JOURNAL OF COMPUTATIONAL PHYSICS 12, 417–421 (1973)

Note

A Conjecture on the Convergence of Numerical Estimates for Multidimensional Integrals with Singular Integrands

Some consideration has been given to error expansions for a number of one-dimensional integrals [1], and to multiple integrals with smooth integrands [2]. However, little attention has been given to the error analysis of multiple integrals with singularities in the integrand.

Multidimensional integrals are commonly evaluated numerically by dividing the region of integration into a number of identical subregions, and applying a quadrature formula to each subregion. The accuracy of the result can be improved by increasing the number of subregions.

In this paper, an asymptotic form is suggested for the convergence of the quadrature results, as the number of subregions is increased, in the case of singular integrands with an isolated singular point. By extrapolating the numerical quadrature estimates, using this asymptotic behavior, the accuracy of a large class of integrals can be increased considerably. The method is particularly useful in the case of integrals with singularities at the boundary of the region of inte-integration, where no method, other than a direct subdivision of the region of integration, is possible.

The asymptotic form for the quadrature is described later, together with an extrapolation procedure to determine the value of the integral as the number of subdivisions is increased indefinitely. Examples of the use of the procedure in the case of a two-dimensional and a three-dimensional integral are also given.

The computer used in these calculations was a CDC 6600. All computations were performed to double precision accuracy, which is greater than 30 significant figures.

Consider an approximation $I(n)$ to a d-dimensional integral over a finite volume obtained by dividing the region of integration into n^d identical subregions and applying a quadrature formula to each subregion. The assumption will be made that the quadrature scheme does not require the evaluation of the integrand at the singular point. The exact value of the integral will be denoted by $I(\infty)$. It is conjectured that for integrands, with a singularity on the boundary of the region of integration, the asymptotic form for the behavior of $I(n)$ is

$$I(n) = I(\infty) + \sum_{r=0}^{\infty} \frac{A_r}{n^{\alpha+r}} + \text{other terms.} \tag{2.1}$$

For large n, the "other terms" are assumed negligible, compared with $\sum_{r=0}^{\infty} A_r/n^{\alpha+r}$. A_r are constants that depend on the integrand, the quadrature formula, and the method of subdivision of the region of integration. Furthermore, it is claimed that the value of α is determined by the magnitude of the contribution from the subregion surrounding the singular point. The contribution from this subregion is $O(1/n^{\alpha})$. The analytic behavior of the integrand will enable α to be determined. Consequently, a knowledge of the position of the singularity and the analytic behavior of the integrand will enable α to be determined.

To evaluate α, it is conjectured that the order of magnitude of the contribution from the subspace occupied by the singularity is determined by the product of the integrand, evaluated with coordinates determined by the order of magnitude of the values bounding the subregion, and the volume of the subspace. The use of this procedure is illustrated in the subsequent examples.

Once the value of α has been derived, together with p values of $I(n)$ for different values of n, it is possible to extrapolate (2.1). This can be done by neglecting the "other terms" in (2.1), and truncating the infinite series after $(p-1)$ terms. The resulting set of equations can be solved for $I(\infty)$.

It is often convenient to have take consecutive integer values, say

$$n = (N-p+1), (N-p+2),..., N,$$

and evaluate the corresponding values of $I(n)$. Retaining only $(p-1)$ unknowns A_r, $r = 0, 1,..., (p-2)$ in the summation in (2.1), one can solve the subsequent set of simultaneous equations to give an "extrapolated" estimate for $I(\infty)$. This we shall call $I_{p,N}(\infty)$. It is given by

$$I_{p,N}(\infty) = \frac{\sum_{r=0}^{p-1} (N-r)^{\alpha+p-2} \binom{p-1}{r} (-1)^r I(N-r)}{\sum_{r=0}^{p-1} (N-r)^{\alpha+p-2} \binom{p-1}{r} (-1)^r}. \tag{2.2}$$

As an example of the use of (2.1) together with the extrapolation procedure (2.2), consider the two dimensional integral

$$I_2 = \int_0^1 \int_0^1 \frac{dx\, dy}{(2-x^2-y^2)^{1/2}}. \tag{3.1}$$

The integral has a singularity at $x = y = 1$. The region of integration is a unit square. I_2 can be evaluated analytically to give

$$I_2 = \pi(1 - \sqrt{2}/2) = 0.92015\ 11845...$$

Here it will be used, solely, to illustrate the conjecture regarding integrals with singular integrands at the boundary region of integration, for the case where no procedure, other than a direct quadrature approach, is possible.

The region of integration can be simply divided into $n \times n$ squares of side $1/n$. To determine α one must examine the contribution to the quadrature sum from the region about the singularity. This arises from the area of the subregion containing the singularity $1/n^2$, and the value of the integrand obtained by the quadrature formula. Since the singularity arises in the region $x \sim (1 - 1/n)$ and $y \sim (1 - 1/n)$, the integrand contribution to the quadrature sum in this subsquare, (3.1), is assumed to be $O(n^{1/2})$. Hence, the total contribution from the singular subregion is $O(1/n^2 \cdot n^{1/2})$, i.e., $O(1/n^{3/2})$. Consequently $\alpha = 3/2$.

The asymptotic form (2.1) becomes

$$I(n) = I(\infty) + \sum_{r=0}^{\infty} \frac{A_r}{n^{3/2+r}} + \cdots. \tag{3.2}$$

TABLE IA

The First Four Quadrature and Extrapolation Results for the Two-Dimensional Integral I_2

n	$I(n)$	n_I	p	$I_{p,4}(\infty)$	Fractional error
1	0.91435 30958	9	1	0.91949 58938	−0.000712
2	0.91823 58214	36	2	0.92017 10107	−0.0000213
3	0.91913 16001	81	3	0.92014 86011	−0.00000305
4	0.91949 58938	144	4	0.92014 90055	−0.00000261

n_I is the number of integrand evaluations.

TABLE IB

The Quadrature and Extrapolation Results Using the 4×4 to 7×7 Subdivision of the Region of Integration for I_2

n	$I(r)$	n_I	p	$I_{p,7}(\infty)$	Fractional error
4	0.91949 58938	144	1	0.91987 17296	−0.000304
5	0.91968 51417	225	2	0.92015 49456	+0.00000384
6	0.91979 80527	324	3	0.92015 09513	−0.000000497
7	0.91987 17296	441	4	0.92015 12008	+0.000000226

n_I is the number of integrand evaluations.

Tables IA and IB contain the numerical quadrature estimates of the integral, using a nine point Gauss product quadrature formula [3] for each subregion. The extrapolated values $I_{p,4}(\infty)$, $p = 1, 2, 3, 4$, are given in Table IA, and $I_{p,7}(\infty)$, $p = 1, 2, 3, 4$ are given in Table IB. The fractional errors $[(I_{p,r}(\infty) - I(\infty))/I(\infty)]$ in the extrapolated values are given in the right column of the tables. It is clear that the extrapolated values improve the direct quadrature sum $I(n)$ by orders of magnitude. The accuracy of the value of $I_{4,7}(\infty)$ is greater than the value of $I(7)$ by 3 orders of magnitude. That given by $I_{4,4}(\infty)$ exceeds, by 2 orders of magnitude, the result $I(4)$.

The second example is,

$$I_3 = \int_0^1 \int_0^1 \int_0^1 \left(1 - \frac{3z^2}{x^2 + y^2 + z^2}\right)^2 dx\, dy\, dz. \tag{4.1}$$

In a similar manner to (3.1), one can extrapolate the quadrature estimates for I_3. The singularity in this case occurs at the origin, and the region of integration is a cube. Dividing the cubical region into n^3 cubes of side $1/n$, one can determine α. The contribution from the volume of the subregion around the origin is $1/n^3$. The quadrature evaluation of the integrand in the subcube at the origin requires $x \sim 1/n$, $y \sim 1/n$, and $z \sim 1/n$. The integrand, (4.1), is $O(n^0)$. Hence the total contribution to the quadrature scheme from the cube at the origin is $O(1/n^3 \cdot n^0)$, i.e., $O(1/n^3)$. Thus $\alpha = 3$, and the asymptotic form for $I(\infty)$ is given by

$$I(n) = I(\infty) + \sum_{r=0}^{\infty} \frac{A_r}{n^{3+r}} + \cdots. \tag{4.2}$$

Table II contains the values of $I(n)$, using a 19 point quadrature formula due to Hammer and Stroud [3], for $n = 4, 5, \ldots, 10$, with extrapolated values $I_{p,10}(\infty)$.

TABLE II

The Three-Dimensional Cubature Results Together with the Extrapolation Results for I_3

n	$I(n)$	n_I	p	$I_{p,10}(\infty)$	$I_{p,10}(\infty)-I_{p-1,10}(\infty)$
4	0.62217 93246 38684	1216	1	0.62220 18739 3036	
5	0.62219 10782 34015	2325	2	0.62220 34165 1516	+0.00000 154..
6	0.62219 62755 22526	4104	3	0.62220 34166 3274	+0.00000 00001 17..
7	0.62219 89193 33254	6517	4	0.62220 34165 6797	−0.00000 00000 647..
8	0.62220 04036 82181	9728	5	0.62220 34165 8479	+0.00000 00000 168..
9	0.62220 13004 86626	13831	6	0.62220 34165 8295	−0.00000 00000 018..
10	0.62220 18739 30360	19000	7	0.62220 34165 8315	+0.00000 00000 002..

n_I is the number of integrand evaluations.

It is not possible to evaluate I_3 exactly, analytically. So, as a measure of the accuracy of the extrapolated values, the right column of Table II contains the differences $[I_{p,10}(\infty) - I_{p-1,10}(\infty)]$ for $p = 5, 6, \ldots, 10$. In the absence of an exact value for the integral, this "measure" of the accuracy is the alternative to no "measure" of the accuracy.

Here also the extrapolated values converge more rapidly than in the original sequence $I(n)$ of quadrature estimates. Using the right column of Table II as a measure of the accuracy, $[I_{7,10}(\infty) - I_{6,10}(\infty)]$ is $O(10^{-13})$, compared with $O(10^{-6})$ for $[I(10) - I_{7,10}(\infty)]$.

A large class of integrals with boundary singularities appear to have the asumptotic behavior suggested by (2.1). The resulting improvement in the convergence of the quadrature approximations, after using an extrapolating scheme such as (2.2), provides estimates for the integrals that exceed by orders of magnitude those obtained directly by multiple applications of a quadrature formula for each subregion.

It is possible to generalize the method for cases in which the integrand is singular along a line or plane.

Acknowledgments

It is a pleasure to thank Mr. G. S. Joyce, Dr. Henry Thacher, and Dr. J. N. Lyness for helpful discussions. The author is indebted to the reviewers for their numerous helpful suggestions.

References

1. L. Fox, *Computer J.* **10** (1967), 87.
2. J. N. Lyness and B. J. J. McHugh, *Computer J.* **6** (1963), 264.
3. A. H. Stroud, "Approximate Calculation of Multiple Integrals," Prentice Hall, NJ, 1971. For the second example, the reference is p. 231, formula C_n : 5–3.

Received: November 10, 1972

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