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Optimum Quadrature Formulas In s Dimensions

Although numerical procedures for functions of more than one variable are of considerable practical importance, they have received relatively little attention. So far as numerical integration is concerned, aside from successive application of appropriate one-dimensional results, as discussed in standard texts, and a few isolated special results for two dimensions, there has been little systematic study of the problem. Tyler [1] has collected a set of formulas of up to seventh degree for integration over rectangular regions in the plane, and up to fifth degree in three dimensions, and also gives a $(2s + 1)$-point third-degree formula for s dimensions. Hammer, Marlowe, Stroud, and Wymore [2, 3, 4] have pointed out useful methods of extending available results for spaces of a given dimension to higher dimensions, and to regions which are related to the given region by affine transformations. They have also developed a number of formulas for simplexes, cones, and spheres in s dimensions.

It is the purpose of the present paper to describe a general approach to the problem which may often yield useful results and to use it to derive formulas in s dimensions using $(s + 1)$ points for second-degree accuracy, and $2s$ points for third-degree accuracy. This method is applicable to any region, although its advantages are most pronounced for regions with a center of symmetry, and in our detailed calculations we will limit ourselves to a hypercube with center at the origin. We will be concerned with formulas of the form

$$(1) \qquad \int_S \cdots \int \varphi(x^{(1)}, \cdots, x^{(s)}) dx^{(1)} \cdots dx^{(s)} = \sum_{i=1}^{m} c_i \varphi(x_i^{(1)}, \cdots, x_i^{(s)}) - R\varphi$$

where $R\varphi$ denotes the error of the formula for a particular function φ. A formula will be said to be of degree n if $R\varphi$ is zero whenever φ is a polynomial of degree n or less in the s variables $x^{(j)}$.

If a formula is of degree n, the c_i and $x_i^{(j)}$ must satisfy the set of equations

$$(2) \qquad \sum_{i=1}^{m} c_i \prod_{j=1}^{s} (x_i^{(j)})^{n_j} = \int_S \cdots \int \prod_{j=1}^{s} (x^{(j)})^{n_j} dx^{(j)} \equiv I_{n_1, \cdots, n_s}$$

for all sets of n_j with sum equal to or less than n. An nth degree formula in s dimensions involves $(n + s)!/n!s!$ such nonlinear inhomogeneous algebraic equations, and each solution to such a set leads to an acceptable nth degree formula. Unfortunately, the task of solving systems of nonlinear algebraic equations is a formidable one, and general solutions have only been obtained in the simplest cases, although special methods have led to single solutions for more complex cases [1].

An instructive formulation of the problem can be obtained by a change in viewpoint. Let us define a set of $m \times m$ diagonal matrices by

$$\mathbf{G} \equiv [\sqrt{c_i}\delta_{hi}] \tag{3}$$

$$\mathbf{X}^{(j)} \equiv [x_i^{(j)}\delta_{hi}]. \tag{4}$$

In terms of these matrices, (2) becomes

$$\operatorname{tr}\{\mathbf{G}\prod_{j=1}^{s}(\mathbf{X}^{(j)})^{n_j}\mathbf{G}\} = I_{n_1,\ldots,n_s}. \tag{5}$$

Although the solution of a set of matrix equations such as (5) is generally no easier than the solution of a set of nonlinear algebraic equations such as (2), this formulation does emphasize certain considerations which are generally used intuitively in solving (2). In the first place, the fact that the validity of a formula of the form of equation (1) is independent of the numbering of the points is reflected in the fact that the trace of a diagonal matrix is unaffected by interchange of diagonal elements. If the region S is symmetric with respect to change of sign of one of the variables, this fact must be reflected by an invariance of (5) to a change of sign of $\mathbf{X}^{(j)}$. If the region S is symmetric with respect to permutation of certain variables, $I_{n_1,\ldots,n_s}$ must be invariant to permutation of the corresponding n_j.

Let us now specialize this to the case of hypercubes with edge length two, and center at the origin. In this case, the $I_{n_1,\ldots,n_s}$ are independent of the order of the subscripts, and

$$I_{n_1,\ldots,n_s} = \begin{cases} 0 & \text{if at least one } n_j \text{ is odd} \\ \dfrac{2^s}{\prod_{j=1}^{s}(n_j+1)} & \text{if no } n_j \text{ is odd.} \end{cases} \tag{6}$$

For a second degree formula, therefore, we have the equations

$$\operatorname{tr}\{\mathbf{GG}\} = 2^s \tag{7}$$

$$\operatorname{tr}\{\mathbf{GX}^{(j)}\mathbf{G}\} = 0 \tag{8}$$

$$\operatorname{tr}\{\mathbf{GX}^{(j)}\mathbf{X}^{(k)}\mathbf{G}\} = \frac{2^s}{3}\delta_{jk}. \tag{9}$$

These equations in the traces may be converted to vector equations if we introduce the m-dimensional column vector with all elements unity, ϵ, and its transpose, ϵ^T. Then if we define the vectors $\xi, \xi_j, \xi_{jk}, \cdots$, by $\xi = \mathbf{G}\epsilon$, $\xi_j = \mathbf{X}^{(j)}\mathbf{G}\epsilon$, $\xi_{jk} = \mathbf{X}^{(j)}\mathbf{X}^{(k)}\mathbf{G}\epsilon$ and so on, (7), (8) and (9) become

$$\epsilon^T\mathbf{G}\mathbf{G}\epsilon = (\mathbf{G}\epsilon)^T(\mathbf{G}\epsilon) = \xi^T\xi = 2^s \tag{10}$$

$$\epsilon^T\mathbf{G}\mathbf{X}^{(j)}\mathbf{G}\epsilon = (\mathbf{G}\epsilon)^T(\mathbf{X}^{(j)}\mathbf{G}\epsilon) = \xi^T\xi_j = 0 \tag{11}$$

$$\begin{aligned}\epsilon^T\mathbf{G}\mathbf{X}^{(j)}\mathbf{X}^{(k)}\mathbf{G}\epsilon &= (\mathbf{X}^{(j)}\mathbf{G}\epsilon)^T(\mathbf{X}^{(k)}\mathbf{G}\epsilon) = \xi_j{}^T\xi_k \\ &= (\mathbf{X}^{(j)}\mathbf{X}^{(k)}\mathbf{G}\epsilon)^T(\mathbf{G}\epsilon) = \xi^T{}_{jk}\xi = \frac{2^s}{3}\,\delta_{jk}.\end{aligned} \tag{12}$$

These, however, will be recognized as merely orthogonality relations among $(s+1)$ vectors, $\xi, \xi_1, \cdots, \xi_s$ and normalization requirements that $|\xi|^2 = 2^s$, $|\xi_j|^2 = 2^s/3$. Now $(s+1)$ orthogonal vectors span a vector space of dimension $(s+1)$ and this space must be a subspace of the vector space of dimension m consisting of all m-dimensional vectors. Thus, a second degree formula of the form of (1) can be obtained with $m = s + 1$, and for any higher value of m.

Our argument has also furnished an explicit algorithm for constructing examples of such formulas by orthogonalizing any linearly independent set of $(s+1)(s+1)$-dimensional vectors, and applying the proper normalization conditions. For example, if we orthogonalize the set, $(1, 1, 1)$, $(3, -\sqrt{3}\tan\vartheta, \sqrt{3}\tan\vartheta)$ and $(3\sqrt{3}\tan\vartheta, 0, 0)$, in that order, we find

$$\xi = (2/\sqrt{3}, 2/\sqrt{3}, 2/\sqrt{3}) \tag{13}$$

$$\xi_1 = \left(\frac{2\sqrt{2}}{3}\cos\vartheta, \frac{2\sqrt{2}}{3}\cos\left(\vartheta + \frac{2\pi}{3}\right), \frac{2\sqrt{2}}{3}\cos\left(\vartheta + \frac{4\pi}{3}\right)\right) \tag{14}$$

$$\xi_2 = \left(\left(\frac{2\sqrt{2}}{3}\right)\sin\vartheta, \frac{2\sqrt{2}}{3}\sin\left(\vartheta + \frac{2\pi}{3}\right), \frac{2\sqrt{2}}{3}\sin\left(\vartheta + \frac{4\pi}{3}\right)\right) \tag{15}$$

so that our integration formula becomes

$$\begin{aligned}&\int_{-1}^{1}\int_{-1}^{1}\varphi(s, t)\,ds\,dt \\ &= \frac{4}{3}\left\{\varphi(\sqrt{\tfrac{2}{3}}\cos\vartheta, \sqrt{\tfrac{2}{3}}\sin\vartheta) + \varphi\left(\sqrt{\tfrac{2}{3}}\cos\left(\vartheta + \frac{2\pi}{3}\right), \sqrt{\tfrac{2}{3}}\sin\left(\vartheta + \frac{2\pi}{3}\right)\right)\right. \\ &\qquad \left. + \varphi\left(\sqrt{\tfrac{2}{3}}\cos\left(\vartheta + \frac{4\pi}{3}\right), \sqrt{\tfrac{2}{3}}\sin\left(\vartheta + \frac{4\pi}{3}\right)\right)\right\} - R_2\varphi\end{aligned} \tag{16}$$

where $R_2\varphi$ vanishes if φ is a polynomial of degree 2 or less. The parameter ϑ is arbitrary, although because of the periodicity of the trigonometric functions it may be taken to lie in the range $-\frac{\pi}{3} \le \vartheta < \frac{\pi}{3}$. The vertices of any equilateral triangle inscribed in a circle of radius $\sqrt{\frac{2}{3}}$ are thus seen to afford a satisfactory set of second-degree integration points.

For higher degree formulas, the orthogonality conditions no longer suffice to define the minimal solution completely, but they still afford a substantial simplification, as can be seen from the following discussion of third-degree formulas. For these, we have, along with (10), (11) and (12), the condition

$$\epsilon^T \mathbf{G} \mathbf{X}^{(j)} \mathbf{X}^{(k)} \mathbf{X}^{(l)} \mathbf{G} \epsilon = (\mathbf{X}^{(j)} \mathbf{X}^{(k)} \mathbf{G} \epsilon)^T (\mathbf{X}^{(l)} \mathbf{G} \epsilon) = \xi^T{}_{jk} \xi_l = 0. \tag{17}$$

Thus, we must consider the $s(s+1)/2$ new vectors ξ_{jk} in addition to ξ and the ξ_j. These new vectors fall into two classes: the s ξ_{jj} are orthogonal to every ξ_l, but not to ξ, while the $s(s-1)/2$ $\xi_{jk} (j \neq k)$ are orthogonal to both sets, or else are null vectors.

Let us consider first the case where all the ξ_{jk} are null vectors. This implies that unless one or more elements of ξ is zero, in which case the basic integration formula includes redundant points with zero weight, only one of the $\mathbf{X}^{(j)}$ can have any given element different from zero. The ξ_{jj} cannot be null vectors, in view of (12), while from (11), unless the c_i differ in sign, $\mathbf{X}^{(j)}$ must include elements of both signs, and thus at least two non-zero elements. We therefore conclude that the dimension of $\mathbf{X}^{(j)}$ must be at least $2s$.

For an equally-weighted formula, $\mathbf{G}$ is a scalar matrix, which we may write as $g\mathbf{E}$, where $\mathbf{E}$ is the identity. From (7), for a $2s$-point formula, g^2 must have the value $2^{s-1}/s$. For the minimum number of points, $\mathbf{X}^{(j)}$ will have but two non-zero elements of opposite sign, and, from (8), of equal magnitude, and these may be arranged in order such that

$$(\mathbf{X}^{(j)})_{hi} = x^{(j)} (\delta_{hi} [\delta_{i,2j-1} - \delta_{i,2j}]) \tag{18}$$

a diagonal matrix with the $(2j-1)$th element equal to $x^{(j)}$ and the $2j$th to $-x^{(j)}$. From (9), it follows that

$$2 x^{(j)2} g^2 = 2^s/3 \tag{19}$$

so that for all j,

$$x^{(j)} = \sqrt{s/3} \tag{20}$$

and we have the family of $2s$-point third-degree integration formulas

$$\int_{-1}^{1} \cdots \int_{-1}^{1} \varphi(x^{(1)}, \cdots, x^{(s)}) dx^{(1)} \cdots dx^{(s)} = \frac{2^{s-1}}{s} \sum_{i=1}^{2s} \varphi(x_i^{(1)}, \cdots, x_i^{(s)}) + R_3 \varphi \tag{21}$$

where

$$x_i^{(j)} = \sqrt{\frac{s}{3}} (\delta_{i,2j-1} - \delta_{i,2j}). \tag{22}$$

The case for s equal to three is included in Tyler's collection [1]. For s greater than three, these formulas have the drawback that they depend upon values of the function outside the range of integration, and thus may have larger remainder terms than are desirable.

If one or more of the ξ_{jk} is non-null, there must be $s + 2$ or more orthogonal vectors, and the minimum value of m must be at least $s + 2$. This lower bound can be attained for s equal to two. In this case, we have a basis of four orthogonal vectors, ξ, ξ_1, ξ_2, and ξ_{12}. If a four-point formula exists, these vectors completely span the space, and we can express ξ_{11} and ξ_{22} as linear combinations of ξ and ξ_{12},

$$\xi_{jj} = a_j\xi + b_j\xi_{12} \tag{23}$$

since ξ_{11} and ξ_{22} are orthogonal to ξ_1 and ξ_2. If we multiply both sides of (23) by ξ^T, it follows from (12) that a_j must be $\frac{1}{3}$. Hence, introducing the definition of ξ_{12}, and rearranging,

$$\mathbf{X}^{(j)}(\mathbf{X}^{(j)} - b_j\mathbf{X}^{(k)})\xi = \tfrac{1}{3}\xi. \tag{24}$$

Thus ξ is an eigenvector, and $\frac{1}{3}$ an eigenvalue of the two matrices, $\mathbf{X}^{(1)}(\mathbf{X}^{(1)} - b_1\mathbf{X}^{(2)})$ and $\mathbf{X}^{(2)}(\mathbf{X}^{(2)} - b_2\mathbf{X}^{(1)})$. Since these matrices are diagonal, all the elements corresponding to non-zero elements of ξ must be equal to $\frac{1}{3}$. In particular, for equally-weighted four-point formulas, the diagonal elements of $\mathbf{X}^{(1)}$ and $\mathbf{X}^{(2)}$ must be the roots of the two equations

$$x^{(1)^2} - b_1x^{(1)}x^{(2)} = \tfrac{1}{3}, \quad x^{(2)^2} - b_2x^{(1)}x^{(2)} = \tfrac{1}{3}, \tag{25}$$

which become

$$x^{(2)} = (x^{(1)^2} - \tfrac{1}{3})/b_1x^{(1)}, \tag{26}$$

and

$$x^{(1)^4} - \frac{2 - b_1b_2 + b_1^2}{3(1 - b_1b_2)}x^{(1)^2} + \frac{1}{9(1 - b_1b_2)} = 0. \tag{27}$$

Now the sum of the squares of the four roots of (27) is equal to -2 times the second term, and if these roots are to satisfy (9)

$$2(2 - b_1b_2 + b_1^2) = 3(1 - b_1b_2)\tfrac{4}{3} \tag{28}$$

so that

$$b_1 = -b_2 \equiv b. \tag{29}$$

Accordingly,

$$x^{(1)^4} - \tfrac{2}{3}x^{(1)^2} + \frac{1}{9(1 + b^2)} = 0 \tag{30}$$

$$x^{(1)} = \pm\left\{\frac{1}{3}\left(1 \pm \sqrt{\frac{b^2}{1 + b^2}}\right)\right\}^{\frac{1}{2}} \tag{31}$$

$$x^{(2)} = \pm \left\{ \frac{1}{3}\left(1 \mp \sqrt{\frac{b^2}{1+b^2}}\right) \right\}^{\frac{1}{2}}. \tag{32}$$

Thus, again we find that the integration points lie on a circle of radius $\sqrt{2/3}$, and that there is a whole family of four-point third-degree cubature formulas, corresponding to the corners of squares inscribed in this circle. In three dimensions, it can be shown that a five-point third-degree formula is impossible, but that the vertices of any regular octahedron inscribed in a sphere of unit radius are satisfactory points for an equally-weighted quadrature formula. Even with matrix notation, the calculations for spaces of higher dimension, or for formulas of higher degree become extremely tedious. However, it seems likely that, as was observed for second- and third-degree formulas, the minimum number of points necessary for a quadrature formula of a given dimension, s, will continue to be of the order of some power of s, and not of the sth power of the number of points for a one-dimensional formula.

It should be noticed that the application of the matrix-vector formulation is not limited to the hypercubical regions with constant weighting function which have been discussed in detail. It is equally helpful in deriving multidimensional analogues of the Gauss-Laguerre and Gauss-Hermite one-dimensional formulas, although the corresponding relations among the vectors are no longer simple orthogonality conditions, but require less obvious methods of solution.

Because of the variety of formulas discussed, the problem of the truncation error for formulas of various degrees and dimension cannot be considered in detail. The more familiar methods for obtaining remainders in one dimension cannot, unfortunately, be extended to multidimensional problems, and Sard's extension [5] of Peano's theorem is one of the very few useful bases for an error estimate. Even so, the expressions are complicated, and depend upon several partial derivatives, thus requiring quite detailed information about the behavior of the integrand, which may often be unavailable.

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HENRY C. THACHER, JR.

Aeronautical Research Laboratory
Wright Air Development Center
Wright-Patterson Air Force Base, Ohio

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