ and ψ regular functions. The error is of order $O(h^l \log h)$. The nodes $x_1, \ldots, x_k$ and weights $w_1, \ldots, w_k$ are found in Table 6.

l	a	v_i	u_i
2	1	1.59154 94309 18953D−01	5.00000 00000 00000D−01
3	2	1.15039 58119 72836D−01	3.91337 37887 53340D−01
		9.36546 45279 49632D−01	1.10866 26211 24666D+00
4	2	2.37964 72841 18974D−02	8.79594 26755 93887D−02
		2.93537 07415 01914D−01	4.98901 71529 13699D−01
		1.02371 51242 51890D+00	9.13138 85795 26912D−01
5	3	2.33901 30272 03800D−02	8.60973 65561 58105D−02
		2.85476 49313 11984D−01	4.84701 96854 17959D−01
		1.00540 33272 20700D+00	9.15298 88691 23725D−01
		1.99497 03039 94294D+00	1.01390 17789 84250D+00
6	3	4.00488 41949 26570D−03	1.67187 96911 47102D−02
		7.74565 53733 36686D−02	1.63695 83714 47360D−01
		3.97284 99935 23248D−01	4.98185 65697 70637D−01
		1.07567 33529 15104D+00	8.37226 62455 78912D−01
		2.00379 69271 11872D+00	9.84173 08440 88381D−01
8	5	6.53181 57085 67918D−03	2.46219 41989 95203D−02
		9.08674 45846 57729D−02	1.70131 58668 54178D−01
		3.96796 65333 75878D−01	4.60925 63586 50077D−01
		1.02785 66405 25646D+00	7.94729 11486 21894D−01
		1.94528 85929 09266D+00	1.00871 04143 37933D+00
		2.98014 79338 89640D+00	1.03609 36497 26216D+00
		3.99886 13499 51123D+00	1.00478 76565 33285D+00
10	6	1.17508 93812 27308D−03	4.56074 68820 84207D−03
		1.87703 41298 31289D−02	3.81060 63223 84757D−02
		9.68646 83914 26860D−02	1.29386 49972 89512D−01
		3.00481 86680 02884D−01	2.88436 03814 08835D−01
		6.90133 15571 73356D−01	4.95811 19143 44961D−01
		1.29369 57380 83659D+00	7.07715 46005 94529D−01
		2.09018 77297 98780D+00	8.74192 43652 85083D−01
		3.01671 93131 49212D+00	9.66136 19865 15218D−01
		4.00136 97478 72486D+00	9.95788 78660 78700D−01
		5.00002 56617 93423D+00	9.99866 57874 23845D−01

Table 8
(*Continued*)

l	a	v_i	u_i
12	7	1.67422 36826 68368D−03	6.36419 07807 20557D−03
		2.44111 00950 09738D−02	4.72396 41432 87529D−02
		1.15385 12974 29517D−01	1.45089 11583 85963D−01
		3.34589 84904 80388D−01	3.02165 94707 85897D−01
		7.32974 05318 07683D−01	4.98427 07397 15340D−01
		1.33230 50485 25433D+00	6.97121 37951 76096D−01
		2.11435 87523 25948D+00	8.57729 56227 57315D−01
		3.02608 45496 55318D+00	9.54413 65543 51155D−01
		4.00316 63012 92590D+00	9.91993 80527 76484D−01
		5.00014 11700 55870D+00	9.99462 18758 22987D−01
		6.00000 10024 41859D+00	9.99993 44080 92805D−01
14	9	9.30518 23685 45380D−04	3.54506 06447 80164D−03
		1.37383 24584 34617D−02	2.68151 40315 76498D−02
		6.63075 27607 79359D−02	8.50409 20350 93420D−02
		1.97997 13976 22003D−01	1.85452 62166 43691D−01
		4.50431 35038 16532D−01	3.25172 43748 83192D−01
		8.57188 86311 01634D−01	4.91155 37472 60108D−01
		1.43450 52296 17112D+00	6.62293 34173 69036D−01
		2.17517 78341 37754D+00	8.13725 45788 40510D−01
		3.04795 50683 86372D+00	9.23559 55149 44174D−01
		4.00497 49068 13428D+00	9.82160 99237 44658D−01
		4.99852 59018 20967D+00	1.00004 73945 96121D+00
		5.99952 30151 16678D+00	1.00090 93366 93954D+00
		6.99996 36178 83990D+00	1.00011 95342 83784D+00
		7.99999 94881 30134D+00	1.00000 28357 46089D+00
16	10	8.37152 98320 14113D−04	3.19091 90866 26234D−03
		1.23938 27255 42637D−02	2.42362 13804 26338D−02
		6.00929 07857 39468D−02	7.74013 55216 53088D−02
		1.80599 12496 01928D−01	1.70488 94202 86369D−01
		4.14283 25990 28031D−01	3.02912 34785 11309D−01
		7.96474 77311 12430D−01	4.65222 08349 14617D−01
		1.34899 38824 67059D+00	6.40148 96370 96768D−01
		2.07347 16602 64395D+00	8.05121 29461 81061D−01
		2.94790 49390 31494D+00	9.36241 19456 98647D−01
		3.92812 92522 48612D+00	1.01435 97753 69075D+00
		4.95720 30865 63112D+00	1.03516 77210 53657D+00
		5.98636 01139 77494D+00	1.02030 86249 84610D+00
		6.99795 77047 91519D+00	1.00479 83974 41514D+00
		7.99988 87575 24622D+00	1.00039 50173 52309D+00
		8.99999 87543 06120D+00	1.00000 71494 22537D+00

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