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Applications of Extrapolation Techniques to Multidimensional Quadrature of Some Integrand Functions with a Singularity*

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Many large scale calculations require the numerical integration of functions that are products of simple functions of a radius with a function readily expressed in cartesian coordinates. The analytic singularity at the origin can cause a relatively expensive calculation when standard methods are employed. The application of known asymptotic expansions to this sort of problem can result in a considerable reduction in expense or increase in accuracy. In this paper, a set of useful expansions are stated. An approach based on extrapolation is described that leads to a method not unlike the Romberg integration. The emphasis here is on applications. For example, the rearrangement of the theory to provide a technique for grid-oriented calculations is discussed; and a full description of the possible effect of numerical instability, how to recognize it and how to alleviate it, is included.

1. INTRODUCTION

A potentially troublesome and expensive problem arises in multidimensional quadrature when the integrand function involves both functions of a radial coordinate and functions of cartesian coordinates. Consider, for example, the three-dimensional function

$$f(x, y, z) = r^{\alpha} g(x, y, z), \qquad \alpha > -3, \tag{1.1}$$

where $r^2 = x^2 + y^2 + z^2$ and $g(x, y, z)$ is analytic. Unless α is an even nonnegative integer, $f(x, y, z)$ is not analytic at the origin, and if the region of integration contains the origin, most standard quadrature rules are very inefficient. To see this clearly, one only needs to consider a simple special case of (1.1), namely,

$$f(\mathbf{x}) = rx = (x^2 + y^2 + z^2)^{1/2}\, x. \tag{1.2}$$

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Quadrature rules are either based on polynomial approximation, or are closely related to it. This function has infinite second derivatives at the origin, and so approximations based on polynomials (all of whose derivatives are finite) are not likely to be efficient.

Often, the best way around this difficulty is to use a hyperspherical coordinate system. Thus, $f(\mathbf{x})$ in (1.2) has the form $r^2 \sin\theta$, which has no singularities in (r, θ) space. In cases in which the integration region is itself spherical, efficient quadrature rules to handle this problem are either available (see e.g. Stroud [4, pp. 267–293]), or can be constructed.

However, in many cases, there are constraints on the overall problem that make it inconvenient or prohibitively expensive to do this.

A familiar situation is one in which an extensive region of integration has been subdivided into an equally spaced cubic mesh. In this case, it is extremely inconvenient to deal with the region near the singularity in an essentially different manner. What is required is a variant quadrature rule, using the same grid of points, which can be used for a cube containing the singularity.

In this paper, a technique for handling this integration without coordinate transformation is described. Specifically, we deal with the integral over the hypercube

$$H: 0 \leqslant x_i \leqslant 1, \qquad i = 1, 2, \ldots, N, \tag{1.3}$$

of an integrand function of the form

$$f(\mathbf{x}) = r^{\alpha}\phi(\boldsymbol{\theta})\, h(r)\, g(x_1, x_2, \ldots, x_N), \qquad \alpha > -N, \tag{1.4}$$

where

$$r^2 = x_1^2 + x_2^2 + \cdots x_N^2,$$

and $(r, \boldsymbol{\theta})$ is a representation of $(\mathbf{x})$ in hyperspherical coordinates.

The functions $\phi(\boldsymbol{\theta})$, $h(r)$ and $g(x_1, x_2, \ldots, x_N)$ are analytic functions of their respective variables.

Once a technique for this problem is available, the overall problem may be handled in a standard manner by breaking up the integration region into hypercubes, 2^N of which have the origin as a vertex. For these 2^N hypercubes, the special technique to be described is used. For the other hypercubes, any standard method may be used.

Briefly, the method consists of extrapolation, eliminating terms in the appropriate error functional expansion. For example, we let $Q^{(m)}f$ stand for the midpoint trapezoidal rule approximation to If based on m^N function values. Let $f(\mathbf{x})$ be the function (1.4). Then, when α is not an integer

$$Q^{(m)}f - If \sim \sum_{i=0} \frac{A_{\alpha+N+i}}{m^{\alpha+N+i}} + \sum_{\substack{s=2 \\ s \text{ even}}} \frac{B_s}{m^s}. \tag{1.5}$$

Here and subsequently, we use the symbol $\sim$ to indicate that the relation is asymptotic. Each summation may be terminated at any point, the remainder having the same order as the first omitted term. This expansion and others like it are derived at length in Lyness [2]. They are listed for convenience in Section 2. Once the form of this expansion is available, and this requires the numerical value of α, an obvious approach is to apply extrapolation to eliminate the early terms in the expansion. The mechanics of this process is described in Section 3. When there is no singularity, i.e., $\alpha =$ an even integer, the terms $A_{\alpha+N+i}$ drop out and this approach is reduced to a variant of Romberg integration. In Section 4, we give some numerical results that confirm that in some problems, this approach is very powerful indeed.

In Section 5, we describe the application of these ideas to a large scale grid-oriented calculation in which the points for function evaluation are specified in advance. In this sort of environment, the extrapolation procedure is used to construct a suitable quadrature rule.

In a less constrained environment in which function values at arbitrary points are allowed, the user has considerable freedom in choosing his mesh sequence (the set of values of m on which to base the extrapolation). He also has freedom to replace $Q^{(m)}f$ by a corresponding m^N-copy of any other quadrature rule. This wide choice is limited by stability considerations and by the necessity of avoiding the use of an excessive number of function values. These questions are discussed in detail in Section 6.

Finally, a word of warning about the scope of this method is in order. It may be applied only if the proper asymptotic expansion is known. To the author's knowledge, there are only two classes of integrand functions for which this is known. One is the class considered here, which is essentially a point singularity r^α or $r^\alpha \ln r$, occurring at the origin. The other is a line singularity x^α along a face of the hypercube, and is an N-dimensional analog of a one-dimensional result in Lyness and Ninham [3]. No results about mixtures of these singularities or more complicated singularities are known to the author, though there are some unconfirmed conjectures.

The importance of this warning is simply that if extrapolation based on an incorrect expansion is used, the results can be very inaccurate and misleading.

2. Some Asymptotic Expansions for the Error Functional

The results stated in this section are proved in Lyness [2]. They are asymptotic expansions for the error functional $Q^{(m)}f - If$, where $Q^{(m)}f$ is an m^N copy of a quadrature rule Qf defined below for integration over the unit hypercube

$$H: 0 \leqslant x_i \leqslant 1, \qquad i = 1, 2, \ldots, N, \tag{2.1}$$

and If represents an exact integral

$$If = \int_H f(\mathbf{x})\, d^N x. \tag{2.2}$$

The most familiar example is the N-dimensional Euler–Maclaurin expansion valid when $f(\mathbf{x})$ is analytic. The significant results below apply to functions $f(\mathbf{x})$ having a point singularity at the origin.

First, we define a *quadrature rule*

$$Qf = Q^{(1)}f = \sum_{j=1}^{n} a_j f(\mathbf{x}_j), \qquad \sum a_j = 1, \tag{2.3}$$

which approximates If. This rule is of *polynomial degree* d if it is exact for all polynomials of degree d or less, i.e.,

$$Qf - If = 0, \qquad f \in \Pi_d\,,\ d = d(Q). \tag{2.4}$$

We term it *symmetric* if it is invariant under reflection about all the hyperplanes $x_i = \frac{1}{2}$, $i = 1, 2, \ldots, N$; i.e.,

$$Qf_i = Qg, \qquad f_i(x_1, \ldots, x_i, \ldots, x_N) = g(x_1, \ldots, 1 - x_i, \ldots, x_N), \qquad i = 1, 2, \ldots, N. \tag{2.5}$$

The m^N *copy of this rule* is the rule obtained by subdividing H into m^N equal hypercubes of side $1/m$ and applying a properly scaled version of Q to each; i.e.,

$$Q^{(m)}f = \frac{1}{m^N} \sum_{\mathbf{l}} \sum_{j} a_j f\left(\frac{\mathbf{x}_j + \mathbf{l}}{m}\right), \tag{2.6}$$

where the sum over $\mathbf{l} = (l_1, l_2, \ldots, l_N)$ includes all m^N distinct vectors for which l_i are nonnegative integers and $\max_i l_i \leqslant m - 1$.

In the expansions listed below, the quantities A_α, B_s, C_s, A_α', and B_s' are independent of m. They depend on the integrand function and the quadrature rule. Integral representations are given in Lyness [2], where these results are proved.

For convenience, in these statements, we assume that Qf does not require an indeterminate function value at the origin. If it does, a minor modification stated in Result 6 below may be required.

Results 1 and 1A below are standard, being the basis for Romberg integration.

Result 1. If $f(\mathbf{x})$ is analytic in all variables within H, then

$$Q^{(m)}f - If \sim \sum_{s=1} B_s/m^s.$$

Result 1A. If $g_p(\mathbf{x})$ together with all its partial derivatives of total order p or less are integrable over H, then

$$Q^{(m)}g_p - Ig_p = \sum_{s=1}^{p-1} B_s/m^s + O(m^{-p}).$$

The next result is the fundamental one.

DEFINITION. $f_\gamma(\mathbf{x})$ is homogeneous of degree γ (with respect to the origin) when

$$f_\gamma(\lambda\mathbf{x}) \equiv \lambda^\gamma f(\mathbf{x}), \qquad \text{for all } \lambda \neq 0. \tag{2.7}$$

Result 2. If $f_\gamma(\mathbf{x})$ has no singularity within the closed hypercube H, except at the origin

$$Q^{(m)}f_\gamma - If_\gamma \sim \frac{A_{N+\gamma}}{m^{N+\gamma}} + \frac{C_{N+\gamma}\ln m}{m^{N+\gamma}} + \sum_{s=1} \frac{B_s}{m^s},$$

with

$$C_{N+\gamma} = 0, \qquad \gamma \neq \text{integer}.$$

Results 2 and 1A may be used to derive similar expansions for any integrand function $f(\mathbf{x})$ that may be expanded in terms of homogeneous functions. For example

Result 3. Let $f(\mathbf{x}) = r^\alpha \phi(\boldsymbol{\theta})\, h(r)\, g(\mathbf{x})$, where $(r, \boldsymbol{\theta})$ is a representation of $\mathbf{x}$ in hyperspherical coordinates and $\phi(\boldsymbol{\theta})$, $h(r)$, $g(x_1, x_2, \ldots, x_N)$ are analytic in their stated variables at all points within H. Then

$$Q^{(m)}f - If \sim \sum_{i=0} \frac{A_{\alpha+N+i} + C_{\alpha+N+i}\ln m}{m^{\alpha+N+i}} + \sum_{s=1} \frac{B_s}{m^s},$$

with

$$C_{\alpha+N+i} = 0, \qquad \alpha \neq \text{integer}.$$

This result follows by using a multivariate Taylor expansion to express $f(\mathbf{x})$ in the form

$$f(\mathbf{x}) = \sum_{i=0}^{p-1} f_{\alpha+i}(\mathbf{x}) + g_p(\mathbf{x}), \tag{2.8}$$

giving

$$Q^{(m)}f - If = \sum_{i=0}^{p-1} (Q^{(m)}f_{\alpha+i} - If_{\alpha+i}) + Q^{(m)}g_p - Ig_p, \tag{2.9}$$

and applying Results 2 and 1A.

When α is not an integer, the coefficients $A_{\alpha+N+i}$ and B_s are locally analytic in α, and one can differentiate Result 3 to obtain

Result 4. Let $F(\mathbf{x}) = f(\mathbf{x}) \ln r = r^\alpha \ln r \phi(\theta)\, h(r)\, g(\mathbf{x})$, with $f(\mathbf{x})$ satisfying the conditions of Result 3; then

$$Q^{(m)}F - IF \sim \sum_{i=0} \frac{A'_{\alpha+N+i} - A_{\alpha+N+i} \ln m}{m^{\alpha+N+i}} + \sum_{s=1} \frac{B_s'}{m^s}, \qquad \alpha \neq \text{integer}.$$

Result 5. When α in Result 4 is an integer, the expansion includes terms in m^{-s}, $m^{-s} \ln m$, and $m^{-s}(\ln m)^2$. For details, refer to Lyness [2].

DEFINITION. The zero modified rule $Q^{[m]}f$ coincides with $Q^{(m)}f$ except that any function value at the origin is ignored. Thus,

$$Q^{[m]}f = Q^{(m)}f - \frac{w_0}{m^N} f(\mathbf{0}), \tag{2.10}$$

where w_0 is the weight assigned by Qf to the origin.

Result 6. When Qf requires a function value at the origin, all results are valid with $Q^{[m]}f$ replacing $Q^{(m)}f$, so long as an additional term K/m^N is included in the expansion. This term is only required in Results 2 and 3 when γ or α, respectively, are integers, and is not required in Result 4.

As mentioned above, the quantities A, B, C, A', B' depend on the quadrature rule and on the integrand function. For special classes of quadrature rules and integrand functions, some of these may be zero.

Result 7. If Q is symmetric

$$B_s' = B_s = C_s = 0, \qquad s \text{ odd}.$$

If Q has polynomial degree $d(Q)$

$$B_s' = B_s = C_s = 0, \qquad 0 < s \leqslant d(Q).$$

Result 8. If $f(\mathbf{x})$ is a polynomial of degree $d(f)$

$$A_i = C_i = 0, \qquad B_s = 0, \qquad s > d(f).$$

Result 9. If $f(\mathbf{x}) = r^\alpha \phi(\theta)\, h(r)\, g(\mathbf{x})$, satisfying the conditions of Result 3 and in addition, $h(r)\, g(\mathbf{x})$ is symmetric (or antisymmetric) about the origin, i.e.,

$$h(r)\, g(\mathbf{x}) \equiv +h(-r)\, g(-\mathbf{x}), \qquad (\text{or } -h(-r)\, g(-\mathbf{x})),$$

then

$$A_i' = A_i = C_i = 0, \qquad i = \alpha + s + N, \; s \text{ odd (or even)}.$$

3. The Mechanics of Extrapolation

In the previous section, a list of results was presented, using which one may construct an error expansion for a certain class of integrand functions. Each error expansion has the form

$$Q^{(m)}f = If + a_1 f_1(m) + a_2 f_2(m) + \cdots + a_p f_p(m) + O(f_{p+1}(m)), \tag{3.1}$$

where a_i stands for a coefficient A, B, or C, and $f_i(m)$ for a simple function of m such as m^{-s}, $m^{-s} \ln m$. The terms in (3.1) are arranged in decreasing order in m, i.e.,

$$\lim_{m\to\infty} f_{s+1}(m)/f_s(m) = 0, \tag{3.2}$$

and it is convenient to set $a_0 = If$ and $f_0(m) = 1$. We now briefly describe the extrapolation process, adapting the notation used in Romberg integration. We require a set of integer values of m, termed the mesh sequence

$$1 \leqslant m_0 < m_1 < m_2 < m_3 < \cdots, \tag{3.3}$$

and we denote a rule sum evaluation by

$$T_{j,0,0} = Q^{(m_j)}f. \tag{3.4}$$

In Romberg integration, one carries out several extrapolations using distinct values of m_j. Thus, extrapolation based on $\{m_k, m_{k+1},..., m_{k+p}\}$ is based on solving the set of linear equations

$$T_{j,0,0} = \sum_{s=0}^{p} T_{k,p,s} f_s(m_j), \qquad j = k, k+1,..., k+p. \tag{3.5}$$

This set is obtained from (3.1) by disregarding the $O(f_{p+1}(m))$ terms. $T_{j,0,0}$ and $f_s(m_j)$ are known and the solutions $T_{k,p,s}$ $(s = 0, 1,..., p)$ are approximations to a_s $(s = 0, 1,..., p)$. We denote the matrix of these equations by $V^{[k,p]}$ and its inverse by $\Gamma^{[k,p]}$, i.e.,

$$\Gamma^{[k,p]} = (V^{[k,p]})^{-1}, \qquad V^{[k,p]}_{j,s} = f_s(m_j). \tag{3.6}$$

(This inverse is of course not calculated as a linear systems solver may be used instead.) Using this notation, the extrapolated value of If may be expressed in the form

$$T_{k,p,0} = \sum_{j=k}^{k+p} \Gamma^{[k,p]}_{j,0} T_{j,0,0} = \sum_{j=k}^{k+p} \gamma_{m_j} Q^{(m_j)} f. \tag{3.7}$$

In conventional Romberg integration, where $f_s(m) = m^{-2s}$, the calculation of approximations $T_{k,p,0}$ may be carried out recursively using the Neville algorithm. Using this, a T-table of approximations to If is formed. However, this can be

used only in cases in which $f_j(m)$ form a geometric progression. In cases where there is a singularity, no convenient algorithm of this type is known to the author.

If the set of mesh ratios form a Geometric progression, then a straightforward algorithm may be constructed for extrapolation for any of these asymptotic expansions. However, even in one-dimension, the use of such a set of mesh ratios is expensive. In two- and three-dimensions, the expense is relatively larger and usually prohibitive.

Thus, in this generalization of Romberg integration, some of the attractive computational features disappear and the use of the Neville algorithm is usually replaced by the use of a linear equation solver. Nevertheless, the saving in terms of function evaluation can be very great, as we show by example in Section 4.

In the rest of this section, we assume that the final term eliminated is an inverse power, that is, that $f_p(m) = m^{-\alpha_p}$. The extrapolation condition number $K_{k,p,0}$ associated with $T_{k,p,0}$ may be defined as

$$K_{k,p,0} = \sum_{j=k}^{k+p} | \Gamma_{j,0}^{[k,p]} | = \sum_{j=k}^{k+p} | \gamma_{m_j} | = \left| \sum_{j=k}^{k+p} \Gamma_{j,0}^{[k,p]} (-1)^j \right|, \tag{3.8}$$

the final equality being valid since the sign of $\Gamma_{j,0}^{[k,p]}$ alternates with j. This is a measure of the amplification of small errors ϵ_j in individual values of $T_{j,0,0}$ that occur as a result of the use of finite precision arithmetic. Thus, if ϵ_τ denotes a bound on the error in $T_{j,0,0}$ and $\epsilon_j = \theta_j \epsilon_\tau$; $| \theta_j | \leqslant 1$, and if the computation of $T_{k,p,0}$ is carried out exactly, then the error is bounded by

$$\sum_{j=k}^{k+p} | \Gamma_{j,0}^{[k,p]} | \epsilon_\tau = K_{k,p,0} \epsilon_\tau . \tag{3.9}$$

In view of (3.8), this condition number $K_{k,p,0}$ may be calculated using precisely the same algorithm as is used to calculate $T_{k,p,0}$, but with initial values $(-1)^j$ replacing $T_{j,0,0}$.

Finally we mention that the elements $\Gamma_{j,0}^{[k,p]}$ depend only on the ratios $m_k : m_{k+1} : \cdots m_{k+p}$. Thus, the condition number $K_{k,p,0}$ is unaltered if all the mesh ratios are altered by a constant factor.

4. Numerical Accuracy

In this section, we give some numerical examples that illustrate the relation between accuracy and expense (in terms of number of function values) using extrapolation. Our first example is

$$If = \int_0^1 \int_0^1 r^{-3/2} e^{-r^2} e^{-x^2} \, dx \, dy \simeq 2.52551,35399,5. \tag{4.1}$$

The reader will recognize a rather brutal, but integrable, singularity at the origin. The expansion provided by result 3 with $\alpha = -3/2$ is valid. When the quadrature rule is symmetric, application of Result 7 leads to

$$Q^{(m)}f - If \sim \frac{A_{1/2}}{m^{1/2}} + \frac{A_{3/2}}{m^{3/2}} + \frac{B_2}{m^2} + \frac{A_{5/2}}{m^{5/2}} + \frac{A_{7/2}}{m^{7/2}} + \frac{B_4}{m^4} + \cdots . \tag{4.2}$$

However, the integrand function is symmetric about the origin, and so application of Result 9 gives

$$Q^{(m)}f - If \sim \frac{A_{1/2}}{m^{1/2}} + \frac{B_2}{m^2} + \frac{A_{5/2}}{m^{5/2}} + \frac{B_4}{m^4} + \frac{A_{9/2}}{m^{9/2}} + \frac{B_6}{m^6} + \cdots . \tag{4.3}$$

These expansions are valid when $Q^{(m)}$ stands for the midpoint trapezoidal rule or the endpoint zero adjusted rule. When Q is replaced by the degree 7 Gaussian rule G_7 we find

$$G_7^{(m)}f - If \sim \frac{A_{1/2}}{m^{1/2}} + \frac{A_{5/2}}{m^{5/2}} + \frac{A_{9/2}}{m^{9/2}} + \frac{A_{13/2}}{m^{13/2}} + \frac{B_8}{m^8} + \frac{A_{17/2}}{m^{17/2}} + \cdots . \tag{4.4}$$

The second example is

$$If = \int_0^1 \int_0^1 r^{1/2} e^{-r^2} e^{-x^2}\, dx\, dy \simeq 0.33865{,}76711, \tag{4.5}$$

and reference to Section 2 gives, for a symmetric rule

$$Q^{(m)}f - If \sim \frac{B_2}{m^2} + \frac{A_{5/2}}{m^{5/2}} + \frac{B_4}{m^4} + \frac{A_{9/2}}{m^{9/2}} + \frac{B_6}{m^6} + \frac{A_{13/2}}{m^{13/2}} + \cdots . \tag{4.6}$$

The third example is

$$If = \int_0^1 \int_0^1 rx\, dx\, dy = \frac{1}{24}(7(2)^{1/2} - 2 + 3\ln(1 + 2^{1/2})) \simeq 0.43931{,}73207{,}36262, \tag{4.7}$$

and

$$Q^{(m)}f - If \sim \frac{B_2}{m^2} + \frac{C_4 \ln m}{m^4} + \frac{A_4}{m^4} + \frac{B_6}{m^6} + \frac{B_8}{m^8} + \frac{B_{10}}{m^{10}} + \cdots . \tag{4.8}$$

In Table I, we list the accuracy, and the number of function values required in various attempts to evaluate these integrals. First, using the endpoint zero-modified trapezoidal rule with no extrapolation. Second, using a 12-point, polynomial degree 7 Gaussian rule (Stroud [4, C_2 : 7–5 p. 255]), and third, using extrapolation based on the endpoint zero-modified trapezoidal rule.

TABLE I

Example →		(4.1)		(4.5)	(4.7)
Q	$\nu(Q)$	$\lvert Qf - If\rvert/If$	$[If = 2.526]$	$\lvert Qf - If\rvert/If$	$\lvert Qf - If\rvert/If$
$R^{[6]a}$	49	0.40	$[Qf = 1.496]$	9.3×10^{-3}	4.5×10^{-3}
$R^{[32]}$	1089	0.17	$[Qf = 2.080]$	2.4×10^{-4}	1.6×10^{-4}
$R^{[128]}$	16,641	0.08	$[Qf = 2.303]$	1.3×10^{-5}	
$G^{(1)b}$	12	0.08	$[Qf = 1.977]$	2.5×10^{-3}	4.0×10^{-5}
$G^{(32)}$	12,288	0.04	$[Qf = 2.428]$	4.0×10^{-7}	3.7×10^{-11}
$G^{(128)}$	196,608	0.02	$[Qf = 2.477]$	1.2×10^{-8}	
$T_{0,3,0}{}^c$	37	1.7×10^{-3}	1.2×10^{-2}	4.0×10^{-5}	2.2×10^{-6}
$T_{0,5,0}$	121	4.5×10^{-5}	2.3×10^{-3}	4.4×10^{-6}	5.3×10^{-9}
$T_{0,9,0}$	1,633	1.3×10^{-10}	2.4×10^{-7}	2.3×10^{-11}	6.2×10^{-14}
Asymptotic expansion		(4.3)	(4.2)	(4.6)	(4.8)

[a] $R^{[m]}$ Trapezoidal rule based on an $(m + 1) \times (m + 1)$ grid.

[b] $G^{(m)}$ 12-point degree 7 Gaussian rule used on each subsquare of side $1/m$.

[c] $T_{0,p,0}$ Result based on extrapolation using $m_0, m_1, \ldots, m_p$, where the mesh sequence is $\{m\} = 1, 2, 3, 4, 6, 8, 12, 16, 24, 32$ based on expansion whose equation number appears in the final row using the trapezoidal rule.

The first six lines of Table I illustrate what might occur in an attempt to "sledgehammer" a result by simply using a standard rule with more and more points. Since the number of points $\nu = O(m^2)$, and the first term in the error expansion (4.2) (or (4.3) or (4.4)) is $E = O(m^{-1/2})$, ultimately, in the first example, $E \sim K\nu^{-1/4}$. To increase the accuracy by a factor of 10, one must increase the number of function values by a factor of 10,000. In passing, we note that subtracting out the singularity involves the separate calculation of $\iint r^{-3/2}\, dx\, dy$, which leads to a difficult special calculation. In the second and third examples, the sledgehammer approach, though expensive, is feasible. Using the trapezoidal rule, $E \sim K\nu^{-1}$ in each case. Using the degree 7 Gaussian rule, $E \sim K\nu^{-5/4}$, and $E \sim K\nu^{-2} \ln \nu$, respectively.

The next set of three lines illustrates the numerical accuracy and cost using extrapolation. For the first example, we give two sets of results, corresponding to the use of asymptotic expansions (4.2) and (4.3), respectively. This illustrates the numerical advantage reaped by a user who notices that the factor $e^{-r^2}e^{-x^2}$ is symmetric about the origin, and so eliminates zero valued terms like $A_{3/2}/m^{3/2}$, using Result 9 instead of eliminating them numerically. This advantage is significant, but not essential to the calculation.

A glance at the table indicates that these examples are arranged in descending order of difficulty. A rough measure of the difficulty is provided by the

"density" of terms in the expansion, or alternatively, the order of the pth term. For example, with $p = 6$, the final term in expansions (4.2), (4.3), (4.6), and (4.8) are

$$B_4/m^4, \quad B_6/m^6, \quad A_{13/2}/m^{13/2}, \quad B_{10}/m^{10},$$

respectively, and these are of successively higher order, indicating that problems requiring these expansions are arranged in descending order of difficulty. The same ordering prevails for all values of p.

It is pertinent to remark once again that the third example with its innocuous looking integrand function rx, while easier than the other examples here, is indeed difficult to integrate numerically over a square because of the singularity at the origin. It is trivial using polar coordinates to integrate this over a circle or the first quadrant of a circle whose center is at the origin. It is also trivial to integrate r^2x, which is a polynomial over either a square or a circle. By the same token, $e^{-\alpha r}g(x, y)$ is difficult and $e^{-\alpha r^2}g(x, y)$ is easy. In practice, it is essential that the user realizes the difficulty of his problem, and this distinction is very important.

5. Application to Large Scale Calculations

In most large scale calculations involving two- or three-dimensional quadrature, constraints on the overall problem prohibit the use of iterative quadrature methods. Features of large scale problems include:

(a) One wishes to calculate a set of integrals.

(b) The same set is calculated a large number of times, incidental parameters in the integrand function being altered between each calculation in an overall iteration towards an acceptable set of parameters.

(c) The integrand functions contain sets of common factors, some common to many of the functions and others independent of some or all of the incidental parameters, and so common to some or all of the iterations.

(d) The domain of integration may be semi-infinite or infinite in some or all directions.

In problems of this type, it is usual to set up a rectangular grid. Since the integrand function is much more intractable near the origin than away from it, the gauge of the grid is often increased several times as one moves away from the origin. The grid is finite and the contribution from the infinite tail is either estimated on the basis of its known asymptotic form or is ignored.

Each point of this grid has a quadrature weight assigned to it (or perhaps several weights for different integrand functions). The quadratures are effected by treating each gridpoint in turn. At each, the various components of the integrand functions

are assembled, assigned their relevant weights and added into a set of running sums.

In an environment of this nature, the direct use of extrapolation that may involve function values at arbitrary points is out of the question. However, the theory of extrapolation may be employed under certain circumstances to provide a more suitable set of weights.

In practice, these weights are frequently determined from simple polynomial based rules such as Simpson's rule or a four panel Newton–Cotes rule. Near the origin, accuracy is maintained only at the considerable expense of using a very fine mesh. In cases in which the nature of the singularity at the origin is known and an asymptotic expansion of type (3.1) is known, this information may be used to construct a more appropriate quadrature rule for use on the part of the grid near the origin. This would obviate the necessity for using an ultrafine mesh there, thus, either reducing the overall expense, or increasing the overall accuracy.

We illustrate the technique for obtaining such a rule in a two-dimensional context. Here there are four squares, each of which has a corner at the origin. Each square is subdivided by the grid. Without loss of generality, we assume that these squares have unit side. It is convenient to choose the grid so that each of these squares contains M^2 subsquares, where M has as many different integer factors as possible but is reasonably small. For illustration, we take $M = 12$ and construct a rule that requires 169 function values for this square. This is based on the endpoint trapezoidal rule

$$Qf = \tfrac{1}{4}(f(0, 0) + f(0, 1) + f(1, 0) + f(1, 1)). \tag{5.1}$$

$Q^{(m)}f$ requires $(m + 1)^2$ function values, all of which lie on the 12×12 grid when $m = 1, 2, 3, 4, 6, 12$. Thus, the result $T_{0,5,0}$ in (3.7) uses only these points, i.e.,

$$T_{0,5,0} = \gamma_1 Q^{(1)}f + \gamma_2 Q^{(2)}f + \gamma_3 Q^{(3)}f + \gamma_4 Q^{(4)}f + \gamma_6 Q^{(6)}f + \gamma_{12} Q^{(12)}f. \tag{5.2}$$

The values of γ_i are determined from (3.6) using the functions $f_s(m)$ from the asymptotic expansion with

$$m_j = 1, 2, 3, 4, 6, 12, \qquad j = 0, 1, 2, 3, 4, 5. \tag{5.3}$$

The m^2-copy of the trapezoidal rule given by (5.1) may be expressed in the form

$$Q^{(m)}f = \frac{1}{m^2} \sum_{i=0}^{m}{}'' \sum_{j=0}^{m}{}'' f\left(\frac{i}{m}, \frac{j}{m}\right), \tag{5.4}$$

where the double prime on the summation symbol indicates that the first and the last terms in the summation (those with index zero and index m) are assigned a

weight factor $\frac{1}{2}$. Substituting (5.4) into (5.2) we find, after some rearrangement, that

$$T_{0,5,0} = \sum_{i=0}^{12} \sum_{j=0}^{12} w(i,j) f\left(\frac{i}{12}, \frac{j}{12}\right). \tag{5.5}$$

The weight matrix is fully symmetric, i.e.,

$$w(a, b) = w(12 - a, b) = w(b, a).$$

For $a \leqslant b \leqslant 6$, the elements are given in terms of

$$\mu_i = \gamma_i / i^2, \qquad i = 1, 2, 3, 4, 6, 12,$$

by

$$\begin{aligned}
w(0, 0) &= \tfrac{1}{4}(\mu_1 + \mu_2 + \mu_3 + \mu_4 + \mu_6 + \mu_{12}),\\
w(2, 2) &= w(2, 4) = w(2, 6) = w(4, 6) = \mu_6 + \mu_{12},\\
w(3, 3) &= w(3, 6) = \mu_4 + \mu_{12},\\
w(4, 4) &= \mu_3 + \mu_6 + \mu_{12},\\
w(6, 6) &= \mu_2 + \mu_3 + \mu_4 + \mu_6 + \mu_{12}.
\end{aligned}$$

Other than those listed above,

$$w(a, b) = \mu_{12}, \qquad a \text{ odd or } b \text{ odd but } (a, b) \neq (3, 3),$$

and

$$w(0, b) = \tfrac{1}{2} w(b, b), \qquad b \geqslant 1.$$

In many problems, one may want to integrate several sets of integrand functions each set having a different asymptotic expansion. To do this efficiently, it might be necessary to construct several different quadrature rules; one for each set of integrand functions. If each were to use the set of points in (5.5) derived from the endpoint two-dimensional trapezoidal rule using mesh ratios $\{1, 2, 3, 4, 6, 12\}$, then the values of γ_j in (5.2) would differ from set to set, but the formulas for $w(a, b)$ in terms of γ_j would be the same for each set.

Sometimes, it is not necessary to do this, if one is prepared for a penalty in terms of accuracy. For example, one may have a situation where one requires 64 different integrands of the form

$$r^{-1/2} h_i(r)\, g_{i,j}(\mathbf{x}), \qquad i, j = 1, 2, \ldots, 8,$$

and while in general the expansion is

$$Q^{(m)} f - If \simeq \frac{A_{3/2}}{m^{3/2}} + \frac{B_2}{m^2} + \frac{A_{5/2}}{m^{5/2}} + \frac{A_{7/2}}{m^{7/2}} + \frac{B_4}{m^4} + \frac{A_{9/2}}{m^{9/2}} + \cdots,$$

for the 15 integrands for which $i = 1$ or $j = 1$ symmetry conditions give

$$A_{5/2} = A_{9/2} = \cdots = 0.$$

While one has the option of two different 169 point rules, the rule designed for the majority of the integrands will also work for the easier 15 integrands, and be equally effective. By choosing not to work out a separate rule for the easier integrands, one has simply omitted obtaining some additional accuracy for those that would have been attainable on the basis of the available function values.

The sort of numerical effect is illustrated in Table I where the accuracy using two different expansions (4.2) and (4.3) in the same example is given.

A related point is that of checking the weights and abscissas. For rules based on polynomial approximation, it is usual to check a list of weights and abscissas for errors by integrating an appropriate set of polynomials and comparing the results with the known exact results. For the rule derived along the lines described above, at present, no complete set of functions for this purpose is known to the author. However, the rule should be exact for the constant function. If terms B_2/m^2, B_4/m^4,..., B_{2t}/m^{2t} are among those eliminated, then the rule should be exact for all polynomials of degree $2t + 1$ or less. However, this constitutes only a partial check, and is not sufficient to find all errors.

6. General Applications and Numerical Stability

In any particular problem that is to be tackled using extrapolation, the overall form of the expansion is determined by the nature of the integrand function. However, the user has to choose a basic quadrature rule Q and a mesh sequence $\{m\}$. In the previous section, we discussed this question in the context of a situation in which one was restricted to function values at points on a grid. In view of this constraint, we suggested a mesh sequence $\{m\} = \{1, 2, 3, 4, 6, 12\}$ using the endpoint trapezoidal rule. In two-dimensions, this choice eliminates five terms of the asymptotic expansion at a cost of 169 function values. Without this constraint, that choice is not the best. For example, the same five terms may be eliminated using the midpoint trapezoidal rule with $\{m\} = \{1, 2, 3, 4, 5, 6\}$ at a cost of only 85 function values, but these are arranged in the square somewhat haphazardly. In this section, we discuss some of the factors that might affect a choice of Q and $\{m\}$.

For purposes of discussion, we shall limit our choice of quadrature rules to three, namely, the endpoint trapezoidal rule, the midpoint trapezoidal rule, and a higher degree Gaussian rule. We shall also limit the choice of mesh sequences to three. These are

$$G\colon \{m\} = 1, 2, 4, 8, 16, 32...,$$

$$F\colon \{m\} = 1, 2, 3, 4, 6, 8, 12...,$$

$$H\colon \{m\} = 1, 2, 3, 4, 5, 6, 7....$$

The Geometric and Harmonic sequences represent extreme choices. In Table II, we list the number of function values required by the midpoint and endpoint trapezoidal rules using the first seven members of these sequences in dimensions 1, 2, 3, and 4. Examination of this table indicates that the use of sequence G is extremely expensive, and that sequence H may be the most economic. However, the accuracy of the results are not commensurate from one sequence to another. The accuracy depends to some extent on the number of function values used, as well as the number of terms eliminated in the asymptotic expansion.

TABLE II

	(1, 2, 3, 4, 5, 6, 7)		(1, 2, 3, 4, 6, 8, 12)		(1, 2, 4, 8, 16, 32, 64)	
	EP	*MP*	*EP*	*MP*	*EP*	*MP*
$N = 1$	19	23	17	36	65	127
$N = 2$	157	133	225	274	4,225	5,461
$N = 3$	1,153	773	2,801	2,556	274,625	299,593
$N = 4$	8,305	4,657	34,497	26,482	17.85×10^6	17.89×10^6

For a given sequence, our experiments have led us to believe that there is no discernable difference in accuracy between the midpoint and endpoint trapezoidal rule. Thus, on the basis of these sort of figures, one would be led to the conclusion that the midpoint rule and the Harmonic sequence might be a nearly optimum choice.

If the calculation were carried out in arbitrarily high precision arithmetic, that would undoubtedly be the proper choice. However, as finite precision arithmetic is used, the overall stability of the calculation has to be considered. As we shall see, the amplification of noise level in function values introduces a component of error in the final result. This amplification is far more severe when the Harmonic mesh sequence is used than when the Geometric sequence is used. The sequence F was introduced by Bulirsch [1] in an attempt to compromise between expense and instability in one-dimensional Romberg integration.

An initial source of computational error arises because the integrand function values are calculated using finite length arithmetic, and so they include a noise component. The routine deals with $(1 + \theta_i\epsilon_f)f(\mathbf{x}_i)$ in place of $f(\mathbf{x}_i)$, where $|\theta_i| < 1$, and ϵ_f is termed the noise level. For very simple integrands, like those in the examples, ϵ_f is two or three units of ϵ_M, the machine accuracy parameter. For more sophisticated integrands, it can be higher.

This error is amplified slightly when sums such as $Q^{(m)}f$ are calculated. If the number of elements in the sum is ν, the relative error in $Q^{(m)}f$ may be as high as

$\nu\epsilon_f$, or if special coding is used, as low as $\epsilon_f \log_2 \nu$. In our experiments, we found this error was usually about $\epsilon_f(\nu)^{1/2}$.

The errors at this point are relatively unimportant and not unexpected. However, this error is seriously amplified by the elimination. Thus, when calculating

$$T_{0,p,0} = \sum_{j=0}^{p} \gamma_{m_j} Q^{(m_j)} f,$$

the computational error ϵ_j in $Q^{(m_j)}f$ could become amplified to $\sum | \gamma_{m_j} | \epsilon_j$. The extrapolation condition number, defined in (3.8) as

$$K_{0,p,0} = \sum | \gamma_{m_j} |$$

is a useful measure of this error. As mentioned in Section 3, this number is readily calculated using the same algorithm as is used to calculate $T_{0,p,0}$. Its value depends on the nature of the asymptotic expansion and on the mesh ratio sequence. Some values are given in Table III.

TABLE III

Table of Values of $K_{0,p,0}$ for Three Mesh Ratio Sequences and Four Error Functional Asymptotic Expansions[a]

Negative powers of m in expansion	p	G	F	H
2, 4, 6, 8	4	1.95	6.2	6.2
10, 12, 14	7	1.96	7.4	55.8
16, 18, 20	10	1.96	9.2	552.8
0.5, 2, 2.5, 4	4	13.9	63	63
4.5, 6, 6.5	7	17.7	250	2,494
8, 8,5, 10	10	18.4	450	107,963
0.5, 1.5, 2, 2.5	4	20	95	95
3.5, 4, 4.5	7	39	883	8,931
5.5, 6, 6.5	10	46	2,720	904,363
0.5, 1,5, 2.5	3	12.2	22	22
3.5, 4.5,	5	20.8	156	291
5.5, 6.5	7	23.8	379	3,783

[a] These have $f_j(m) = m^{-s_j}$ the values of s_j appearing in the first column.

In many cases, the high condition number associated with the Harmonic sequence may compromise the accuracy of the result to an unacceptable extent. Whether this is likely to happen depends on the accuracy required by the user and on the machine precision being used. As an extreme example, if accuracy $\epsilon_{\text{req}} = 10^{-4}$ is required, and one is using a double precision program for which $\epsilon_M = 10^{-16}$, the loss of seven or eight decimal places is not important and one could normally use the Harmonic sequence. However, in the same problem using a single precision program for which $\epsilon_M = 10^{-6}$, considerable care might be necessary, possibly necessitating the use of the far more expensive Geometric sequence.

In cases in which numerical stability might pose a problem, this effect may be alleviated by using a Gaussian rule of moderate polynomial degree in place of the trapezoidal rule.

Leaving aside stability criteria, the results of our numerical experiments indicate that there is little significant difference in quality of results when measured on an accuracy per number of function value basis between using Gaussian rules and the trapezoidal rules. Whatever mesh sequence is used, the effect of removing some of the terms B_{2s}/m^2 leaves a more stable calculation. This comparison is illustrated in Table III. The fourth expansion is identical with the third except that $B_2 = B_4 = B_6 = 0$, and corresponds to the same problem using a degree 7 Gaussian rule in place of the trapezoidal rule. When one extrapolates to eliminate all terms up to a fixed order, the figures for the condition numbers are directly comparable. In a sense, by using a Gaussian rule, one has carried out some of the extrapolation analytically, and so less further extrapolation is required. A glance at the table indicates that there is a considerable reduction in the condition number. However, if the Gaussian rule involves negative weights an additional factor in the overall condition number $\sum | a_i | / \sum a_i$ should be included.

The user must distinguish clearly between the noise level and the accuracy of function values. Thus, a user may wish to integrate a function $\phi(\mathbf{x})$ to accuracy 10^{-3}. Since $\phi(\mathbf{x})$ is cumbersome to evaluate, he replaces it by an easier function $\psi(\mathbf{x})$, and he knows perhaps that $| \phi(\mathbf{x}) - \psi(\mathbf{x})| < 10^{-5}$. The user tends to think of the accuracy of the function values as being 10^{-5}. However, the noise level simply depends on how $\psi(\mathbf{x})$ is calculated, and if $\psi(\mathbf{x})$ is a straightforward function, it may be near the machine accuracy parameter ϵ_M. It is this noise level that is amplified by the computation. The difference $| \phi(\mathbf{x}) - \psi(\mathbf{x})|$ is quite irrelevant in this context.

If the calculation is carried out using a linear equation solver, the user must remember that the condition number associated with the matrix may be much higher than the condition number $K_{0,p,0}$, which is associated only with the first element in the solution. Thus, it can happen that the linear equation solver breaks down and returns an error condition in cases where a solution is quite feasible.

In the discussion presented in this section, we have done little more than to outline briefly some of the many considerations that might go into choosing a mesh sequence and quadrature rule for a specific problem. For the reader who would like a specific answer, the following approach is suggested.

(i) Decide on a limit on the number of function values.

(ii) Employ the mesh sequence F and the midpoint trapezoidal rule.

(iii) Code this iteratively and in such a way that later on, one can alter the mesh sequence if desired.

(iv) Arrange the program so that it returns the condition number together with the approximate result at each stage.

This will produce a set of results $(T_{0,p,0}, K_{0,p,0})$ $p = 0, 1, 2, \ldots, \bar{p}$. Human examination of these results is necessary. The accuracy may be roughly estimated by the agreement between the final two values of $T_{0,p,0}$. If this estimate is not acceptable, the value of $K_{0,p,0}$ should indicate whether this is due to instability or not. On the basis of this information and the remarks in this section, he is now in a position to plan a new strategy.

7. Concluding Remarks

Multidimensional quadrature is an expensive component in many large scale calculations. At the present time, it appears that any method with widespread application is likely to be too inefficient for use in particular problems. The future trend is likely to be towards special methods for different classes of frequently encountered problems.

In this paper, one class of problem is treated, this being the one that occurs when the integrand function is a product of a simple function of a radius r, like $r^\alpha \ln r$, with a well-behaved function of cartesian coordinates. The theory is based on known asymptotic expansions for the error functional. Our emphasis is on the application of these in the context of large scale calculations with a computer.

There remain many avenues for future research. One involves widening the class of allowed integrand functions by deriving corresponding expansions for perhaps functions $x^\alpha r^\beta$. In another direction, an efficient algorithm for solving the particular class of linear equations involved here (to replace the general linear equation solver) would be welcome. The impetus necessary to instigate such work may result from more widespread use of the present results. It is the author's hope that this paper might help to bring this about.

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