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NUMERICAL INTEGRATION ON THE SPHERE

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Abstract

This is a discussion of some numerical integration methods for surface integrals over the unit sphere in $\mathbf{R}^3$. Product Gaussian quadrature and finite-element type methods are considered. The paper concludes with a discussion of the evaluation of singular double layer integrals arising in potential theory.

1. Introduction

This is a discussion of some numerical integration methods for the surface integral

$$I(f) = \int_U f(Q)\, d\sigma, \tag{1.1}$$

with U the unit sphere in $\mathbf{R}^3$. The integration formulae will include product Gaussian quadrature and some methods based on breaking U into smaller triangular elements with various associated low order integration schemes.

The motivation for discussing such methods arises from the desire to solve integral equations defined over simple smooth surfaces S in $\mathbf{R}^3$,

$$\lambda\rho(P) - \int_S K(P, Q)\rho(Q)\, d\sigma(Q) = \psi(P), \qquad P \in S. \tag{1.2}$$

Such equations can arise in a variety of applications, although we are particularly interested in those equations arising from solving potential theory problems in $\mathbf{R}^3$. To deal with integrals over a general surface S, we assume there is a smooth 1-1 mapping of U onto S; then an integral over S can be transformed into one of the form (1.1).

The product Gaussian quadrature formula is discussed and illustrated in Section 2. Methods for triangulating the sphere and some associated integration formulas are given in Section 3. Since most kernel functions $K(P, Q)$, in (1.2), are singular in potential theory applications, we discuss the evaluation of one such integral in Section 4.

For a review of integration methods on the sphere, see Keast and Diaz [6], Lebedev [7], and Stroud [13, Sections 2.6 and 8.4]. The methods discussed in the present paper are not optimal, but they are well-suited to the solution of integral equations. Moreover, the theory of optimal methods is far from complete, as has been noted in [7]; consequently it would not be possible to carry out a complete error analysis of the resulting numerical methods for solving (1.2).

2. Product Gaussian quadrature

Let $I(f)$ be written using spherical coordinates

$$I(f) = \int_0^{2\pi} \int_0^{\pi} F(\theta, \phi) \sin \theta \, d\theta \, d\phi, \tag{2.1}$$

with $f(\theta, \phi) \equiv f(x, y, z)$. The integral is approximated by

$$I_m(f) = \frac{\pi}{m} \sum_{j=1}^{2m} \sum_{i=1}^{m} w_i f(\theta_i, \phi_j). \tag{2.2}$$

The $\{\theta_i\}$ are chosen so that $\{\cos(\theta_i)\}$ and $\{w_i\}$ are the Gauss-Legendre nodes and weights on $[-1, 1]$. The points ϕ_j are evenly spaced on $[0, 2\pi]$ with spacing π/m; usually

$$\phi_j = j\pi/m \qquad \text{or} \qquad \left(j - \frac{1}{2}\right)\pi/m. \tag{2.3}$$

With this choice of node points and weights, $I_m(f)$ integrates exactly any polynomial $f(x, y, z)$ of degree less than $2m$; see [13, page 40] for a proof. For an integration formula, the degree of precision is n if the formula is exact for some polynomial of degree $n + 1$. Hence $I_m(f)$ has degree of precision $2m - 1$.

The formula $I_m(f)$ is less efficient than the optimal formulae of [7], but not badly so. For methods of an increasing degree of precision, Lebedev introduces the efficiency index

$$\eta(n) = (n + 1)^2/(3N(n)), \tag{2.4}$$

where n is the degree of precision and $N(n)$ the number of associated node points on U. The larger the index for a given n, the more efficient is the method. The formulae developed by Lebedev satisfy $\eta(n) \to 1$ as $n \to \infty$. The above Gaussian formula has index $\eta(2m - 1) = 2/3$ for $m > 1$. Lebedev's formulae use only $2/3$ the number of node points used by $I_m(f)$. This is not a large difference and it is offset somewhat by the ease with which $I_m(f)$ is constructed.

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Convergence results for $I_m(f)$ can be obtained from an approximation theorem of Ragozin [11]. Using this, it is straightforward to show that, if $f(x, y, z)$ is k times continuously differentiable on U, then

$$|I(f) - I_m(f)| \leq C/\left((2m-1)^k\right) \qquad \text{for } m \geq 1. \tag{2.5}$$

This bound shows the same rapid convergence associated with Gaussian quadrature for one variable integration. A short proof of (2.5) is given in [1].

EXAMPLES. Four numerical examples will be given, and they will be referenced by the four different surfaces S_i that are used. The first two examples are

$$\int_{S_i} e^x \, d\sigma, \qquad i = 1, 2, \tag{2.6}$$

with S_i the ellipsoidal surface $(x/a)^2 + (y/b)^2 + (z/c)^2 = 1$, where S_1 uses $(a, b, c) = (1, 1, 2)$ and S_2 uses $(1, 2, 5)$. The last two examples are to calculate the surface area of S_i,

$$\int_{S_i} d\sigma, \qquad i = 3, 4, \tag{2.7}$$

with S_i a 'peanut-shaped' region given by

$$(x, y, z) = R(\theta)\,(a \cos\phi \sin\theta, b \sin\phi \sin\theta, \cos\theta)$$

where

$$R(\theta) = \left[\cos(2\theta) + \left[c - \sin^2(2\theta)\right]^{1/2}\right]^{1/2}.$$

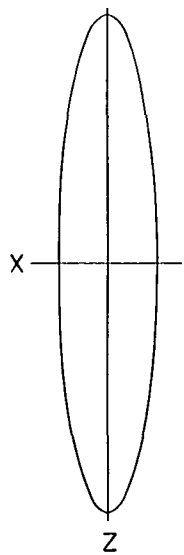

Figure 1. *Cross-section of the ellipsoid* S_2.

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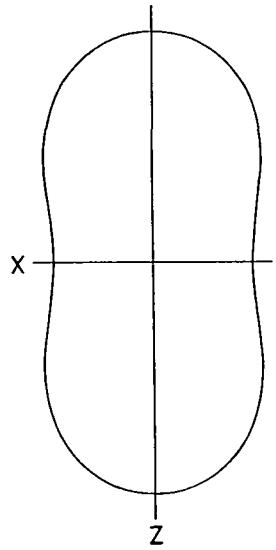

Figure 2. Cross-section of the surface S_3.

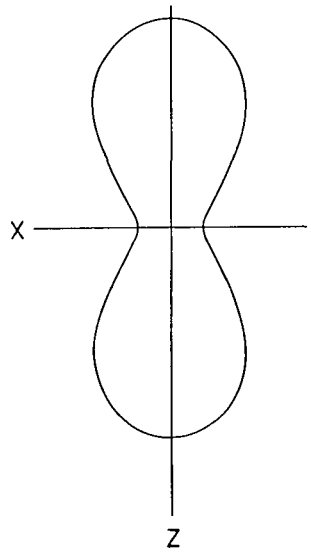

Figure 3. Cross-section of the surface S_4.

Surface S_3 uses $(a, b, c) = (1, 2, 2)$ and S_4 uses $(1, 2, 1.1)$. The cross-sections in the x, z-plane of the surfaces S_2, S_3, and S_4 are shown in Figures 1 to 3. Surfaces S_2 and S_4 are somewhat more ill-behaved than S_1 and S_3.

Table 1 contains the numerical results for the four integrals. The column n gives the number of integration nodes. As expected, the convergence is rapid.

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TABLE 1
Errors for product Gaussian quadrature

		Relative error for the integration over S_i			
m	n	$i = 1$	$i = 2$	$i = 3$	$i = 4$
4	32	−3.0E-4	−1.5E-3	7.8E-3	−3.4E-2
8	128	−1.3E-6	−8.6E-5	1.4E-4	−2.2E-2
12	288	−9.0E-9	−7.3E-6	−3.3E-6	−5.9E-3
16	512	<5.0E-12	−7.9E-7	−3.7E-7	−1.4E-3
20	800	<5.0E-12	−9.9E-8	−1.2E-8	−3.7E-4

3. Finite element integration

Letting $\{\Delta_1, \ldots, \Delta_n\}$ be a triangulation of U, we can write

$$I(f) = \sum_{j=1}^{n} \int_{\Delta_j} f(Q)\, d\sigma. \tag{3.1}$$

We will consider numerical approximations to $I(f)$ based on approximating each integral over Δ_j using a fixed low order integration rule. First, we discuss how to triangulate U.

The usual manner of subdividing U is based on using a rectangular or triangular grid on the rectangle $\{(\theta, \phi) | 0 \leqslant \theta \leqslant \pi,\ 0 \leqslant \phi < 2\pi\}$, and this is mapped onto a triangulation of U using the standard spherical coordinates formula. The advantage of this method is its simplicity, and usually it is rapid to implement. The main disadvantage is that it results in a very nonuniform distribution of nodes and elements on U; usually there are relatively more nodes near the poles $z = \pm 1$. The elements are also quite varied in shape and size, in general. For these reasons, we consider another method of subdivision.

Create an initial triangulation of U by inscribing a tetrahedron, octahedron, or icosahedron inside U, and then project it outward onto the surface U. This gives a uniform subdivision of equilateral spherical triangles, with 4, 8, or 20 faces, respectively. To subdivide an existing triangulation $\{\Delta_i\}$, we divide each face Δ_i into four smaller triangles: find the midpoints of the sides of Δ_i, and then connect them by great circle paths. If Δ_i is not too large, then the four new triangles created from Δ_i will be almost congruent, and will be nearly similar to Δ_i. This triangulation method leads to a fairly uniform subdivision of U, particularly when the initial subdivision is an icosahedron. Denote the three triangulation schemes by $T_{t,n}$, $T_{o,n}$, and $T_{i,n}$, depending on whether the initial

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triangulation uses a tetrahedron, octahedron, or icosahedron, The subscript n indicates the number of faces.

THE CENTROID RULE. The simplest method for estimating the integral over Δ_i is

$$\int_{\Delta_i} f(Q)\, d\sigma \approx f(Q_i) \cdot \text{Area}(\Delta_i), \tag{3.2}$$

where Q_i is the centroid of Δ_i. If v_1, v_2 and v_3 denote the vertices of Δ_i, define

$$Q_i = (v_1 + v_2 + v_3)/|v_1 + v_2 + v_3|. \tag{3.3}$$

Using this in (3.1), we obtain

$$I(f) \approx \sum_{i=1}^{n} f(Q_i)\, \text{Area}(\Delta_i) \equiv C_n(f), \tag{3.4}$$

and we shall call this the 'centroid rule'. This simple rule is surprisingly accurate, especially when certain triangulations of U are being used.

If $f(Q)$ is twice continuously differentiable on U, then a bound on the rate of convergence is given by

$$|I(f) - C_n(f)| \leqslant k_1/n. \tag{3.5}$$

A proof is sketched later in this section. The numerical results given below also seem to confirm the correctness of the order.

Nonetheless, the method has another interesting aspect. Table 2 gives the degree of precision d of $C_n(f)$ for the various polyhedral triangulation schemes. These are somewhat surprising results for such a simple method. Clearly, this triangulation method is important, as other nonuniform triangulations generally have only degree of precision 0 or 1. The results of Table 2 can be proved in a straightforward way, based on the results of [12].

TABLE 2
Degree of precision of the centroid rule

Triangulation	$T_{t,n}$	$T_{o,n}$	$T_{i,n}$
Degree of Precision	2	3	5

EXAMPLES. We use the integrals (2.6) and (2.7) that were used for the product Gaussian quadrature. The triangulation method is $T_{i,n}$, and the results are given in Tables 3 and 4.

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TABLE 3
Numerical examples 1 and 2 for the centroid rule

	Surface S_1		Surface S_2	
n	Relative error	Ratio	Relative error	Ratio
20	−1.2E-3		−4.7E-3	
		−10		66
80	1.1E-5		−7.0E-5	
		5.9		−4.10
320	1.8E-6		1.8E-5	
		5.1		4.6
1280	3.6E-7		3.8E-6	

TABLE 4
Numerical examples 3 and 4 for the centroid rule

	Surface S_3		Surface S_4	
n	Relative error	Ratio	Relative error	Ratio
20	−1.1E-2		−2.8E-1	
		6.4		75
80	−1.7E-3		−3.8E-3	
		118		−2.2
320	−1.5E-5		1.7E-3	
		2.2		−16
1280	−6.8E-6		−1.0E-4	

With most examples, including the ones shown here, the error first decreases very rapidly and then settles down to a slower rate of decrease, usually one more consistent with the theoretical bound of $O(1/n)$. When the triangulations $T_{t,n}$ and $T_{o,n}$ are used, similar behaviour holds, but the errors are not as small as with $T_{i,n}$.

AN ISOPARAMETRIC METHOD. We use the isoparametric mapping approach of the finite element method. Let σ_0 denote the unit simplex in $\mathbf{R}^2$, $\sigma_0 = \{(s, t) | 0 \leqslant s, t, s + t \leqslant 1\}$. Let Δ_i be a spherical triangle with vertices v_1, v_2 and v_3. Define

$$p(s, t) = v_1 + t(v_2 - v_1) + s(v_3 - v_1)$$

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and

$$q(s, t) = p(s, t)/|p(s, t)|, \qquad \text{for } (s, t) \in \sigma_0. \tag{3.6}$$

It is straightforward to show that p is a 1-1 mapping of σ_0 onto the planar triangle determined by v_1, v_2 and v_3 and that q is a 1-1 mapping of σ_0 onto Δ_i.

Using (3.6), we can write

$$\int_{\Delta_i} f(Q)\, d\sigma = \int_{\sigma_0} f(q(s, t))|q_s \times q_t|\, ds\, dt, \tag{3.7}$$

with q_s and q_t denoting the partial derivatives of $q(s, t)$. We now integrate this numerically with an integration method of degree of precision 3:

$$\int_{\sigma_0} g(s, t)\, ds\, dt \approx \frac{1}{40}[\, g(0, 0) + g(1, 0) + g(0, 1)\,] + \frac{1}{15}\left[\, g\left(0, \tfrac{1}{2}\right) + g\left(\tfrac{1}{2}, 0\right) + g\left(\tfrac{1}{2}, \tfrac{1}{2}\right)\right] + \frac{9}{40} g\left(\tfrac{1}{3}, \tfrac{1}{3}\right). \tag{3.8}$$

Under the mapping q, the points $\{(0, 0), (0, 1), (1, 0)\}$ map into v_1, v_2 and v_3, the points $\{(\frac{1}{2}, 0), (0, \frac{1}{2}), (\frac{1}{2}, \frac{1}{2})\}$ map into the centroid Q_i of Δ_i. We apply (3.8) to the right side of (3.7) for each Δ_i and call the sum of the resulting numerical integrals $J_n(f)$.

For the convergence of $J_n(f)$, we show later that, if $f(x, y, z)$ is four times continuously differentiable on U, then

$$|I(f) - J_n(f)| \leqslant k_2/n^2. \tag{3.9}$$

Thus this method should be an improvement on the centroid method. In actual examples, however, the centroid method has almost always been much superior, provided $T_{i,n}$ was used with $n \leqslant 1280$, which was the bound on n in most computations.

EXAMPLES. As before, we evaluate the integrals (2.6) and (2.7), and use $T_{i,n}$. The results are given in Tables 5 and 6, where 'Nodes' gives the number of integration node points on U. The work with $J_n(f)$ is about the same as for $C_{4n}(f)$, since the triangulation $T_{i,4n}$ is needed to obtain the nodes used in $J_n(f)$.

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TABLE 5
Numerical examples 1 and 2 for the isoparametric method

		Surface S_1		Surface S_2	
n	Nodes	Relative error	Ratio	Relative error	Ratio
20	62	-2.8E-2		-3.0E-2	
			13.7		14.3
80	242	-2.0E-3		-2.1E-3	
			15.3		16.0
320	962	-1.3E-4		-1.3E-4	

TABLE 6
Numerical examples 3 and 4 for the isoparametric method

		Surface S_3		Surface S_4	
n	Nodes	Relative error	Ratio	Relative error	Ratio
20	62	-3.2E-2		-1.8E-1	
			11		31
80	242	-2.9E-3		-5.8E-3	
			12		-6.9
320	962	-1.3E-4		8.4E-4	

Based on our examples, the centroid rule should be used in preference to the isoparametric method $J_n(f)$, provided n is not too large and $T_{i,n}$ is used. With other values of n or other triangulations, $J_n(f)$ is much more competitive, and possibly superior. Comparing with the other examples for the product Gaussian quadrature, the latter is generally superior in accuracy to $C_n(f)$, especially at moderate to high error tolerances.

ERROR BOUND DERIVATIONS. We will give only a sketch of the proof of (3.9); the details are straightforward, but algebraically complicated. First, note that the integration rule (3.8) is exact for all polynomials $g(s, t)$ of degree ≤ 3. For a general differentiable function $g(s, t)$, an error formula can be found in the standard way: expand $g(s, t)$ in a Taylor series through the third degree plus a remainder term, and apply the error functional for (3.8) to this equation. The error will be proportional to the fourth derivatives of g.

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To apply this to deriving (3.9), first assume that $f(x, y, z)$ is defined in a neighborhood of U, with continuous and bounded fourth order derivatives. Since (3.8) is applied to (3.7), consider the fourth derivative of the integrand in (3.7). It can be shown that

$$\left| \frac{\partial^4}{\partial s^k \partial t^{4-k}} [f(q(s, t))|q_s \times q_t|] \right| \leqslant C \max\{|v_1 - v_2|^6, |v_1 - v_3|^6\}. \quad (3.10)$$

In addition, the following results can be shown for our triangulations $T_{i,n}$, $T_{o,n}$, and $T_{t,n}$:

$$c_1/n \leqslant \text{Area}(\Delta_i) \leqslant c_2/2, \qquad \text{for } i = 1, \ldots, n, \quad (3.12)$$

where c_1 and $c_2 > 0$ and independent of n; furthermore,

$$c_3 \max\{|v_1 - v_2|^2, |v_2 - v_3|^2, |v_3 - v_1|^2\} \leqslant \text{Area}(\Delta_i) \leqslant c_4 \min\{|v_1 - v_2|^2, |v_2 - v_3|^2, |v_3 - v_1|^2\}, \quad (3.12)$$

with $i = 1, \ldots, n$, v_1, v_2 and v_3 the vertices of Δ_i, and c_3 and $c_4 > 0$ independent of n. Combining all of these results with the error formula for (3.8), derived using a Taylor series, we obtain (3.9).

For functions $f(Q)$ defined only on U, if they are four times differentiable using a local parametrization on U, then they can be extended to a new function on a neighborhood of U; and the extensions can be chosen to have the same degree of differentiability. For a discussion of this, see [4, pages 13, 100].

The proof of (3.5) is quite similar. We write

$$\begin{aligned} e_i &= \int_{\Delta_i} f(Q)\, d\sigma - f(Q_i)\,\text{Area}(\Delta_i) \\ &= \int_{\sigma_0} f(q(s, t))|q_s \times q_t|\, ds\, dt - \frac{1}{2} f\left(q\left(\frac{1}{3}, \frac{1}{3}\right)\right)\left|q_s\left(\frac{1}{3}, \frac{1}{3}\right) \times q_t\left(\frac{1}{3}, \frac{1}{3}\right)\right| \\ &\quad + f(Q_i)\left[\frac{1}{2}\left|q_s\left(\frac{1}{3}, \frac{1}{3}\right) \times q_t\left(\frac{1}{3}, \frac{1}{3}\right)\right| - \int_{\sigma_0} |q_s \times q_t|\, ds\, dt\right] \\ &= E_i^{(1)} + E_i^{(2)}. \end{aligned} \quad (3.13)$$

The point $(\frac{1}{3}, \frac{1}{3})$ is the centroid of σ_0, and $Q_i = q(\frac{1}{3}, \frac{1}{3})$. The integration rule

$$\int_{\sigma_0} g(s, t)\, ds\, dt \approx \frac{1}{2} g\left(\frac{1}{3}, \frac{1}{3}\right) \quad (3.14)$$

has degree of precision 1. Using the same kind of proof as that given for (3.9), it follows that

$$E_i^{(1)} = O(1/n^2). \quad (3.15)$$

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For $E_i^{(2)}$, repeat the same argument, with $g(s, t) = |q_s \times q_t|$ in (3.14). Using the boundedness of f on U, we obtain $E_i^{(2)} = O(1/n^2)$. Thus $E_i = O(1/n^2)$, and the sum of the errors over $\{\Delta_i\}$ is $O(1/n)$.

4. Evaluation of a singular integral

The use of integral equations in the solution of potential theory problems in $\mathbf{R}^3$ leads to the evaluation of singular surface integrals; for example, see Jaswon and Symm [5]. As an example of the treatment of such integrals, we will consider the evaluation of

$$\int_S d(B) \frac{\partial}{\partial \nu(A)} \left[\frac{1}{|B - A|} \right] d\sigma(A), \qquad B \in S, \tag{4.1}$$

with S a smooth boundary surface for a simply connected region, $\nu(A)$ the inner normal to S at A, and $d(B)$ a smooth density function (called the double layer density). This integral arises from the representation of harmonic functions as double layer potentials in $\mathbf{R}^3$; the singularity in (4.1) is of order $1/|A - B|$. Unfortunately, there does not seem to be any way to remove the singularity using a change of variables, and it must be treated directly. There is another formulation in terms of solid angles: for example, see Mikhlin [10, page 349], but that too has significant problems when trying to calculate the solid angles, especially when B is near to A.

As before, assume there is a 1-1 mapping of U onto S and then use it to change the integral in (4.1) to one over U. This leads to the integral operator

$$\mathcal{K}\rho(P) = \int_U K(P, Q)\rho(Q)\, d\sigma(Q), \qquad P \in U. \tag{4.2}$$

The kernel K includes the original kernel of (4.1) and the change of the surface area differential.

A PRODUCT GAUSSIAN QUADRATURE FORMULA. Begin by applying the well-known identity

$$2\pi = \int_S \frac{\partial}{\partial \nu(B)} \left[\frac{1}{|A - B|} \right] d\sigma(B), \qquad A \in S, \tag{4.3}$$

to obtain

$$\mathcal{K}\rho(P) = 2\pi\rho(P) + \int_U K(P, Q)[\rho(Q) - \rho(P)]\, d\sigma. \tag{4.3}$$

The new integrand is bounded at $Q = P$, although it will still be discontinuous.

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If we were now to change to spherical coordinates for Q, then the point P would become a singular point internal to the integration region $[0, \pi] \times [0, 2\pi]$. Most numerical integration methods perform poorly in such a situation, and that will be true here. To avoid this, we first rotate the coordinate system,

$$Q' = HQ, \tag{4.5}$$

with H a Householder orthogonal matrix. It is to be chosen so that $P' = HP$ is $(0, 0, 1)$ or $(0, 0, -1)$. We use a spherical coordinates representation for Q', and apply the product Gaussian quadrature with respect to this new representation. The singularity in the integrand occurs along either $\theta = 0$ or $\theta = \pi$. This change of variables results in much improved accuracy and, moreover, there is now a regular behaviour to the error as the integration parameter m is increased.

EXAMPLE. (1) We choose $S = U$ and, to have a test case, use the result that $\mathcal{K}\rho = 2\pi/(2k + 1)\rho$, for $k \geqslant 0$, for any spherical harmonic of degree k. (See [9, page 69] for the definition of spherical harmonics). We choose the spherical harmonics

$$\rho^{(1)}(P) = z \quad \text{and} \quad \rho^{(2)}(P) = z^2 - (x^2 + y^2)/2. \tag{4.6}$$

For P, we have

$$(-.30353, .93417, .18759). \tag{4.7}$$

The index of integration is m, and the number of nodes is $n = 2m^2$. The numerical results are given in Table 7.

TABLE 7
Gaussian rule: example 1 for singular integral

m	n	Error for $\mathcal{K}\rho^{(1)}$	Ratio	Error for $\mathcal{K}\rho^{(2)}$	Ratio
4	32	1.4E-3		−1.0E-2	
			6.9		7.1
8	128	2.0E-4		−1.4E-3	
			7.4		7.4
16	512	2.7E-5		−1.9E-4	
			7.7		7.7
32	2048	3.5E-6		−2.5E-5	

(2) We use the surface S_3 with the density functions of (4.6) and let P be the point on S_3 corresponding to the point of (4.7) on U, $P = (-.20036, 1.23330, .12383)$. The errors in Table 8 were calculated using a very accurate value of $\mathcal{K}\rho(P)$, obtained with a much larger value of m.

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TABLE 8
Gaussian rule: example 2 for singular integral

m	n	Error for $\mathcal{K}\rho^{(1)}$	Ratio	Error in $\mathcal{K}\rho^{(2)}$	Ratio
4	32	−5.2E-2		5.6E-2	
			92		−93
8	128	−5.7E-4		−6.0E-4	
			11		20
16	512	−5.4E-5		−3.0E-5	
			7.4		7.4
32	2048	−7.2E-6		−4.0E-6	

In these examples and with all other examples we calculated, the error has the asymptotic form

$$c/(m^3) + O(1/m^4). \tag{4.8}$$

As the surface becomes more ill-behaved, the value of m must be larger before the behaviour (4.8) becomes apparent. With surfaces S_2 and S_4, this happens with $m = 64$, but the error is still quite small with smaller values of m. With an error of the form (4.8), Richardson extrapolation can be used to accelerate the convergence, and that should be an important tool with these singular problems. A similar strategy is suggested by Lyness [8].

A FINITE ELEMENT INTEGRATION FORMULA. Most numerical methods for evaluating (4.1) are based on first writing it as a sum of smaller integrals, based on some triangulation of S,

$$\sum_{j=1}^{n} \int_{\Delta_j} d(B) \frac{\partial}{\partial \nu(B)} \left[\frac{1}{|A - B|} \right] do(B).$$

Usually each integral over Δ_j is approximated by the central rule, and the surface area of Δ_j is approximated by the area of the planar triangle determined by the vertices of Δ_j. For examples, see Jaswon and Symm [5, page 233], Birtles *et al.* [3], and Wait [14, page 303]; the last paper also uses a quadratic isoparametric method, with improved results. This is a very flexible approach to the evaluation of integrals like (4.1), but it also leads to greater inaccuracy than if the special nature of the kernel and surface were taken into account.

We approximate (4.2) using the centroid rule, with a crude modification to avoid elements containing the singular point P, using

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$$\mathcal{K}\rho(P) \approx \sum_{P \notin \Delta_j} K(P, Q_j)\rho(Q_j)\ \text{Area}(\Delta_j) + \left[2\pi - \sum_{P \notin \Delta_j} K(P, Q_j)\ \text{Area}(\Delta_j)\right]\rho(V), \tag{4.9}$$

where Q_j is the centroid of Δ_j, and V is some centrally located point in the union of all elements Δ_j containing P. The approximation uses (4.3). Empirically, the behaviour of this method is best when P is a centroid of one of the triangles Δ_j.

EXAMPLE. (1) We let $S = U$, and let ρ and P be given by (4.6) and (4.7). The triangulation $T_{i,n}$ is used, and P is a centroid of one of the faces of $T_{i,20}$. The results are given in Table 9.

TABLE 9
Centroid rule: example 1 for singular integral

n	Error in $\mathcal{K}\rho^{(1)}$	Ratio	Error in $\mathcal{K}\rho^{(2)}$	Ratio
20	−5.7E-3		4.2E-2	
		6.1		6.2
80	−9.4E-4		6.8E-e	
		7.0		7.0
320	−1.4E-4		9.8E-4	
		7.1		7.1
1280	−1.9E-5		1.4E-4	
		6.7		6.6
5120	−2.9E-6		2.1E-5	

(2) We use the same surface S_3, density ρ, and point P as with example 2 for product Gaussian quadrature. The results are given in Table 10.

TABLE 10
Centroid rule: example 2 for singular integral

n	Error in $\mathcal{K}\rho^{(1)}$	Ratio	Error in $\mathcal{K}\rho^{(2)}$	Ratio
20	1.6E-1		1.2	
		−2.7		−83
80	−5.9E-2		−1.4E-2	
		−3.7		−4.0
320	1.6E-2		3.5E-3	
		−3.8		−28
1280	−4.1E-3		−1.3E-4	
		−4.0		−.7
5120	1.0E-3		1.9E-4	

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As can be seen, the error is quite regular when $S = U$, but not otherwise. This has been borne out with all other examples computed to date. Empirically, for $S = U$, the error is about $O(1/n^{1.5})$, which is equivalent to the result (4.8) for product Gaussian quadrature. There seems to be a fortuitous cancellation of errors taking place in this case. For all other surfaces, the uniform rate is mostly lost.

To compare the two methods of evaluating (4.2), the product Gaussian formula has proved much more regular in convergence than the centroid rule and, usually, the Gaussian formula has been much more accurate as well. In our programs, the Gaussian formula has required less memory storage, the programs have been simpler, and generally it has performed much more efficiently.

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