The evaluation of multidimensional integrals

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A critical examination is made of a class of formulae which have been used to carry out multidimensional integrations. It is shown that certain familiar assumptions under which these formulae have been constructed are not valid and that their general use may produce results seriously in error. It is suggested that the repeated application of one dimensional integration formulae is still likely to be the most satisfactory method for evaluating multidimensional integrals both as regards accuracy and economy.

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1. Introduction

In this paper an investigation is made of multidimensional quadrature formulae which evaluate integrals of the form $\int_{-1}^{1} \dots \int_{-1}^{1} f(x_1, x_2, \dots x_n) dx_1 \dots dx_n$. In general an integral can be reduced to this form by an appropriate transformation of the variables.

The most natural approach to the evaluation of an n-dimensional integral is through the repeated application to each variable of a one-dimensional formula of degree of precision k yielding what is called a Cartesian product formula. A one-dimensional formula of degree of precision k is defined as one which integrates exactly all powers of x not greater than x^k. Thus a Cartesian product formula based on a one-dimensional formula of degree of precision k would integrate exactly all products of powers of the variables, $x_1^{i_1} x_2^{i_2} \dots x_n^{i_n}$, called *monomials*, such that $0 \leqslant i_j \leqslant k$ for $j = 1, 2, \dots, n$. Such a formula would require k^n evaluations of the integrand.

This strong dependence of the number of integrand evaluations on the value of n has led to the development of multidimensional integration formulae, which would require fewer integrand evaluations than the Cartesian product formulae, and based on an extension of the definition of the degree of precision. A multidimensional formula of degree of precision k is defined to be one which integrates exactly all monomials of power not greater than k. A monomial of power p is defined to be a monomial, $x_1^{i_1} x_2^{i_2} \dots x_n^{i_n}$, such that $i_1 + i_2 + \dots + i_n = p$. All multivariate polynomials of degree not greater than k would be integrated exactly by a multidimensional formula of degree of precision k. The multivariate polynomial of degree k is defined as a linear sum of monomials, as distinct from powers as in the one-dimensional case, of power not greater than k. For example the general multivariate polynomial of degree three in two dimensions is

$$a_1 x_1^3 + a_2 x_2^3 + a_3 x_1^2 x_2 + a_4 x_1 x_2^2 + a_5 x_1^2 + a_6 x_2^2 + a_7 x_1 x_2 + a_8 x_1 + a_9 x_2 + a_{10}$$

where $a_1, a_2, \dots a_{10}$ are constants. The general multivariate polynomial of degree k in n dimensions has $\binom{n+k}{k}$ terms (Hammer, 1959). A multidimensional formula based on this definition of degree of precision was developed in the last century by Clerk-Maxwell (1877) and over the last several years many more formulae have been derived (e.g. Tyler, 1957; Stroud, 1957, 1960; Miller, 1960).

The use of the definition, degree of precision, to categorize multidimensional integration formulae suggests that the accuracy of the formulae and their degree of precision are closely related. It will be shown later that certain previously unemphasized properties of the Taylor expansion of a multivariate function, which forms the foundation for the development of the multidimensional formulae, precludes any meaningful relationship between degree of precision and accuracy. As a result the application of these integration formulae is likely to yield unreliable results.

2. The construction of multidimensional integration formulae

The multidimensional integration formulae for evaluating the n-dimensional integral

$$I = \int_{-1}^{1} \dots \int_{-1}^{1} f(x_1, \dots, x_n) dx_1 \dots dx_n \tag{1}$$

are constructed, as in the one-dimensional case, by approximating (1) by a weighted sum of the values of the integrand at certain specified points. The general formula can be written as

$$I \approx \sum_{t=1}^{L} A_t \sum_P f(a_{1,t}, a_{2,t}, \dots, a_{n,t}) \tag{2}$$

where $\sum_P$ denotes the sum over all permutations including sign changes of $a_{1,t}, a_{2,t}, \dots a_{n,t}$. It is clear that these points should be given equal weight, A_t, since the range of integration is symmetrical and there is no reason to

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distinguish one variable from another in the general integrand. The quantity $\{a_{1,t}, \ldots a_{n,t}\}$ is sometimes referred to as a *generator*.

The technique for calculating the abscissae and weights of (2) was first introduced by Clerk-Maxwell (1877) and latei developed by Tyler (1953), Stroud (1957), Hammer and Stroud (1958) and Miller (1960). It consists of expanding both (1) and (2) as Taylor series about the origin and choosing the weights and abscissae such that the expansions agree for all terms associated with monomials of power not greater than k. The resulting formulae are said to be of degree of precision k. Three formulae of degree of precision five and one of degree of precision seven are given in the Appendix and will be referred to later.

Such integration formula of degree of precision k will integrate exactly all monomials of power k. If, however, they are to integrate monomials of higher power with acceptable accuracy, it is required that the Taylor expansion of the integral should converge rapidly and that terms which have not been taken account of exactly in the expansion of (1) (that is, those associated with monomials of power greater than k) should not affect the result unacceptably. It will be shown in the next section that in general neither of these requirements is likely to be satisfied.

3. The Taylor expansion of multivariate functions

The Taylor expansion of $f(x_1, x_2, \ldots x_n)$ about the origin can be written as

$$f(x_1, x_2, \ldots x_n) = \sum_{i_1=0}^{\infty} \sum_{i_2=0}^{\infty} \ldots \sum_{i_n=0}^{\infty} D_{i_1, i_2, \ldots, i_n} x_1^{i_1} x_2^{i_2} \ldots x_n^{i_n} \quad (3)$$

and repeated partial differentiation shows that

$$D_{i_1, i_2, \ldots i_n} = \frac{1}{i_1! i_2! \ldots i_n!} \cdot \frac{\partial^{i_1 + i_2 + \ldots + i_n} f(0, 0, \ldots, 0)}{\partial^{i_1} x_1 \, \partial^{i_2} x_2 \ldots \partial^{i_n} x_n}. \quad (4)$$

As Hammer and Wymore (1957) have noted, for the purposes of integration, monomials of the same power contribute equally so that all permutations of the indices in $x_1^{i_1} x_2^{i_2} \ldots x_n^{i_n}$ can be grouped together. For example $x_1^4 x_2^2$ makes the same contribution as $x_1^2 x_2^4$. In addition, since the range of integration in each variable is symmetrical only even powers of the individual variables need be considered. The integrand can thus be written as

$$f(x_1, x_2, \ldots, x_n) = f(0, 0, \ldots, 0) + \sum_{i=1}^{\infty} \frac{1}{(2i)!} S_{2i} x_1^{2i} + \sum_{i=1}^{\infty} \sum_{j=i}^{\infty} \frac{1}{(2i)!(2j)!} S_{2i,2j} x_1^{2i} x_2^{2j} + \sum_{i=1}^{\infty} \sum_{j=i}^{\infty} \sum_{k=j}^{\infty} \frac{1}{(2i)!(2j)!(2k)!} S_{2i,2j,2k} x_1^{2i} x_2^{2j} x_3^{2k} + \ldots \quad (5)$$

$$= f_0 + \frac{1}{2!} S_2 x_1^2 + \left(\frac{1}{4!} S_4 x_1^4 + \frac{1}{2!}\frac{1}{2!} S_{2,2} x_1^2 x_2^2\right) + \left(\frac{1}{6!} S_6 x_1^6 + \frac{1}{4!2!} S_{4,2} x_1^4 x_2^2 + \frac{1}{2!2!2!} S_{2,2,2} x_1^2 x_2^2 x_3^2\right) + \left(\frac{1}{8!} S_8 x_1^8 + \frac{1}{6!2!} S_{6,2} x_1^6 x_2^2 + \frac{1}{4!4!} S_{4,4} x_1^4 x_2^4 + \frac{1}{4!2!2!} S_{4,2,2} x_1^4 x_2^2 x_3^2 + \frac{1}{2!2!2!2!} S_{2,2,2,2} x_1^2 x_2^2 x_3^2 x_4^2\right) + \ldots \quad (6)$$

where $S_{l_1, l_2, \ldots l_s}$ is defined by

$$S_{l_1, l_2, \ldots, l_s} = \sum_{m=1}^{\binom{n}{s}} \sum_{l} \frac{\partial^{(l_1 + l_2 + \ldots + l_s)} f(0, 0, \ldots, 0)}{\partial^{l_1}_{x_{m1}} \partial^{l_2}_{x_{m2}} \ldots \partial^{l_s}_{x_{ms}}} \quad (7)$$

the summation being over all the $\binom{n}{s}$ choices of s variables from n and over all distinct permutations of $l_1, l_2, \ldots, l_s$ not taking account of order. The total number of terms in (7) is $\binom{n}{s} \dfrac{s!}{n_1! n_2! \ldots n_r!}$ where $n_1, n_2, \ldots, n_r$ are the numbers of the $l_1, l_2, \ldots, l_s$ which are equal to each other. For example 2,2,4,4,4, would have $r = 2$ and $n_1 = 2$ and $n_2 = 3$.

The expansion of the multidimensional integral is obtained directly from (6) by integrating over all the variables, giving

$$J = 2^{-n} \int_{-1}^{1} \ldots \int_{-1}^{1} dx_1 \ldots dx_n f(x_1, x_2, \ldots, x_n)$$

$$= f_0 + \frac{1}{3!} S_2 + \left(\frac{1}{5!} S_4 + \frac{1}{3!3!} S_{2,2}\right) + \left(\frac{1}{7!} S_6 + \frac{1}{5!3!} S_{4,2} + \frac{1}{3!3!3!} S_{2,2,2}\right) + \left(\frac{1}{9!} S_8 + \frac{1}{7!3!} S_{6,2} + \frac{1}{5!5!} S_{4,4} + \frac{1}{5!3!3!} S_{4,2,2} + \frac{1}{3!3!3!3!} S_{2,2,2,2}\right) + \ldots \quad (8)$$

In both (6) and (8) the terms associated with the same monomial power have been grouped together in brackets. The convergence of the Taylor expansion (5) is directly reflected in expansion (8), and the properties of this series will now be discussed. **Table 1** lists the coefficients, multiplying the $S_{i,j,k,\ldots}$ terms in (8), in their decreasing order of magnitude. The rather slow convergence is to be noted. Apart from the first few values the successive coefficients generally differ by much less than a factor of two. Another astonishing fact which emerges is that ordering in terms of monomial power is completely lost after the first few terms. For example, the first fourteen coefficients in the ordering are associated with monomials of powers 0,2,4,4,6,6,8,8,6,10,8,10,10 and 12.

Table 1

Coefficients of the Taylor expansion (8) of the text. The coefficients are referred to by their associated subscripts and are grouped such that the first coefficient of a given order is at least a factor of 10 greater than the first coefficient of the next order. The coefficients within each order are in decreasing order of magnitude.

ORDER	COEFFICIENTS
1	0 2
10^{-1}	2,2 4 2,2,2
10^{-2}	2,4 2,2,2,2 2,2,4 6
10^{-3}	2,2,2,2,2 4,4 2,2,2,4 2,6 2,2,2,2,2,2
10^{-4}	2,4,4 2,2,2,2,4 2,2,6 2,2,2,2,2,2,2 8 2,2,4,4 4,6
10^{-5}	2,2,2,2,2,4 2,2,2,6 2,2,2,2,2,2,2,2 4,4,4 2,8 2,2,2,4,4 2,4,6 2,2,2,2,2,2,4 2,2,2,2,6
10^{-6}	2,2,2,2,2,2,2,2,2 2,4,4,4 2,2,8 2,2,2,2,4,4 2,2,4,6 6,6 2,2,2,2,2,2,2,4 2,2,2,2,2,6 10 4,8 2,2,2,2,2,2,2,2,2,2 2,2,4,4,4 4,4,6 2,2,2,8
10^{-7}	2,2,2,2,2,4,4 2,2,2,4,6 2,6,6 2,2,2,2,2,2,2,2,4 4,4,4,4 2,2,2,2,2,2,6 2,10 2,4,8 2,2,2,4,4,4 2,4,4,6 2,2,2,2,8 2,2,2,2,2,2,4,4 2,2,2,2,4,6 2,2,6,6
10^{-8}	2,2,2,2,2,2,2,2,2,4 2,4,4,4,4 2,2,2,2,2,2,2,6 2,2,10 2,2,4,8 6,8 2,2,2,2,4,4,4 2,2,4,4,6 2,2,2,2,2,8 4,6,6 2,2,2,2,2,2,2,4,4 2,2,2,2,2,4,6 4,10 4,4,8 2,2,2,6,6 12 2,2,4,4,4,4 2,2,2,2,2,2,2,2,6 2,2,2,10 4,4,4,6 2,2,2,4,8 2,6,8

So far the effect of the actual values of the derivatives on the convergence has not been discussed. It is conceivable that the S terms could decrease sufficiently rapidly with increasing monomial power to produce satisfactory convergence, but this is in fact a property of very smooth functions. Thus in such circumstances the Cartesian product formulae would probably be competitive with the multidimensional formulae. However, such a property of the S terms is unlikely to be met by a general function.

It is of interest to investigate the ordering of monomials for some specific integrands, hopefully those which might be representative of the range of variation encountered in practice.

The ten-dimensional integrands $\prod_{i=1}^{10} \cos \lambda x_i$, $\prod_{i=1}^{10} \frac{1}{(1+\lambda x_i)}$ and $\left(1 + \sum_{i=1}^{10} x_i\right)^{20}$ have derivatives given by the following expressions:

$$\prod_{i=1}^{10} \cos \lambda x_i : |S_{l_1, l_2, \ldots, l_s}| = \frac{\lambda^{(l_1 + l_2 + l_s)} 10!}{(10 - s)! n_1! n_2! \ldots n_r!} \quad (9)$$

$$\prod_{i=1}^{10} \frac{1}{(1 + \lambda x_i)} : S_{l_1, l_2, \ldots, l_s} = \frac{\lambda^{(l_1 + l_2 + l_s)} 10! l_1! l_2! \ldots l_s!}{(10 - s)! n_1! n_2! \ldots n_r!} \quad (10)$$

$$\left(1 + \sum_{i=1}^{10} x_i\right)^{10} : S_{l_1, l_2, \ldots, l_s} = \frac{\lambda^{(l_1 + l_2 + \ldots l_s)} 10! 20!}{(20 - l_1 - l_2 - \ldots - l_s)!(10 - s)! n_1! n_2! \ldots n_r!}$$
$$= 0 \text{ if } l_1 + l_2 + \ldots + l_s > 20. \quad (11)$$

The quantities $n_1, n_2, \ldots, n_r$ have been defined in connection with (7). The contributions of the various terms of (8) in decreasing order of magnitude for these integrands are presented in Tables 2, 3, 4, 5 and 6.

Table 2 gives the contributions to (8) from the integrand $\prod_{i=1}^{10} \cos \lambda x_i$ for $\lambda = 1$. It is clear that ordering in terms of monomial power is completely disrupted and that an integration formula based on monomial power would give poor results. Neglecting a factor of 2^{10}, Formula 3 of the Appendix using 201 integrand

Table 2

Contribution of terms of (8) of the text for the integrand $\prod_{i=1}^{10} \cos x_i$. The terms are referred to by their associated subscripts and are grouped such that the first term of a given order is at least a factor of 10 greater than the first term of the next order. The terms within each order are in decreasing order of magnitude.

ORDER	TERMS
1	2 2,2 0 2,2,2
10^{-1}	2,2,2,2 2,4 2,2,4 4 2,2,2,2,2 2,2,2,4
10^{-2}	2,2,2,2,4 2,2,2,2,2,2 2,4,4 4,4 2,6 2,2,4,4 2,2,6 6 2,2,2,2,2,4
10^{-3}	2,2,2,4,4 2,2,2,6 2,2,2,2,2,2,2 2,4,6 2,2,2,2,6 2,2,2,2,4,4 2,2,2,2,2,2,4 4,6 2,2,4,6
10^{-4}	2,4,4,4 4,4,4 2,8 2,2,4,4,4 2,2,2,4,6 2,2,2,2,2,6 2,2,8 8 2,2,2,2,2,2,2,2 2,2,2,2,2,4,4 2,2,2,4,4,4 2,2,2,2,2,2,2,4 2,2,2,8
10^{-5}	2,2,2,2,4,6 2,4,4,6 4,4,6 2,2,2,2,2,2,6 2,2,4,4,6 2,4,8 2,2,2,2,8 2,6,6 4,8 2,2,2,2,4,4,4 2,2,2,2,2,2,4,4 6,6 2,2,4,8 2,2,6,6 2,2,2,2,2,4,6 2,4,4,4,4 4,4,4,4 2,2,2,2,2,2,2,2,2
10^{-6}	2,2,2,4,4,6 2,2,2,4,8 2,2,2,6,6 2,2,2,2,2,8 2,2,2,2,2,2,2,2,4 2,2,4,4,4,4 2,10 2,2,2,2,2,2,2,6 2,2,10 10 2,2,2,2,2,4,4,4 2,4,6,6 2,2,2,2,4,4,6 4,6,6 2,2,2,2,4,8 2,2,2,10 4,4,4,6 2,4,4,4,6 2,2,2,2,6,6 2,2,2,4,4,4,4 2,2,2,2,2,2,2,4,4 2,2,2,2,2,2,4,6

evaluations gives the result of 0·545 for this integral, while the exact value is about 0·179. For comparison, the 2-point repeated one-dimensional Gauss formula using 1024 integrand evaluations gives the result 0·171. Improvement of Formula 3 by subdivision is out of the question since the number of integrand evaluations would increase by a factor of 2^{10}. The respectable performance of the 2-point Gauss formula is a result of the predominance of low valued subscript terms early in the expansion. This tends to be a characteristic of multidimensional integrands and suggests that accurate results may generally be obtainable using repeated one-dimensional Gauss formulae of low degree. It would be expected that as λ is made smaller, viz. as the integrand becomes smoother, that ordering in terms of monomial power would not be disrupted so early in the expansion and that the convergence would be more rapid. **Table 3**, which shows the contribution from the individual terms of (8) for the integrand $\prod_{i=1}^{10} \cos \frac{x}{2}$ verifies this. As expected Formula 3 gives a satisfactory result, 0·665 compared with the exact value of about 0·657. If, however, it were necessary to improve this result by using a multidimensional formula of higher degree the disruption of ordering in monomial power later in the expansion would again produce inaccuracies.

Table 4 lists the contributions to (8) of the integrand (10) for $\lambda = 0\cdot9$ which varies rapidly close to the limits of integration. In this case not only is there extreme disruption of monomial ordering but in addition the convergence is extremely slow. Again as λ is reduced the reordering becomes less pronounced and the convergence is more rapid. **Table 5** illustrates this, showing the contribution to (8) of the integrand (10) for $\lambda = 0\cdot5$. Again Formula 3 gives a result of the correct order, 0·241, compared to the exact value of about 0·256.

Finally **Table 6** shows the contributions to (8) for integrand (11) and indicates how extreme the reordering of monomial powers can be. In this case a multidimensional formula of degree 18 would be required to handle the first term alone. It is notable that a three-point Gauss formula would exactly integrate all but eight of the first twenty-four terms and gives a value of

Table 3

Contribution of terms of (8) of the text for the integrand $\prod_{i=1}^{10} \cos \frac{1}{2} x_i$. The terms are referred to by their associated subscripts and are grouped such that the first term of a given order is at least a factor of 10 greater than the first term of the next order. The terms within each order are in decreasing order of magnitude.

ORDER	TERMS
1	0 2
10^{-1}	2,2 2,2,2
10^{-2}	4 2,4 2,2,2,2
10^{-3}	2,2,4
10^{-4}	2,2,2,2,2 2,2,2,4 6 4,4 2,6 2,4,4
10^{-5}	2,2,2,2,4 2,2,6 2,2,2,2,2,2 2,2,4,4
10^{-6}	2,2,2,6 4,6 8 2,2,2,2,2,4 2,2,2,4,4 2,4,6 2,8 2,2,2,2,2,2,2
10^{-7}	4,4,4 2,2,2,2,6 2,2,4,6 2,2,8 2,4,4,4 2,2,2,2,4,4 2,2,2,2,2,2,4
10^{-8}	2,2,2,8 2,2,4,4,4 2,2,2,4,6 4,8 2,2,2,2,2,6 6,6 2,2,2,2,2,2,2,2 4,4,6 10 2,4,8 2,6,6 2,10 2,4,4,6 2,2,2,2,2,4,4
10^{-9}	2,2,2,4,4,4 2,2,2,2,2,2,2,4 2,2,2,2,8 2,2,2,2,4,6 2,2,4,8 2,2,6,6 4,4,4,4 2,2,10 2,2,2,2,2,2,6 2,2,4,4,6
10^{-10}	2,4,4,4,4 2,2,2,2,2,2,2,2,2 6,8 2,2,2,4,8 4,6,6 2,2,2,2,4,4,4 2,2,2,2,2,2,4,4 2,2,2,6,6 2,2,2,2,2,8 2,2,2,10 4,10 4,4,8 2,2,2,2,2,4,6 2,6,8 2,2,2,4,4,6 2,4,6,6 2,2,2,2,2,2,2,2,4 2,2,4,4,4,4 12

$1 \cdot 46 \times 10^{14}$ compared with the exact result of about $1 \cdot 57 \times 10^{14}$ (again neglecting a factor of 2^{10}).

With the exception of (11), the integrands that have been discussed have been separable in terms of the variables. Due to the difficulty of obtaining expressions for the derivatives of non-separable integrands it was not possible to derive tables for the contribution to (8) even for simple cases. However, two three-dimensional non-separable test integrands were evaluated using Formulae 1, 2, 3 and 4 of the Appendix. It would be expected that the strong appearance of cross terms would make integrals of this type difficult to handle with high accuracy by multidimensional formulae based on monomial power, and this is indeed borne out by the results shown in **Table 7**. For comparison, the result of the repeated Gauss formula of fifth degree has been given; this uses approximately the same number of points as the other formulae. A point which should be stressed is that a multidimensional formula which does not contain at least one generator (see Section 2) having non-zero elements in each dimension will give zero for monomials containing all the variables. The occurrence of this undesirable feature for formulae 1 and 3 is evident in Table 7 for the integrand $\sin x^2y^2z^2$ whose leading term contains all three variables.

The multidimensional formulae could of course be made more accurate by subdividing the domain of integration and summing the results of the application of the formulae to each subdomain. Unless, however, some of the abscissae lie on the boundary of the domain of integration and thus contribute to more than one of the partial sums, the amount of labour is likely to increase out of all proportion to the gain in accuracy. For example, Miller (1960) subdivides the range of Formula 3 and applies the resulting 152-point formula to integrate $\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} \cos x \cos y \cos z \, dx \, dy \, dz$ obtaining an error of $0 \cdot 000384$. This is much inferior to the

Table 4

Contribution of terms of (8) of the text for the integrand $\prod_{i=1}^{10} \frac{1}{(1+0\cdot 9x_i)}$. The terms are referred to by their associated subscripts and are grouped such that the first term of a given order is at least a factor of 2 greater than the first term of the next order. The terms within each order are in decreasing order of magnitude.

ORDER	TERMS
1	2,2,4 2,2 2,4 2 2,2,2 2,2,2,4 2,2,6 2,4,6 2,6 2,2,4,6
2^{-1}	2,4,4 2,2,4,4 4 2,2,2,6 2,2,8 2,4,8 2,8 2,2,4,8 2,2,2,2 0 2,2,2,4,6 4,6 2,4,4,6 2,2,2,2,4 2,2,2,4,4
2^{-2}	2,2,10 2,4,10 2,2,2,8 4,4 2,10 2,2,4,10 6 2,2,4,4,6 2,6,8 2,2,6,8 2,4,6,8 2,2,2,4,8 2,2,12 4,8 2,4,4,8 2,6,6 2,4,12 2,2,6,6 2,12 2,2,4,6,8 2,2,2,10 2,2,4,12 2,4,6,6 2,4,4,4 2,2,2,2,6 8 4,4,6 2,6,10 2,2,4,4,8 2,2,6,10 2,4,6,10 2,2,4,6,6
2^{-3}	2,2,4,4,4 2,2,2,4,10 2,2,14 2,4,14 4,10 2,4,4,10 2,14 2,2,4,14 2,2,2,2,2 2,2,2,6,8 2,2,2,12 2,2,4,6,10 4,6,8 2,2,2,2,4,6 6,8 2,2,2,4,4,6 2,6,12 2,2,2,2,8 10 2,2,6,12 2,2,4,4,10 4,4,8 2,8,10 2,4,6,12 2,2,2,2,4,4 2,2,2,6,6 2,2,2,4,12 2,2,8,10 4,6,6 4,4,4 2,4,8,10 6,6 4,12 2,4,4,6,8 2,4,4,12 2,2,2,14 2,2,2,6,10 2,2,4,6,12 2,2,2,4,6,8 4,6,10 2,6,14 2,8,8 2,2,4,8,10 12 6,10 2,2,6,14 2,2,2,2,10 2,2,2,2,4,8 2,2,8,8

four-point Gauss formula which gives an error of 0·00002 using only 64 points. In any case the application of subdivision does not necessarily produce uniform convergence so that probably more than one subdivision would have to be applied. A further improvement in accuracy could be obtained by the use of extrapolation methods but again several subdivisions would be necessary with a consequent large increase in labour.

4. Conclusions

An analysis of the Taylor expansion of multidimensional integrands indicate that multidimensional integration formulae derived on the basis of exact integration of monomials up to a particular power are likely to produce very unreliable results. It is suggested that the repeated application of one-dimensional Gauss quadrature formulae of low degree may be the most accurate and economical means of carrying out multidimensional integration due to the tendency for monomials containing low powers of the variables to dominate the Taylor expansion of the integrand.

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Table 5

Contribution of terms of (8) of the text for the integrand $\prod_{i=1}^{10} \frac{1}{(1 + 0 \cdot 5x_i)}$. The terms are referred to by their associated subscripts and are grouped such that the first term of a given order is at least a factor of 10 greater than the first term of the next order. The terms within each order are in decreasing order of magnitude.

ORDER	TERMS
1	0 2 2,2 4
10^{-1}	2,4 2,2,2 2,2,4 6 2,6 2,2,2,2
10^{-2}	4,4 2,2,2,4 2,2,6 2,4,4 8 2,8 4,6 2,4,6 2,2,4,4 2,2,2,6 2,2,8 2,2,2,2,2 10 2,2,2,2,4
10^{-3}	2,10 4,8 2,2,4,6 2,4,8 4,4,4 2,2,2,4,4 6,6 2,2,10 2,2,2,8 12 2,6,6 2,12 2,4,4,4 2,2,2,2,6 4,4,6 4,10 2,2,4,8 6,8 2,2,2,4,6 2,4,4,6 2,2,2,2,2,2
10^{-4}	2,4,10 2,2,2,2,2,4 2,6,8 2,2,12 2,2,6,6 2,2,2,10 14 2,2,4,4,4 2,14 2,2,2,2,8 4,4,8 2,2,2,2,4,4 4,6,6 4,12 2,2,4,10 2,2,4,4,6 6,10 2,2,6,8 2,2,2,4,8 2,4,4,8 2,4,12 2,4,6,6 2,6,10 2,2,2,2,2,6 2,2,14 2,2,2,12 16 4,6,8 2,2,2,2,4,6 8,8 2,2,2,6,6 2,16
10^{-5}	2,8,8 2,2,2,2,10 4,4,4,4 2,4,6,8 4,4,10 2,2,2,4,4,4 4,14 2,2,4,12 6,12 4,4,4,6 2,2,4,4,8 2,2,2,2,2,2,4 8,10 2,2,6,10 2,2,2,2,2,2,2 2,2,4,6,6 2,2,2,4,10 2,4,14 2,4,4,10 2,2,2,6,8 2,4,4,4,4 2,2,2,4,4,6 2,6,12 2,8,10 2,2,16 2,2,2,2,2,8 18 2,2,2,14 2,4,4,4,6 4,6,10 2,2,2,2,4,8 2,2,8,8 2,2,2,2,2,4,4 2,18 6,6,6 2,2,4,6,8 2,2,2,2,12 4,4,12 2,4,6,10 4,16 4,4,6,6 2,2,4,14 4,8,8 6,14 2,6,6,6 6,6,8 2,2,2,2,6,6 8,12 2,2,6,12 2,2,4,4,10 4,4,4,8 2,2,2,4,12 2,2,8,10 2,4,16 2,2,2,2,2,2,6 2,4,4,12 2,2,2,6,10

Appendix

Some multidimensional integration formulae

Formula 1

An n-dimensional fifth degree formula comprising $4n^2 - 2n + 1$ integrand evaluations is

$$J \simeq K = \frac{(10n^2 - 106n + 180)}{180} f(0, 0, \ldots, 0) + \frac{(14 - 5n)}{90} \sum_P f(1, 0, \ldots, 0) + \frac{(5n - 7)}{180(n-1)} \sum_P f(1, 1, 0, \ldots, 0) + \frac{8}{45(n-1)} \sum_P f\left(\frac{1}{2}, \frac{1}{2}, 0, \ldots, 0\right).$$

Formula 2

This fifth degree formula which is applicable to three or more dimensions and uses $(8n^3 - 24n^2 + 22n + 3)/3$ integrand evaluations takes the form

$$J \approx K = \frac{(10n^2 - 124n + 270)}{270} f(0, 0, 0, \ldots, 0) + \frac{(23 - 5n)}{180} \sum_P f(1, 0, 0, \ldots, 0) + \frac{(5n - 9)}{360(n-1)(n-2)} \sum_P f(1, 1, 1, 0, \ldots, 0) + \frac{8}{45(n-1)(n-2)} \sum_P f\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 0, \ldots, 0\right).$$

Table 6

Contribution of terms of (8) of the text for the integrand $\left(1 + \sum_{i=1}^{10} x_i\right)^{20}$. The terms are referred to be their associated subscripts and are grouped such that the first term of a given order is at least a factor of 10 greater than the first term of the next order. The terms within each order are in decreasing order of magnitude.

ORDER	TERMS
1	2,2,2,2,2,4,4 2,2,2,2,4,4 2,2,2,2,2,2,4 2,2,2,4,4,4 2,2,2,2,2,2,2,4 2,2,2,2,4,6 2,2,2,2,4,4,4 2,2,2,2,2,4 2,2,2,2,2,2,4,4 2,2,2,2,2,2,6 2,2,4,4,4 2,2,2,4,6 2,2,4,4,6 2,2,2,2,2,6
10^{-1}	2,2,2,4,4 2,2,2,2,2,2,2,2 2,2,2,2,2,4,6 2,2,2,4,4,6 2,2,2,2,2,2,2 2,4,4,4,4 2,2,2,2,2,2,2,2,2 2,2,2,2,2,2,2,2,4 2,2,4,4,4,4 2,2,2,2,6 2,2,2,4,8 2,2,2,2,2,2,2,6 2,4,4,6 2,2,2,6,6 2,2,2,2,2,8 2,2,2,2,4 2,2,4,6
10^{-2}	2,4,4,4 2,2,2,2,8 2,2,2,2,2,2 2,2,2,2,4,8 2,4,4,4,6 2,2,2,2,6,6 2,2,4,6,6 2,4,6,6 2,2,4,8 2,2,4,4 2,2,6,6 2,2,2,2,2,2,8 4,4,4,6 4,4,4,4 2,2,4,4,8 2,4,4,8 2,2,2,6 2,2,6,8 2,2,2,2,2,2,2,2,2,2 2,2,2,8 2,2,2,6,8 2,2,2,2,10
10^{-3}	4,4,4,4,4 2,2,2,4 2,2,2,2,2 2,2,4,10 4,4,6 2,4,6 4,6,6 2,2,2,4,10 2,2,2,10 2,2,2,2,2,10 2,4,8 2,4,6,8 4,4,6,6 2,6,6 4,4,8 2,6,8 4,4,4 4,6,8 4,4,4,8 2,4,4 2,6,6,6 2,4,10
10^{-4}	2,4,4,10 2,2,8 2,2,6 6,6,6 2,2,10 2,2,6,10 2,2,2,2 4,4,10 2,2,2,12 2,6,10 2,2,8,8 2,8,8 2,2,4 2,2,2,2,12 2,2,4,12 2,4,12
10^{-5}	6,8 2,2,12 4,8 6,6 4,6 6,6,8 4,6,10 4,10 4,8,8 6,10 8,8 2,8 2,10 2,8,10

Table 7

% error obtained using Formulae 1, 2, 3 and 4 of the Appendix and the three-point Gauss formula to calculate $\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} f(x, y, z)\, dx\, dy\, dz$.

$f(x, y, z)$	FORMULA				GAUSS 27 points
	1 31 points	2 23 points	3 19 points	4 27 points	
$\cos(xyz)$	$-1 \cdot 8$	$1 \cdot 8$	$-1 \cdot 8$	$-0 \cdot 03$	$-0 \cdot 0002$
$\sin(x^2y^2z^2)$	100	-84	100	$-1 \cdot 2$	$-0 \cdot 5$

Formula 3

A fifth degree formula using only $2n^2 + 1$ integrand evaluations is

$$J \approx K = \frac{(25n^2 - 115n + 162)}{162} f(0, 0, \ldots, 0)$$

$$+ \frac{5(14 - 5n)}{162} \sum_P f\left\{\sqrt{\left(\tfrac{3}{5}\right)}, 0, \ldots, 0\right\}$$

$$+ \frac{25}{324} \sum_P f\left\{\sqrt{\left(\tfrac{3}{5}\right)}, \sqrt{\left(\tfrac{3}{5}\right)}, 0, \ldots, 0\right\}.$$

Formula 4

A seventh degree formula for three dimensions using 27 integrand evaluations can be obtained in the form

$$J \approx K = A_0 f(0, 0, 0) + A_1 \sum_P f(x_1, 0, 0) + A_2 \sum_P f(x_2, x_2, 0) + A_3 \sum_P f(x_3, x_3, x_3).$$

There are two possible choices for A_0, A_1, A_2, A_3, x_1, x_2 and x_3, thus:

$A_0 = 0\cdot1184868$ or $0\cdot1821729$
$A_1 = 0\cdot0053074$ $\quad 0\cdot0466670$
$A_2 = 0\cdot0629095$ $\quad 0\cdot0049431$
$A_3 = 0\cdot0118472$ $\quad 0\cdot0598136$
$x_1 = 1\cdot2795819$ $\quad 0\cdot8484180$
$x_2 = 0\cdot7000973$ $\quad 1\cdot1064129$
$x_3 = 0\cdot8550443$ $\quad 0\cdot6528165$

These formulae have the undesirable feature that one of the abscissae lies outside the range of integration.

Estimate of the maximum error in best polynomial approximations

By G. M. Phillips*

By using Chebyshev's equioscillation theorem and the well-known error formula for the interpolating polynomial, inequalities are derived for the minimax error in polynomial approximation. These results are extended to piecewise polynomial approximations.

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1. Approximations over a single interval

Suppose a function $f(x)$ is defined on $[a, b]$ and that $f^{(n+1)}(x)$ exists and is continuous on that interval. Let $p_n(x)$ be the polynomial of degree not greater than n which is the best approximating polynomial for $f(x)$ on $[a, b]$ in the Chebyshev sense. By the equioscillation theorem (see, for example, Davis (1963)), $\exists$ at least $n + 2$ points on which

$$\max_{a \leqslant x \leqslant b} | f(x) - p_n(x) |$$

is attained, with the error $f(x) - p_n(x)$ alternating in sign over those points. Hence, by continuity, $\exists$ at least $n + 1$ distinct points, say $x_0, x_1, \ldots, x_n$, on $[a, b]$, where $f(x) - p_n(x) = 0$, and so we may write the usual estimate for the error in the interpolating polynomial,

$$f(x) - p_n(x) = \frac{(x - x_0) \ldots (x - x_n)}{(n + 1)!} f^{(n+1)}(\xi_x), \quad (1)$$

where ξ_x is some function of x.

Now let $x_0^*, x_1^*, \ldots, x_n^*$ be the zeros of $T_{n+1}((2x - b - a)/(b - a))$, where $T_{n+1}(x)$ is the Chebyshev polynomial $\cos((n + 1)\cos^{-1} x)$. If we let $q_n(x)$ be the interpolating polynomial for $f(x)$ constructed at $x_0^*, x_1^*, \ldots, x_n^*$, we will have

$$f(x) - q_n(x) = \frac{(x - x_0^*) \ldots (x - x_n^*)}{(n + 1)!} f^{(n+1)}(\eta_x), \quad (2)$$

η_x being some function of x. Therefore

$$\max_{a \leqslant x \leqslant b} |f(x) - q_n(x)| \leqslant \frac{1}{(n + 1)!} \max_{a \leqslant x \leqslant b} |(x - x_0^*) \ldots (x - x_n^*)| \cdot \max_{a \leqslant x \leqslant b} |f^{(n+1)}(x)|. \quad (3)$$

Putting $y = (2x - b - a)/(b - a)$ and

$$y_r^* = (2x_r^* - b - a)/(b - a) \text{ for } r = 0, 1, \ldots, n,$$

$$\max_{a \leqslant x \leqslant b} |(x - x_0^*) \ldots (x - x_n^*)| = \left(\frac{b - a}{2}\right)^{n+1} \cdot \max_{-1 \leqslant y \leqslant 1} |(y - y_0^*) \ldots (y - y_n^*)|. \quad (4)$$

Thus the inequality (3) gives

$$\max_{a \leqslant x \leqslant b} |f(x) - q_n(x)| \leqslant \frac{(b - a)^{n+1}}{2^{2n+1}(n + 1)!} \cdot \max_{a \leqslant x \leqslant b} |f^{(n+1)}(x)|. \quad (5)$$

From the definition of $p_n(x)$, it follows that

$$\max_{a \leqslant x \leqslant b} |f(x) - p_n(x)| \leqslant \frac{(b - a)^{n+1}}{2^{2n+1}(n + 1)!} \cdot \max_{a \leqslant x \leqslant b} |f^{(n+1)}(x)|. \quad (6)$$

Also, from (1),

$$\max_{a \leqslant x \leqslant b} | f(x) - p_n(x)| \geqslant \frac{1}{(n + 1)!} \max_{a \leqslant x \leqslant b} |(x - x_0) \ldots (x - x_n)| \cdot \min_{a \leqslant x \leqslant b} |f^{(n+1)}(x)| \quad (7)$$

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