High-Order Corrected Trapezoidal Quadrature Rules for Functions with a Logarithmic Singularity in 2-D

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Abstract

In this report we construct correction coefficients to obtain high-order trapezoidal quadrature rules to evaluate 2-dimensional integrals with a logarithmic singularity of the form

$$J(v) = \int_D v(x,y)\ln(\sqrt{x^2+y^2})dxdy,$$

where the domain D is a square containing the point of singularity $(0,0)$ and v is a C^∞ function defined on the whole plane $\mathbb{R}^2$. The procedure we use is a generalization to 2-D of the method of central corrections for logarithmic singularities described in [1]. As in 1-D, the correction coefficients are independent of the number of sampling points used to discretize the square D. When v has compact support contained in D, the approximation is the trapezoidal rule plus a local weighted sum of the values of v around the point of singularity. These quadrature rules give an efficient, stable and accurate way of approximating $J(v)$. We provide the correction coefficients to obtain corrected trapezoidal quadrature rules up to order 20.

1 Introduction

Some important mathematical models of a physical problem in 2-D involve the evaluation of an integral of the form

$$J(v) = \int_D v(x,y)\ln(\sqrt{x^2+y^2})dxdy, \tag{1}$$

where v is a C^∞ function defined on the whole plane $\mathbb{R}^2$, and the domain D is a square containing the point $(0,0)$ of singularity. An example where an integral of the type (1) appears is the Lippmann-Schwinger equation of the scattering problem associated with the Helmholtz equation in 2-D (see [2] for example). A stable, accurate, and efficient

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evaluation of the integral (1) is desirable to approximate the solution efficiently in such applications. In [1] it is described a corrected trapezoidal quadrature rule to approximate integrals with a logarithmic singularity in 1-D. The method we use is a generalization of the method of central corrections of [1]. An important feature of these quadrature rules is that they remain stable for very high-orders (see [1]). Another feature is that the correction added to the trapezoidal rule involves a weighted sum of a few values of v, where the weights are independent of the number of points used to discretize the square D (assuming that the sampling points are distributed uniformly on D). In some instances the function v has compact support contained in D; this produces some reduction in the computational cost. This important case is also described.

2 Definitions and notation

In this section we describe the definitions and notation that will be used in this work . For the remaining of this report $D = [a_1, b_1] \times [a_2, b_2]$ will denote a square that contains the point $(0, 0)$, $v : \mathbb{R}^2 \to \mathbb{R}$ will be a C^∞ function, and $f : \mathbb{R}^2 \backslash \{(0, 0)\} \to \mathbb{R}$ a function defined as

$$f(x, y) = v(x, y) \ln(\sqrt{x^2 + y^2}). \tag{2}$$

Therefore our goal is to approximate the integral

$$J(v) = \int_D f(x, y) dxdy \tag{3}$$

using a corrected trapezoidal rule. We first discretize the square $D = [a_1, b_1] \times [a_2, b_2]$ using a uniform grid containing n points on each side. Thus $h = (b_1 - a_1)/(n - 1)$ is the distance between sampling points, and the square D is discretized using the n^2 grid points

$$P_{i,j} = (a_1 + ih, a_2 + jh), \qquad i, j = 0, \ldots, n - 1. \tag{4}$$

In this report we will assume that the square D contains the point $(0, 0)$ and that $(0, 0)$ is one of the grid points of $\{P_{i,j}\}$. The trapezoidal rule applied to a function $g : \mathbb{R}^2 \to \mathbb{R}$ on the square D and with respect to the set of grid points $\{P_{i,j}\}$ will be denoted by $T_h(g)$ and can be defined as successive applications of the trapezoidal rule in 1-D, that is,

$$T_h(g) = h^2 \left(\sum_{j=1}^{n-2} S_j + \frac{1}{2}(S_0 + S_{n-1}) \right), \tag{5}$$

where

$$S_j = \sum_{i=1}^{n-2} g(P_{i,j}) + \frac{1}{2}(g(P_{0,j}) + g(P_{n-1,j})) \quad \text{for } j = 0, \ldots, n - 1. \tag{6}$$

As it is well-known, if the function g has m continuous derivatives and if either g is periodic in $\mathbb{R}^2$ with period equal to the length of each side of the square D or if g has compact support contained in D, then it follows from the Euler-Maclaurin summation formula (see [3], [4], [5]) that $T_h(g)$ converges to the integral $\int_D g(x, y) dxdy$ at the rate

$$\int_D g(x, y) dxdy - T_h(g) = O(h^m). \tag{7}$$

If g is either non-smooth or non-periodic then $\int_D g(x,y)dxdy - T_h(g)$ is at most $O(h^2)$. Since the type of functions f we want to integrate in this report are both non-periodic and singular (with a logarithmic singularity), there will be two type of corrections to the trapezoidal rule:

1) *Boundary correction* to account for the non-periodicity of f
2) *Logarithmic correction* to account for the logarithmic singularity of f at $(0,0)$.

We will specify in the next section both type of corrections. In the remaining of this section we will describe some definitions and notation used by the logarithmic correction. Let $\{P_{i,j}\}$ be the set of grid point that discretize D (see formula (4)). Assuming that $(0,0)$ is one grid point, we can extend the set of grid points $\{P_{i,j}\}$ to the whole plane by defining

$$G = \{(ph, qh) | p, q \in \mathbf{Z}\}. \tag{8}$$

Consider now a partition of the set of grid points G into groups according to their distance to the origin: two grid points (p_1h, q_1h) and (p_2h, q_2h) belong to the same group if they are located at the same distance from the origin, $p_1^2 + q_1^2 = p_2^2 + q_2^2$ (see Figure 1). Each group contains exactly one grid point (sh, th) such that the integers s and t satisfy $s \geq 0$ and $0 \leq t \leq s$; such group will be designated as the $r-th$ group, where r and the grid point (sh, th) are related by the formula

$$r = \frac{s(s+1)}{2} + t + 1. \tag{9}$$

We will denote the $r-th$ group by G_r or by $G_{(s,t)}$ (see Figure 1). To each group $G_{(s,t)}$ we associate the monomial function

$$g_r(x,y) = x^{2s}y^{2t}. \tag{10}$$

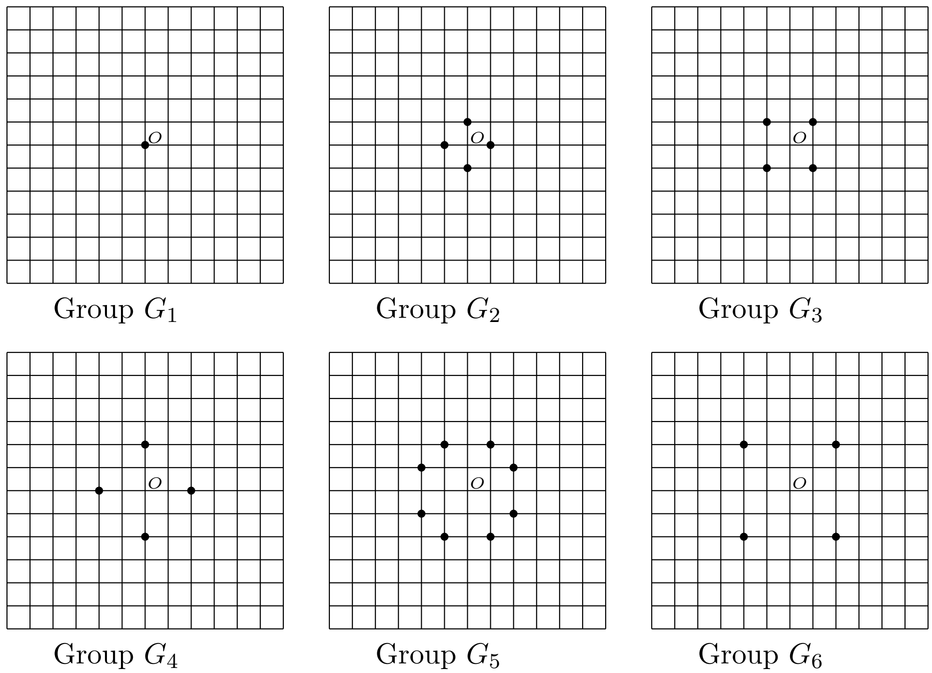


Figure 1: The set $G = \{(ph, qh)|p, q \in \mathbf{Z}\}$ of grid points is partitioned into groups. Two grid points belong to the same group if they are located at the same distance from the origin $O = (0, 0)$. Thus $G_1 = \{(0, 0)\}$, $G_2 = \{(h, 0), (-h, 0), (0, h), (0, -h)\}$, and so on.

In the next sections we will use the previous notation and definitions to describe a corrected trapezoidal rule that approximates the integral (1).

3 Boundary and logarithmic correction

The corrected trapezoidal rule with a logarithmic singularity requires two type of corrections. The first correction is on the boundary of the domain D; this correction is used when the integrand f of (1) is non-periodic. The other type of correction is due to the singularity of logarithm at $(0, 0)$.

3.1 Boundary correction

Boundary correction is discussed in [1] for smooth functions defined on the real line $\mathbb{R}$; boundary correction in 2-D is just successive applications of the 1-D case: according to the notation of ([1]), let m be a positive odd integer and β_k^m, $k = 1, \ldots, (m-1)/2$

be the $(m-1)/2$ coefficients for boundary correction (see [1]). If $\{P_{i,j}\}$ is the grid used to discretize the square D (as defined in (4)) and $g : \mathbb{R}^2 \to \mathbb{R}$ is a function, then the boundary corrected trapezoidal rule applied to g is denoted by $T^n_{\beta^m}(g)$, n being the number of equally spaced sampling points on each side of the square D, and is given by the formula

$$T^n_{\beta^m}(g) = h^2 \sum_{j=1}^{n-2} S_j + \frac{h^2}{2}(S_0 + S_{n-1}) + h^2 \sum_{k=1}^{\frac{m-1}{2}} \left(-S_{-k} + S_k + S_{n-1-k} - S_{n-1+k}\right) \beta^m_k \quad (11)$$

where

$$\begin{aligned} S_j &= \sum_{i=1}^{n-2} g(P_{i,j}) + \frac{1}{2}(g(P_{0,j}) + g(P_{n-1,j})) \\ &+ \sum_{k=1}^{\frac{m-1}{2}} \left(-g(P_{-k,j}) + g(P_{k,j}) + g(P_{n-1-k,j}) - g(P_{n-1+k,j})\right) \beta^m_k, \end{aligned} \quad (12)$$

for $j = -(m-1)/2, \ldots, n-1+(m-1)/2$.

If the function g has $m+1$ continuous derivatives then (see [1])

$$\int_D g(x,y)dxdy - T^n_{\beta^m}(g) = O(h^{m+1}). \quad (13)$$

Thus the boundary corrected trapezoidal rule $T^n_{\beta^m}(g)$ consists of the trapezoidal rule plus a weighted sum of values of g evaluated at grid points close to the boundary of the square $D = [a_1, b_1] \times [a_2, b_2]$. For a boundary correction of order $m+1$ the correction takes place near the boundary of the square $[-(m-1)h/2 + a_1, b_1 + (m-1)h/2] \times [-(m-1)h/2 + a_2, b_2 + (m-1)h/2]$ (see Figure 2).

To use the boundary corrected trapezoidal rule when the function is of the form $f(x,y) = \ln(\sqrt{x^2+y^2})v(x,y)$, which is not defined at $(0,0)$, define the punched boundary corrected trapezoidal rule as

$$T^n_{0,\beta^m}(f) = T^n_{\beta^m}(\tilde{f}) \quad (14)$$

where

$$\tilde{f}(x,y) = \begin{cases} f(x,y) & \text{if } (x,y) \neq (0,0) \\ 0 & \text{if } (x,y) = (0,0). \end{cases} \quad (15)$$

Since $\tilde{f}$ is not smooth at $(0,0)$, the boundary corrected trapezoidal rule $T^n_{\beta^m}(\tilde{f})$ gives a poor approximation to the integral (1). A logarithmic correction term needs to be added to the boundary correction term in order to improve the order of convergence. This correction is described in the next section.

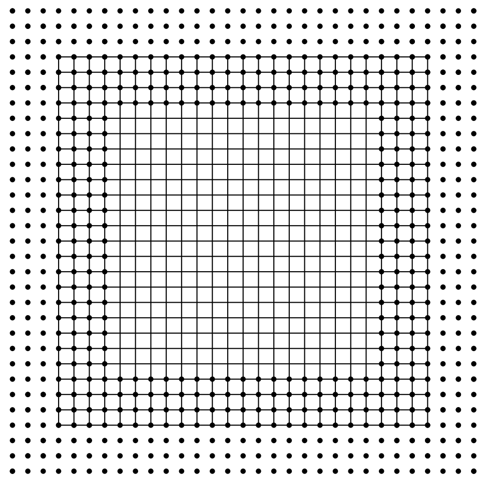


Figure 2: Boundary correction is done on the grid points near the boundary of the square $D = [a_1, b_1] \times [a_2, b_2]$ and on some grid points outside D. In the figure it is illustrated the case $m = 7$ or 8th order boundary correction. The extended grid shown corresponds to the set of grid points $\{P_{i,j}\}$ for $i, j = -(m-1)/2, , ..., n-1+(m-1)/2$, with $P_{i,j}$ as defined in (4).

3.2 Logarithmic correction

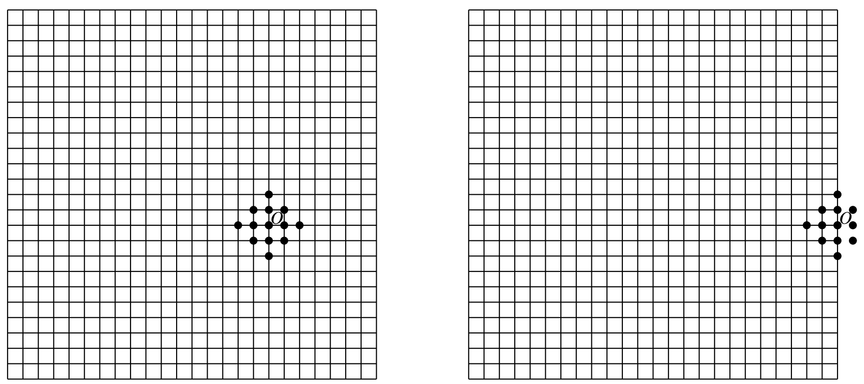
Logarithmic correction is needed due to the singularity of the function f at $(0, 0)$. This type of correction added to the boundary correction $T^n_{0,\beta^m}(f)$ will increase the rate of convergence to the integral (1). If v is the C^∞ function related to f by the formula (2), the logarithmic correction is computed by means of a weighted sum of the values of v at neighboring points of $(0, 0)$. The way we define such weighted sum is an extension to 2-D of the method of central corrections in 1-D described in [1]. More explicitly, we will find a vector of k correction coefficients $\mathbf{c}^k = (c_1, \ldots, c_k)$ so that the logarithmic correction $L^n_{\mathbf{c}^k}(v)$, defined as

$$L^n_{\mathbf{c}^k}(v) = h^2 \log(h) v(0, 0) + h^2 \left(\sum_{r=1}^{k} c_r \sum_{(ph,qh) \in G_r} v(ph, qh) \right), \tag{16}$$

has the property that

$$J(v) = T^n_{0,\beta^m}(f) + L^n_{\mathbf{c}^k}(v) + O(h^{\min(m+1,4+2p)}), \tag{17}$$

where p is the largest integer such that $1 + p(p + 1)/2 \leq k$. As in 1-D, the correction coefficients $c_1, \ldots, c_k$ are independent of the distance h between sampling points, independent of v, and independent of the square D. In order to achieve a correction of order $4 + 2p$ in (17) it is necessary that $m \leq 3 + 2p$. On the other hand our numerical experiments indicate that the minimum number k of logarithmic correction coefficients needed to achieve a correction of order $4 + 2p$ is $k = 1 + p(p+1)/2$. The integer p represents how big is the square centered at $(0,0)$ on which the logarithmic correction is performed. More specifically, the correction is done on all grid points located in the interior of the square $[-ph, ph] \times [-ph, ph]$ plus a correction on the grid points that belong to the group G_k which are the points $(0, ph)$, $(0, -ph)$, $(ph, 0)$, and $(-ph, 0)$ when $k = 1 + p(p+1)/2$ (see Figures 3 and 4).



a) b)

Figure 3: Logarithmic correction is a weighted sum of values of v around the point of singularity $O = (0,0)$. In the figure it is illustrated an 8th order correction which requires of $k = 4$ correction coefficients ($p = 2$ in this case). In a) the point O of logarithmic singularity is located on the interior of the square D, while in b) it is located on the boundary of the square D.

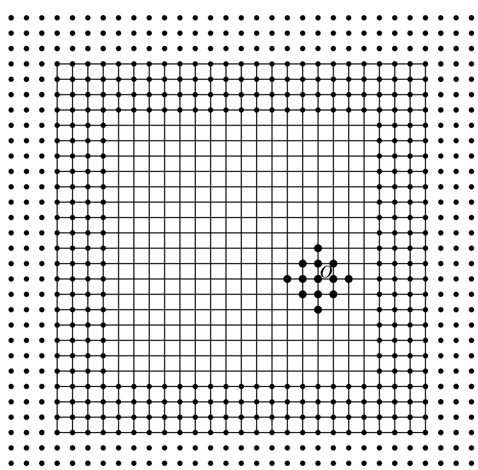


Figure 4: Boundary and logarithmic correction. In the figure it is illustrated the grid points needed for an 8th order boundary correction of the function f, and for an 8th order logarithmic correction of the function v. In this case $m = 7$ and $p = 2$.

3.3 Correction of functions with compact support

As is well-known, if a function g is C^∞ and g and all its derivatives vanish at the boundary of the square D, then it follows from the Euler-Maclaurin summation formula that the rate of convergence of the trapezoidal rule $T_h(g)$ is superalgebraic. In this case there in no necessity of boundary correction. Thus if the smooth function v and its derivatives have compact support contained in D, Formula (17) is simplified as

$$J(v) = T_h(\tilde{f}) + L^n_{\mathbf{c}^k}(v) + O(h^{4+2p}). \tag{18}$$

Hence when the function v has compact support, the integral (1) is approximated with the trapezoidal rule plus a local correction around the point of singularity $(0, 0)$. The order of convergence is $4+2p$ when we use $k = 1+p(p+1)/2$ coefficients for logarithmic correction, with $p \geq 0$.

3.4 Computation of the logarithmic correction coefficients

To compute the first k logarithmic correction coefficients $\mathbf{c}^k$ we take as v in Equation (17) the C^∞ monomial functions g_r defined in Equations (10) and (9), and we take as domain of integration a square centered at $(0, 0)$, say $D = [-1, 1] \times [-1, 1]$, and neglet the error term in (17). That is, let $v_r = g_r$ and $f_r(x, y) = v_r(x, y) \ln(\sqrt{x^2 + y^2})$ for $r = 1, \ldots, k$. Set $m = 41$, that is 20 coefficients for boundary correction (see [1]). The next step is to find the solution $\mathbf{c}^k_h = (c_{1,h}, \ldots, c_{k,h})$ of the resulting linear system of k equations

$$J(v_r) = T^n_{0,\beta^m}(f_r) + L^n_{\mathbf{c}^k_h}(v_r), \quad r = 1, \ldots, k. \tag{19}$$

Such solution $\mathbf{c}^k_h$ approximates the vector $\mathbf{c}^k$ of logarithmic correction coefficients. In our numerical calculation we obtained by setting $h = 1/20$ that $\mathbf{c}^k_h$ and $\mathbf{c}^k$ agree in at least 16 digits for several values of the number k of correction coefficients (k=1, 2, 4, 7, 11, 16, and 37).

The integrals $J(v_r)$ of the system of equations (19) are computed analytically. The system of equations (19) is very ill-conditioned, and to obtain the correction coefficients with a precision of 16 digits, we used the LU decomposition in extended arithmetic with 100 digits of precision. The calculations where carried out using a Fortran based multipresicion system (see [6]). According to our results, the number k of logarithmic correction coefficients of interest are of the form $k = 1 + p(p + 1)/2$ in order to obtain an order of convergence of $4 + 2p$, where $p \geq 0$.

The logarithmic correction coefficients are tabulated below for k = 1, 2, 4, 7, 11, 16, and 37, giving orders of convergence between 4 and 20. In the next section we give some numerical examples testing the quadratures obtained with the tabulated coefficients.

$k = 1$, order 4	$k = 16$, order 14	$k = 37$, order 20
-1.3105329259115095d0	-1.1646982357508747d0	-1.1564478673399723d0
	-3.5890328129867669d-2	-3.8126710449913075d-2
	-9.5074099436320872d-3	-1.1910098717735232d-2
$k = 2$, order 6	8.4541772191636749d-3	1.0946813560280918d-2
-1.2133459579012365d0	1.0979359740499282d-3	1.8459370374209805d-3
-2.4296742002568231d-2	-1.1783003516981361d-5	-2.6130060578859742d-5
	-1.6023206924446483d-3	-2.9040233795126303d-3
	-1.6849437585541639d-4	-4.9701596518365230d-4
$k = 4$, order 8	3.3320425168508138d-6	1.2749931410650803d-5
-1.1882171416684368d0	-9.8490563660380440d-7	-6.5820750987412075d-6
-3.0413000735379221d-2	2.2604824606510965d-4	7.3301436931546191d-4
-3.3900200171833950d-3	1.2470171982677393d-5	1.0733577004383499d-4
3.2240746917944449d-3	-1.7168213185329377d-7	-1.9458112583293086d-6
	6.6801225895094825d-8	1.3143856331004638d-6
	-4.3347365473805450d-9	-2.5402660668233166d-7
$k = 7$, order 10	-1.6344859129100059d-5	-1.5475173218203846d-4
-1.1765131626655374d0		-1.7683396386845410d-5
-3.3070930145520950d-2		2.6480195544534095d-7
-6.1598611771676465d-3		2.6480195544534095d-7
5.5343086429652787d-3		-2.1443542291607470d-7
3.4587810881957096d-4		4.1096136734188740d-8
1.7601808923023545d-7		-6.6696462836304480d-9
-5.0039036749807269d-4		2.4751027705921126d-5
		1.9206904724678774d-6
		-2.4935555816866533d-8
$k = 11$, order 12		2.3124001225072397d-8
-1.1694962171857752d0		-4.3978037096882189d-9
-3.4698254694377585d-2		7.1457202698992097d-10
-8.1243444153848045d-3		-7.6547561188576653d-11
7.1885293443181541d-3		-2.6158207181242810d-6
7.4595382605746944d-4		-1.0183222363887877d-7
-5.5672375863432573d-6		1.1918930487773071d-9
-1.0668259664240182d-3		-1.2213737542214254d-9
-6.6934093317098417d-5		2.3104783998729453d-10
1.0591321235750506d-6		-3.7578874163491022d-11
-1.9350916131464208d-7		4.0255398498327133d-12
8.7321567454452694d-5		-2.1171431666402956d-13
		1.3551691363041958d-7

Table 1: Correction coefficients $\mathbf{c}^k$ for a logarithmic singularity, $k = 1, 2, 4, 7, 11, 16$, and 37.

4 Numerical tests

One interesting application of the quadrature rules (17) is the integration of functions of the form $f(x, y) = \ln(\sqrt{x^2 + y^2})v(x, y)$ where v is smooth and highly oscillatory. This situation is found for example in the Lippman-Schwinger equation in 2-D that models the scattering of acoustic waves with large wave numbers in an inhomogeneous medium of compact support (see [2]).

To test the quadratures defined in (17), we present two examples using functions that are highly oscillatory on the square $D = [-\pi, \pi] \times [-\pi, \pi]$,

$$v(x, y) = \frac{\sin(50r)}{50r}, \quad \text{and} \quad v(x, y) = J_0(100r),$$

where $r = \sqrt{x^2 + y^2}$, and J_0 is the Bessel function of the first kind of order 0 (see [7]). In these examples, the funtion v oscillates 50 and 100 times respectively on the interval $[-\pi, \pi]$. The minimum requirement to resolve each oscillation is to discretize using at least two points per wavelength, that is 100 and 200 points respectively on each side of the square $[-\pi, \pi] \times [-\pi, \pi]$. For the first example, Table (2) shows the relative errors obtained with the quadratures (17) for different orders and using n^2 grid points to discretize the square $[-\pi, \pi] \times [-\pi, \pi]$, and for the values $n = 100$ and $n = 160$. For the second example, the relative errors are shown in Table (3) for $n = 200$ and $n = 300$. Except for a method of order 2 (where there is no correction at all), in these examples we used a value of m for boundary correction that satisfies $m \geq 3 + 2p$, so that the order of the method is $4 + 2p$, for $p \geq 0$.

Order	$n = 100$, Relative Error	$n = 160$, Relative Error
2	1.1×10^{-1}	5.0×10^{-2}
4	3.7×10^{-3}	5.4×10^{-4}
6	5.6×10^{-4}	3.4×10^{-5}
8	1.4×10^{-4}	3.6×10^{-6}
10	4.4×10^{-5}	4.7×10^{-7}
12	1.5×10^{-5}	6.7×10^{-8}
14	5.2×10^{-6}	1.0×10^{-8}
20	3.0×10^{-7}	4.9×10^{-11}

Table 2: Relative errors produced by applying the quadratures (17) to the function $f(x, y) = \ln(r)\sin(50r)/(50r)$, with $r = \sqrt{x^2 + y^2}$. Here the domain of integration is the square $D = [-\pi, \pi] \times [-\pi, \pi]$, and n^2 is the number of equally spaced grid points used to discretize D.

Order	$n = 200$, Relative Error	$n = 300$, Relative Error
2	5.3×10^{-1}	2.4×10^{-1}
4	2.7×10^{-2}	5.2×10^{-3}
6	5.1×10^{-3}	4.5×10^{-4}
8	1.5×10^{-3}	6.3×10^{-5}
10	4.9×10^{-4}	1.0×10^{-5}
12	1.8×10^{-4}	1.8×10^{-6}
14	6.8×10^{-5}	3.3×10^{-7}
20	4.5×10^{-6}	2.6×10^{-9}

Table 3: Relative errors produced by applying the quadratures (17) to the function $f(x, y) = \ln(r)J_0(100r)$, with $r = \sqrt{x^2 + y^2}$. Here the domain of integration is the square $D = [-\pi, \pi] \times [-\pi, \pi]$, and n^2 is the number of equally spaced grid points used to discretize D.

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