High-Order Quadratures for Integral Operators with Singular Kernels

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Abstract

A numerical integration method that has rapid convergence for integrands with known singularities is presented. Based on endpoint corrections to the trapezoidal rule, the quadratures are suited for the discretization of a variety of integral equations encountered in mathematical physics. The quadratures are based on a technique introduced by Rokhlin (*Computers Math. Applic.* **20**, pp. 51-62, 1990). The present modification controls the growth of the quadrature weights and permits higher-order rules in practice. Several numerical examples are included.

Abbreviated Title. Quadratures for Integral Equations

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1 Introduction

The discretization of a linear Fredholm integral equation of the second kind,

$$f(x) + \int_a^b K(x,t)\, f(t)\, dt = g(x), \tag{1}$$

where the kernel K is in $L^2([a,b]^2)$ and the right hand side g and unknown f are in $L^2([a,b])$, is typically obtained either by projection of the equation onto an n-dimensional subspace of L^2 (Galerkin method or method of moments), or by approximation of the integral at n points $\{x_1, \ldots, x_n\} \subset [a,b]$ by a quadrature,

$$\int_a^b K(x_i,t)\, f(t)\, dt \approx \sum_{j=1}^{n} w_{ij}\, K(x_i,x_j)\, f(x_j), \qquad i = 1,\ldots,n \tag{2}$$

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(Nyström method). Both methods lead to a system of n linear algebraic equations in n unknowns, which are then solved by one of a variety of techniques. It is well known that the rate of convergence of the Galerkin method is determined by the convergence of the subspace projections to the underlying functions, as well as the accuracy of the computed projection coefficients (inner products) for K and g. Also known, though perhaps less widely appreciated, is the fact that the Nyström solution converges, as a function of n, to the true solution f at a rate equal to the rate of convergence of the quadrature to the integral (see, e.g., Mikhlin [5]).

For a large variety of physical problems, the kernel K is singular for $x = t$, dooming most conventional quadrature schemes to slow convergence. Often, however, the kernel is derived from a Green's function with singularity of known type. For this case Rokhlin [6] constructed quadratures based on corrections to the trapezoidal rule. His scheme achieves kth order convergence by altering $2k$ weights to exactly integrate the functions $t^i \cdot s(x-t) + t^j$, for $i, j = 0, \ldots, k-1$, where the function s contains the singularity of K. Rokhlin's method is restricted to fairly low orders of convergence, due to explosive growth in magnitude of the altered weights with k. Starr [7] constructed quadratures based on points at Chebyshev nodes on subintervals of $[a, b]$, with quadrature weights again determined so that the functions $t^i \cdot s(x-t) + t^j$ are integrated exactly for $i, j = 0, \ldots, k-1$. To prevent the rapid growth of the quadrature weights with k, he allowed extra weights (e.g., $3k$ weights for $2k$ constraining equations) and minimized their sum of squares.

This paper introduces quadrature rules inspired by the rules of Rokhlin and Starr. Global rules are developed, based on corrections to the trapezoidal rule, that achieve arbitrary order convergence, with weights of small magnitude, for integrands with known singularities. The rules are constructed as follows:

1. For differentiable integrands on $[a, b]$, the trapezoidal rule is corrected at the endpoints according to the Euler-Maclaurin formula. The derivatives at a and b appearing in the Euler-Maclaurin formula are computed to the necessary order by finite-difference expressions of the integrand. The coefficients in the expressions are limited in magnitude by using values of the integrand at more points than dictated by the order of convergence.

2. For an integrand with a singularity of known type at x, the interval of integration is divided into subintervals $[a, x]$ and $[x, b]$ so that the singularity lies at one endpoint of each subinterval. The trapezoidal rule for each interval is corrected at the differentiable end according to 1. At the singular end, corrections are made so that the functions $t^i \cdot s(x-t) + t^j$ are integrated exactly, for $i, j = 0, \ldots, k-1$. Here the integrand is assumed to have the form $f(t) \cdot s(x-t) + g(t)$, where f and g have multiple continuous derivatives. As in 1., the correction weights are limited in magnitude by allowing more than $2k$ weights and minimizing their sum of squares.

We define these quadrature rules in §2, establish their analytical properties in §3, present numerical examples in §4, and conclude with a brief discussion in §5.

2 Corrected Trapezoidal Rules

It is well known that the trapezoidal rule for integration can be modified at the ends via the Euler-Maclaurin summation formula to a rapidly convergent rule, provided that the integrand is sufficiently differentiable. We will suppose, instead, that the integrand is singular at one end of the interval and the form of the singularity is known. In this case a modification at that end may be determined so that the corrected trapezoidal rule is rapidly convergent. In the following subsection, we define endpoint corrections, for differentiable integrands, that depend on the node spacing h for the trapezoidal rule with n subintervals, the order k of the corrected rule, the number of correction weights m, and the node spacing $h' = h/c$ of the corrections. In the following subsection, we use these corrections at the smooth end and define corrections at the singular end with order k', number of correction weights m', and correction node spacing $h'' = h/c'$.

2.1 Differentiable Integrands

We begin with the assumption that the integrand is differentiable throughout the interval of integration. For k an even positive integer, m a positive integer with $m > k$, and $c \in \mathbf{R}$, $c > 0$, we define the $1 \times m$ vector d_{ck}^m by the formula

$$d_{ck}^m = v_{ck} \cdot (M_k^m)^I, \tag{3}$$

where the $1 \times (k-1)$ vector v_{ck} is defined by

$$v_{ck} = \left\langle 0,\ \frac{B_2}{2!}c^2,\ 0,\ \frac{B_4}{4!}c^4,\ \ldots,\ 0,\ \frac{B_{k-2}}{(k-2)!}c^{k-2},\ 0 \right\rangle, \tag{4}$$

the $m \times (k-1)$ matrix M_k^m is defined by

$$M_k^m = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 1 & 1 & \frac{1}{2!} & \cdots & \frac{1}{(k-2)!} \\ 1 & 2 & \frac{2^2}{2!} & \cdots & \frac{2^{k-2}}{(k-2)!} \\ \vdots & & & & \vdots \\ 1 & m-1 & \frac{(m-1)^2}{2!} & \cdots & \frac{(m-1)^{k-2}}{(k-2)!} \end{pmatrix}, \tag{5}$$

B_j denotes the jth Bernoulli number (see, e.g., [1]), and superscript I denotes pseudoinverse (see, e.g., [3]). We define the linear operator $T_n(\cdot, a, b)$ by the formula

$$T_n(f,a,b) = h \cdot \left(\frac{1}{2}f(a) + f(a+h) + \ldots + f(b-h) + \frac{1}{2}f(b) \right), \tag{6}$$

and the linear operator $D_{ck}^{mn}(\cdot, a, b)$ by the formula

$$D_{ck}^{mn}(f,a,b) = h \cdot d_{ck}^m \cdot \begin{pmatrix} f(a) + f(b) \\ f(a+h') + f(b-h') \\ \vdots \\ f(a+(m-1)h') + f(b-(m-1)h') \end{pmatrix} \tag{7}$$

where $h = (b-a)/n$ and $h' = h/c$. For differentiable functions f, the expression $D_{ck}^{mn}(f,a,b)$ is a kth order correction to the trapezoidal rule.

Theorem 2.1 *Suppose the function $f : [a,b] \to \mathbf{R}$ is k times continuously differentiable. Then there exists $C > 0$ independent of n such that*

$$\left| \int_a^b f(x)\,dx - T_n(f,a,b) - D_{ck}^{mn}(f,a,b) \right| < \frac{C}{n^k}. \tag{8}$$

Proof. The Euler-Maclaurin formula (see, e.g., [3]) states

$$\begin{aligned} \int_a^b f(x)\,dx &= T_n(f,a,b) + \sum_{i=1}^{k/2-1} h^{2i}\,\frac{B_{2i}}{(2i)!}\,\left(f^{(2i-1)}(a) - f^{(2i-1)}(b)\right) \\ &\quad + h^k\,\frac{B_k}{k!}(a-b)f^{(k)}(\zeta), \end{aligned} \tag{9}$$

for some $\zeta \in [a,b]$. Taylor's expansion of f about a is

$$f(a + i\,h') = \sum_{j=0}^{k-2} f^{(j)}(a)\frac{(i\,h')^j}{j!} + f^{(k-1)}(\nu_i)\frac{(i\,h')^{k-1}}{(k-1)!}, \tag{10}$$

with $a \le \nu_i \le a + i\,h'$, for $i = 0, 1, \ldots, m-1$, which can be written in matrix form as

$$\begin{pmatrix} f(a) \\ f(a+h') \\ \vdots \\ f(a+(m-1)h') \end{pmatrix} = M_k^m \cdot \begin{pmatrix} f(a) \\ f'(a) \\ \vdots \\ f^{(k-2)}(a) \end{pmatrix} + \epsilon_{h'}, \tag{11}$$

where M_k^m is defined in (5) and $\epsilon_{h'}$ is a $(k-1) \times 1$ vector with elements of order $O((h')^{k-1})$. Similarly, we obtain

$$\begin{pmatrix} f(b) \\ f(b-h') \\ \vdots \\ f(b-(m-1)h') \end{pmatrix} = M_k^m \cdot \begin{pmatrix} f(b) \\ -f'(b) \\ \vdots \\ (-1)^{(k-2)}f^{(k-2)}(b) \end{pmatrix} + \epsilon'_{h'}. \tag{12}$$

The matrix M_k^m is of rank $k-1$, for the functions $x^j/j!$, for $j = 0, 1, \ldots$, form a Chebyshev system; hence

$$(M_k^m)^I\, M_k^m = I_{k-1}, \tag{13}$$

the identity matrix of dimension $k-1$. Combination of (7), (9), (11), (12), and (13) yields (8). □

Remark 2.2 Theorem 2.1 does not address the form of the dependence of C on f, a, b, k, c, and m. It is not difficult to see that C depends on $f^{(k)}(\zeta)$, for some $\zeta \in [a,b]$. It also depends on the accuracy of the finite-difference approximations to the odd derivatives of f, as represented by D_{ck}^{mn}. While the order of these approximations is $O(h^k)$, the constant depends on m/c, as will be seen in the examples. For m/c small, the error is dominated by the Euler-Maclaurin error $h^k f^{(k)}(\zeta)(a-b)B_k/k!$.

2.2 Singular Integrands

We now consider integrands of the form

$$f(x) = \phi(x) \cdot s(x) + \psi(x) \tag{14}$$

for all $x \in (0,b]$, where $\phi, \psi \in C^k([0,b])$ and the function $s \in C^k((0,b])$ is singular at 0, but integrable on the interval $[0,b]$. We assume that the numerical separation of f into the two summands of (14) is unavailable in practice; for quadratures in the contrary case see Kress [4]. We will see that endpoint corrections of the trapezoidal rule which make the quadrature exact for functions $x^i \cdot s(x) + x^j$, for $i,j = 0,\ldots,k-1$, are in general kth order convergent. We define the right-end corrected rule $R_{ck}^{mn}(\cdot, b)$ by the formula

$$R_{ck}^{mn}(f,b) = T_n'(f,b) + h \cdot d_{ck}^m \cdot \begin{pmatrix} f(b) \\ f(b-h') \\ \vdots \\ f(b-(m-1)h') \end{pmatrix}, \tag{15}$$

where the linear operator $T_n'(\cdot, b)$ is defined by

$$T_n'(f,b) = h \cdot \left(f(h) + f(2h) + \cdots + f(b-h) + \frac{1}{2} f(b) \right) \tag{16}$$

and d_{ck}^m is defined by (3); $h = b/n$ and $h' = h/c$. We denote the error of the right-end corrected rule as follows:

$$E_{ck}^{mn}(f,b) = \int_0^b f(x)\,dx - R_{ck}^{mn}(f,b). \tag{17}$$

For positive integers k' and m', and $c' \in \mathbf{R}$, $c' > 0$, we define the $1 \times m'$ vector $\delta_{ckc'k'}^{mm'n}$ by the formula

$$\delta_{ckc'k'}^{mm'n} = h^{-1} \cdot u_{ckk'}^{mn} \cdot (L_{c'k'}^{m'n})^I, \tag{18}$$

where the $1 \times 2k'$ vector $u_{ckk'}^{mn}$ is defined by

$$\begin{aligned} u_{ckk'}^{mn} = \; & \Big\langle E_{ck}^{mn}(1,b), \ldots, E_{ck}^{mn}(x^{k'-1}, b), \\ & E_{ck}^{mn}(s(x),b), \ldots, E_{ck}^{mn}(x^{k'-1} \cdot s(x), b) \Big\rangle, \end{aligned} \tag{19}$$

and the $m' \times 2k'$ matrix $L^{m'n}_{c'k'}$ is defined by

$$L^{m'n}_{c'k'} = \begin{pmatrix} 1 & h'' & \cdots & (h'')^{k'-1} & s(h'') & \cdots & (h'')^{k'-1} \cdot s(h'') \\ 1 & 2h'' & \cdots & (2h'')^{k'-1} & s(2h'') & \cdots & (2h'')^{k'-1} \cdot s(2h'') \\ \vdots & & & \vdots & \vdots & & \vdots \\ 1 & m'h'' & \cdots & (m'h'')^{k'-1} & s(m'h'') & \cdots & (m'h'')^{k'-1} \cdot s(m'h'') \end{pmatrix}, \quad (20)$$

where $h'' = h/c'$ and $h = b/n$. We define the linear operator $\Delta^{mm'n}_{ckc'k'}(\cdot, b)$ by the formula

$$\Delta^{mm'n}_{ckc'k'}(f, b) = h \cdot \delta^{mm'n}_{ckc'k'} \cdot \begin{pmatrix} f(h'') \\ f(2h'') \\ \vdots \\ f(m'h'') \end{pmatrix}, \quad (21)$$

and the following theorem holds. Its proof is based on the observation that the integrand f is the sum of two parts, one integrated exactly, and the other vanishing at 0 along with several of its derivatives. The proof directly follows that of Theorem 2.1 in [6], and is omitted.

Theorem 2.3 *Suppose the function $f : [a, b] \to \mathbf{R}$ is given by (14), and that the elements of $\delta^{mm'n}_{ckc'k'}$ defined in (18) are bounded with respect to n. Then there exists $C > 0$ independent of n such that*

$$\left| \int_0^b f(x)\, dx - R^{mn}_{ck}(f, b) - \Delta^{mm'n}_{ckc'k'}(f, b) \right| < \frac{C}{n^{\min(k,k')}}. \quad (22)$$

We will see that the condition on $\delta^{mm'n}_{ckc'k'}$ is met if $k' < k$, i.e., if the correction at the smooth end is of higher order than the correction at the singular end. In this case, then, we obtain quadrature rules with order of convergence k', which is arbitrary. In the next section we demonstrate that the other parameters determining the quadrature weights can be chosen so that the convergence is not overshadowed by roundoff error.

3 The Size of the Correction Weights

It is well known that Newton-Cotes quadrature rules, with n equispaced nodes, and weights determined so as to exactly integrate polynomials of degree less than n, are impractical for large n due to explosively growing weights (see, e.g., [8]). It might be expected that finite-difference approximations to the high-order Euler-Maclaurin corrections to the trapezoidal rule would suffer a similar fate, which is indeed the case. But the size of the weights can be controlled by using more weights than the order of the rule and (for the Euler-Maclaurin corrections) by increasing the spacing between correction nodes. The following theorem governs the behavior of the elements of d^m_{ck} as c and m are varied.

Theorem 3.1 *Suppose the vector d^m_{ck} of correction coefficients is defined by (3). Then we have the limit*

$$\lim_{m\to\infty} \max_{1\le i\le m} |(d^m_{ck})_i| = 0; \quad (23)$$

furthermore, for any $\gamma \in \mathbf{R}$, $\gamma > 0$, the value

$$\max_{1 \le i \le m} |(d^m_{\gamma \cdot m, k})_i| \tag{24}$$

is bounded with respect to m.

Proof. Let $\gamma = c/m$ (not necessarily a constant). We rearrange equation (3) for d^m_{ck} to obtain

$$d^m_{ck} = \left\langle 0, \frac{B_2}{2}\gamma^2, \ldots, \frac{B_{k-2}}{k-2}\gamma^{k-2}, 0 \right\rangle \cdot m \cdot \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 1 & \frac{1}{m} & \cdots & (\frac{1}{m})^{k-2} \\ \vdots & & & \vdots \\ 1 & \frac{m-1}{m} & \cdots & (\frac{m-1}{m})^{k-2} \end{pmatrix}^I, \tag{25}$$

where we denote the vector on the right hand side by $\tilde{v}_{\gamma k}$ and the matrix by $(\tilde{M}^m_k)^I$. We denote the sequence of orthonormal (shifted and scaled Legendre) polynomials for the interval $[0,1]$ by $p_0, p_1, \ldots$; the moments β_{ij} are defined by the formula

$$\beta_{ij} = \int_0^1 p_i(x)\, x^j \, dx, \qquad i, j = 0, 1, 2, \ldots, \tag{26}$$

the $(k-1) \times (k-1)$ matrix β_k by

$$\beta_k = \{\beta_{ij}\}_{i=0,\ldots,k-2;\, j=0,\ldots,k-2}, \tag{27}$$

and the $(k-1) \times m$ matrix $\mathcal{M}^m_k$ by

$$\mathcal{M}^m_k = \{p_i(j/m)\}_{i=0,\ldots,k-2;\, j=0,\ldots,m-1}. \tag{28}$$

We obtain

$$\lim_{m \to \infty} \frac{1}{m} \cdot \mathcal{M}^m_k \cdot \tilde{M}^m_k = \beta_k \tag{29}$$

from the observation that each element of the matrix on the left is a rectangular-rule quadrature for the corresponding element on the right. For a vector v we let $\|v\|$ denote $\max_i |v_i|$. Combining (25) and (29) we have

$$\begin{aligned} \lim_{m \to \infty} \|d^m_{ck}\| &= \lim \left\| \tilde{v}_{\gamma k} \cdot m \cdot (\tilde{M}^m_k)^I \right\| \\ &\le \lim \left\| \tilde{v}_{\gamma k} \left((m^{-1} \tilde{M}^m_k)^I - {\beta_k}^{-1} \mathcal{M}^m_k \right) \right\| + \lim \left\| \tilde{v}_{\gamma k} \cdot {\beta_k}^{-1} \mathcal{M}^m_k \right\| \\ &= \lim \left\| \tilde{v}_{\gamma k} \cdot {\beta_k}^{-1} \mathcal{M}^m_k \right\|, \end{aligned}$$

if γ is bounded. If γ is a constant, the latter limit is bounded by $\left\| \tilde{v}_{\gamma k} \cdot {\beta_k}^{-1} \right\| \cdot (k-1) \sup |p_i(x)|$, where the supremum is taken over $x \in [0,1]$ and $i \le k-2$, giving (24); if $\gamma \to 0$ as $m \to \infty$, then the limit is 0, yielding (23). □

Theorem 3.1 implies that we can choose the number of correction weights m and their relative spacing $c = h/h'$ such that c/m, and magnitude of the largest correction weight, is as small as desired. The tradeoff is that the quadrature error constant increases as c/m decreases; our experiments indicate, however, that a favorable balance is possible. A similar situation exists for the singularity correction weights $\delta^{mm'n}_{ckc'k'}$.

Theorem 3.2 *Suppose that for $s(x) = x^\alpha$ with $0 < |\alpha| < 1$, the vector $\delta^{mm'n}_{ckc'k'}$ of correction weights is defined by (18), with $k' < k$. Then for any $\gamma \in \mathbf{R}$, $\gamma > 0$, the value*

$$\max_{1 \le i \le m'} |(\delta^{m,m',n}_{c,k,\gamma \cdot m',k'})_i| \tag{30}$$

is bounded with respect to m' and n, and furthermore, we have the limit

$$\lim_{m' \to \infty} \max_{1 \le i \le m'} |(\delta^{mm'n}_{ckc'k'})_i| = 0. \tag{31}$$

Proof. Let $\gamma = c'/m'$. We rearrange (18) to obtain

$$\delta^{mm'n}_{ckc'k'} = h^{-1} \cdot \tilde{u}^{mm'n}_{ckc'k'} \cdot (\tilde{L}^{m'}_{k'})^I, \tag{32}$$

where the $1 \times 2k'$ vector $\tilde{u}^{mm'n'}_{ckc'k'}$ is defined by

$$\begin{aligned} \tilde{u}^{mm'n'}_{ckc'k'} = & \Big\langle E^{mn}_{ck}(1,b)/1, \ldots, E^{mn}_{ck}(x^{k'-1},b)/(m'h'')^{k'-1}, \\ & E^{mn}_{ck}(x^\alpha,b)/(m'h'')^\alpha, \ldots, E^{mn}_{ck}(x^{\alpha+k'-1},b)/(m'h'')^{\alpha+k'-1} \Big\rangle, \end{aligned} \tag{33}$$

and the $m' \times 2k'$ matrix $\tilde{L}^{m'}_{k'}$ is defined by

$$\tilde{L}^{m'}_{k'} = \begin{pmatrix} 1 & \frac{1}{m'} & \cdots & (\frac{1}{m'})^{k'-1} & (\frac{1}{m'})^\alpha & \cdots & (\frac{1}{m'})^{\alpha+k'-1} \\ 1 & \frac{2}{m'} & \cdots & (\frac{2}{m'})^{k'-1} & (\frac{2}{m'})^\alpha & \cdots & (\frac{2}{m'})^{\alpha+k'-1} \\ \vdots & & & \vdots & \vdots & & \vdots \\ 1 & 1 & \cdots & (1)^{k'-1} & (1)^\alpha & \cdots & (1)^{\alpha+k'-1} \end{pmatrix}. \tag{34}$$

We now use the observation (see [6]) that for $p > -1$ and a quadrature $R^{mn}_{ck}(x^p, b)$ of right-end order $k \ge 2$, there is a constant $C > 0$ such that for $p < k$,

$$\left| \int_0^b x^p \, dx - R^{mn}_{ck}(x^p, b) \right| < \frac{C}{n^{p+1}}. \tag{35}$$

Combining (17), (33), and (35) we obtain

$$\left|(\tilde{u}^{mm'n'}_{ckc'k'})_i\right| = \frac{\left|E^{mn}_{ck}(x^{i-1},b)\right|}{(m'h'')^{i-1}} < \frac{C_i}{n(b/\gamma)^{i-1}}, \tag{36}$$

$$\left|(\tilde{u}^{mm'n'}_{ckc'k'})_{i+k}\right| = \frac{\left|E^{mn}_{ck}(x^{\alpha+i-1},b)\right|}{(m'h'')^{\alpha+i-1}} < \frac{C_{i+k}}{n(b/\gamma)^{\alpha+i-1}}, \tag{37}$$

for $i = 1, \ldots, k'$. The pseudoinverse of $\tilde{L}^{m'}_{k'}$ is bounded, as can be shown by a derivation similar to that in the proof of Theorem 2.3. The combination of (32), (36), (37), and the bound for $(\tilde{L}^{m'}_{k'})^I$ yields (30), for γ bounded, and (31), if $c' = \gamma \cdot m$ is a constant. □

4 Numerical Examples

4.1 Differentiable Integrands

The well-known fourth order quadrature formula (see, e.g., [9])

$$\int_a^b f(x)\,dx \;\approx\; h\cdot\left(\frac{3}{8}f(a)+\frac{7}{6}f(a+h)+\frac{23}{24}f(a+2h)+f(a+3h)+\cdots\right.$$
$$\left.+\,f(b-3h)+\frac{23}{24}f(b-2h)+\frac{7}{6}f(b-h)+\frac{3}{8}f(b)\right)$$

is the rule $T_n(f,a,b)+D_{ck}^{mn}(f,a,b)$ with $c=1$ and $m=k-1=3$. In this case, $d_{ck}^m = \langle -1/8, 1/6, -1/24\rangle$. Various other values of d_{ck}^m are given in Table 1.

We have tested the convergence of these rules for the function $f(x)=\sin(23x)+\cos(24x)$ on the interval $[0,1]$. The errors for various parameter choices are shown in Table 2, as computed with double precision arithmetic. It can be seen that the rules perform well and the expected order of convergence is achieved in each case. The close spacing of the corrections for $c=k$ reduces the error considerably, compared with $c=1$. The largest correction weight for $c=k=m/2=12$ has magnitude $\approx 3h/2$, so cancellation errors are minimal.

Table 1: *Endpoint corrections transform the familiar trapezoidal rule into a high-order quadrature for functions with several continuous derivatives. The quadrature rules are given by the formula* $\int_a^b f(x)\,dx = T_n(f,a,b) + h\sum_{i=1}^m (d_{ck}^m)_i\,[f(a+(i-1)\,h') + f(b-(i-1)\,h')] + O(h^k)$*, where* $h=(b-a)/n$*,* $h'=h/c$*, and* $T_n(f)=h\,[\frac{1}{2}f(a)+f(a+h)+\cdots+f(b-h)+\frac{1}{2}f(b)]$*. The elements* $(d_{ck}^m)_i$ *are tabulated as* N_i/D*.*

$c=1 \qquad m=k-1$

	$k=2$	$k=4$	$k=6$	$k=8$	$k=10$	$k=12$
D	1	24	1,440	120,960	7,257,600	958,003,200
N_1	0	−3	−245	−23,681	−1,546,047	−216,254,335
N_2		4	462	55,688	4,274,870	679,543,284
N_3		−1	−336	−66,109	−6,996,434	−1,412,947,389
N_4			146	57,024	9,005,886	2,415,881,496
N_5			−27	−31,523	−827,7760	−3,103,579,086
N_6				9,976	5,232,322	2,939,942,400
N_7				−1,375	−2,161,710	−2,023,224,114
N_8					526,154	984,515,304
N_9					−57,281	−321,455,811
N_{10}						63,253,516
N_{11}						−5,675,265

Table 2: *Errors for the application of the corrected trapezoidal rules* $T_n(f,a,b)+D_{ck}^{mn}(f,a,b)$ *to the function* $f(x)=\sin(23x)+\cos(24x)$ *on the interval* $[a,b]=[0,1]$*, as computed using double precision arithmetic.*

	$c=1$	$m=k-1$		$c=k$	$m=2k$	
n	$k=4$	$k=8$	$k=12$	$k=4$	$k=8$	$k=12$
10	1.70E−02	1.83E−02	—	1.49E−02	6.92E−4	1.10E−06
20	5.32E−04	1.78E−04	4.43E−04	3.79E−04	3.07E−07	3.75E−10
40	1.21E−05	4.33E−06	1.17E−07	1.35E−05	5.10E−10	5.34E−14
80	2.38E−06	9.83E−09	9.14E−11	2.13E−06	1.83E−13	2.90E−15
160	1.99E−07	9.60E−12	1.51E−14	1.72E−07	3.00E−16	3.00E−16
320	1.39E−08	2.85E−14	2.20E−15	1.20E−08	3.80E−15	1.00E−16

Table 3: *Limiting values as* $n\to\infty$ *of endpoint corrections* $\delta_{ckc'k'}^{mm'n}$ *for three different singularities. Here* $c=k=m/3=16$ *and* $k'=4$.

$c'=8 \qquad m'=8$

$s(x)=x^{-1/2}$	$s(x)=\log(x)$	$s(x)=x^{1/2}$
.7889576157976986E+01	.3093483401777122E+01	.1761384695584808E+01
−.1014839102693306E+03	−.3101788376740790E+02	−.1382118344852977E+02
.4982052353339497E+03	.1362059155903270E+03	.5459150117813370E+02
−.1241778604543411E+04	−.3147474808724214E+03	−.1173574845498706E+03
.1751093993580452E+04	.4215054127612634E+03	.1507790199321616E+03
−.1419085152097947E+04	−.3287854038787327E+03	−.1147784911579322E+03
.6179863268019096E+03	.1388011671370668E+03	.4762309598361213E+02
−.1123274649636003E+03	−.2455521037187227E+02	−.8297842633159577E+01

$c'=4 \qquad m'=16$

$s(x)=x^{-1/2}$	$s(x)=\log(x)$	$s(x)=x^{1/2}$
.8462579989929540E+01	.3448173692662518E+01	.2050559756045592E+01
−.5435908661112594E+02	−.1601143873638304E+02	−.6865912494117176E+01
.1004033238128716E+03	.2427502641368332E+02	.8491285270322254E+01
−.1562169259798149E+02	.4722206428800859E+00	.1705242848943216E+01
−.6374313277726896E+02	−.1447823711138307E+02	−.4604469053907677E+01
−.3072510651936008E+02	−.9989335956026066E+01	−.4354220712239432E+01
.2115143836148849E+02	.2211594559407416E+01	−.3188321047055960E+00
.4683397742937565E+02	.1043094039079357E+02	.3251630138161534E+01
.3502121990978420E+02	.9802590813947814E+01	.3885773620301128E+01
−.1616432670704066E+00	.2167076760778314E+01	.1580226691059038E+01
−.3336312819210096E+02	−.6661869944148136E+01	−.1806976420043709E+01
−.4173860435447336E+02	−.1034071990767905E+02	−.3745300019759054E+01
−.1641816344862332E+02	−.5384782825493895E+01	−.2450268607844168E+01
.2850714644518526E+02	.5793630843054246E+01	.1662082464711006E+01
.4919461810492213E+02	.1228302599763183E+02	.4590184679455359E+01
−.3294374628555238E+02	−.7517895633725869E+01	−.2571006056382313E+01

4.2 Singular Integrands

Several examples have been computed for singular integrands. The test function $f(x) = \sin(23x) + \cos(24x) + s(x)(\sin(21x) + \cos(22x))$ was used, for the singular part $s(x)$ one of the functions $x^{-1/2}$, $\log(x)$, and $x^{1/2}$. The correction coefficients were computed using REAL *16 (quadruple precision) arithmetic, due to the poor conditioning of the small scale linear systems to be solved. Note that although the correction coefficients differ for various n, they reach limiting values as $n \to \infty$ (see [6]); this property enables us to compute them for several n and obtain them for other values of n by interpolation.

Table 3 shows the limiting values of the correction coefficients for $k' = 4$. For each of the three singularities, two values of the pair (c', m') were used. These results demonstrate that while the correction coefficients are rather large for $k' = 4$, their size can be controlled (to avoid cancellation errors) by decreasing c' and increasing m'. Table 4 displays the quadrature errors resulting from using the correction coefficients on the test function. The quadrature computations were made using double precision arithmetic. These examples demonstrate that with appropriate choices of the parameters c, k, c', k', m and m', effective, high-order quadratures for known singularities are practical.

Table 4: *Errors for the application of the corrected trapezoidal rules* $R^{mn}_{ck}(f,b) + \Delta^{mm'n}_{ckc'k'}(f,b)$ *to the function* $f(x) = \sin(23x) + \cos(24x) + s(x)(\sin(21x) + \cos(22x))$*, for three choices of the singular function* $s(x)$*, on the interval* $[0,b] = [0,1]$*, as computed using double precision arithmetic. Here* $c = k = m/3 = 16$.

$c' = m' = 2k'$

	$s(x) = x^{-1/2}$		$s(x) = \log(x)$		$s(x) = x^{1/2}$	
n	$k = 4$	$k = 8$	$k = 4$	$k = 8$	$k = 4$	$k = 8$
10	2.97E−02	2.04E−05	6.70E−03	1.91E−06	9.12E−03	9.83E−07
20	1.27E−03	1.51E−08	3.59E−05	4.06E−10	7.86E−07	3.34E−10
40	1.41E−05	3.36E−09	4.78E−07	7.49E−11	1.53E−07	9.15E−12
80	5.12E−07	3.21E−09	7.01E−10	1.58E−10	4.46E−09	4.55E−11
160	1.73E−08	1.34E−10	2.71E−10	5.21E−12	1.12E−10	2.87E−14
320	6.12E−10	1.36E−11	1.61E−11	3.83E−13	2.88E−12	7.19E−15

$c' = k \quad m' = 4k'$

	$s(x) = x^{-1/2}$		$s(x) = \log(x)$		$s(x) = x^{1/2}$	
n	$k = 4$	$k = 8$	$k = 4$	$k = 8$	$k = 4$	$k = 8$
10	1.07E+01	2.17E+00	2.29E−01	1.14E−01	2.75E−01	4.51E−02
20	1.81E−01	8.13E−04	8.01E−03	2.20E−05	3.32E−03	1.55E−05
40	2.97E−03	7.98E−07	1.83E−04	3.29E−08	7.93E−05	7.63E−09
80	4.76E−05	2.26E−10	4.99E−06	1.45E−11	3.77E−07	3.45E−12
160	2.68E−06	3.67E−12	5.31E−08	1.51E−13	2.45E−08	1.26E−14
320	9.35E−08	6.62E−14	4.67E−10	1.64E−14	6.58E−10	3.08E−16

5 Discussion

In this paper we have developed quadratures based on the trapezoidal rule that achieve high-order convergence for integrands with known singularities. These rules, with quadrature nodes that are equispaced except for the correction terms, are well suited to the evaluation of integral operators, which typically must be evaluated at multiple points. We remark that the locations of the density values can be equispaced, with the values at correction nodes determined by local interpolation (see, e.g., [2]).

The quadratures presented here overcome a limitation of similar quadratures developed by Rokhlin [6], namely that the correction weights grow rapidly with increasing order. The slowdown in growth is achieved by allowing more correction weights than required by the number of constraining equations and minimizing their sum of squares.

We have demonstrated the asymptotic behavior of the quadratures and the quadrature weights analytically, while giving numerical examples to demonstrate their effectiveness for typical parameter values.

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