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1. P. C. HAMMER & A. W. WYMORE, "Numerical integration over higher dimensional regions." Unpublished manuscript.
2. G. SZEGÖ, *Orthogonal Polynomials*, Am. Math. Soc. *Colloquium Publications*, v. 23, New York, 1939.
3. G. W. TYLER, "Numerical integration of functions of several variables," *Canadian J. Math.*, v. 5, 1953, p. 393–412.

Numerical Integration over Simplexes

1. Introduction. Integration formulae for numerical evaluation of integrals over the simplex in n-space have been given inductively by Hammer, Marlowe, and Stroud [1] so that it is possible in principle to determine a formula holding exactly for the kth degree polynomial in n variables. In the same paper certain affinely symmetric integration formulae are given for the triangle and tetrahedron. Using the theory proposed by Hammer and Wymore [2], it is possible to extend the usefulness of methods developed by transformations of the regions and by use of Cartesian products.

In this paper we give two integration formulae of affinely symmetric type for the simplex in n-space which respectively hold exactly for the quadratic polynomial and the cubic polynomial in n variables. The method for establishing the exact values of integrals needed we believe is new in that the "numerical" formulae are used for the purpose.

2. The formula for cubic polynomials. Let the vertices of the n-simplex, S_n, be $V_0, \cdots, V_n$ and then its centroid is given by $C = \sum_1^n V_i/(n+1)$. Let Δ_n be the hypervolume of S_n.

THEOREM *1: An integration formula exact for the general cubic polynomial over S_n for $n \geq 1$ is given by*

$$\int_{S_n} f dv_n = a_n \sum_0^n f(U_i) + c_n f(C) \tag{1}$$

where

$$a_n = \frac{(n+3)^2}{4(n+1)(n+2)} \Delta_n \quad c_n = \frac{-(n+1)^2}{4(n+2)} \Delta_n$$

and

$$U_i = \frac{2}{n+3} V_i + \frac{n+1}{n+3} C \quad i = 0, \cdots, n.$$

Proof: It may first be remarked that the points U_i are on the median lines of S_n and that the statement of the theorem is in symmetric form. In particular, under an affine transformation taking S_n onto itself, the set of points $\{U_i\}$ is invariant and the centroid C is fixed. Since there exists an affine transformation mapping any simplex in E_n onto any other we may choose any particular simplex S_n to carry out the proof. Our choice is specified by vertices as follows:

$$V_0 = (0, \cdots, 0), \qquad V_1 = (1, 0, \cdots, 0),$$
$$V_2 = (1, 1, 0, \cdots, 0), \cdots, \quad V_n = (1, 0, \cdots, 0, 1).$$

It is simply verified that the formula given holds for $n = 1$ and $n = 2$. Hence we assume that it holds for E_{n-1} and proceed to show that it also holds for E_n where $n - 1 \geq 2$. Let f be a cubic polynomial in $x_1, x_2, \cdots, x_n$. Then $f|_{x_1=1}$ is a cubic polynomial in $x_2, \cdots, x_n$. Now using a result established in [1] we may write

$$(2) \quad \int_{S_n} f dv_n = \int_0^1 \left(\int_{x_1 S_{n-1}} f dv_{n-1} \right) dx_1$$
$$= \int_0^1 x_1^{n-1} [a_{n-1} \sum_1^n f(x_1 \bar{U}_i) + c_{n-1} f(x_1 \bar{C}_i)] dx_1$$

where S_{n-1} is the $(n - 1)$-simplex with vertices $V_1, \cdots, V_n$ in the hyperplane $x_1 = 1$, $\bar{C} = 1/n \sum_1^n V_i$, $\bar{U}_i = \dfrac{2}{n+2} V_i + \dfrac{n}{n+2} \bar{C}$, $i = 1, 2, \cdots, n$ and a_{n-1} and c_{n-1} are the weights as indicated in the theorem with n replaced by $n - 1$. It is observed that the hypervolume Δ_{n-1} is $1/(n - 1)!$ and Δ_n is $1/n!$. Let f be the monomial $x_1^i x_2^j x_3^k$ where $0 \leq i + j + k \leq 3$. Using (2) we find on substitution and simplification that:

$$(3) \quad \int_{S_n} x_1^i x_2^j x_3^k dv_n = \frac{\Delta_n [(n + 2)^{2-j-k} (3^j + 3^k + n - 2) - n^{3-j-k}]}{4(n + 1)(n + i + j + k)}.$$

On the basis of our assumption, (3) gives the value of the integral indicated. On the other hand, formula (1) applied to $f = x_1^i x_2^j x_3^k$ gives

$$(4) \quad \frac{\Delta_n}{4(n+1)(n+2)} \{ (n+3)^{2-i-j-k} [n^i + (n+2)^i (3^j + 3^k + n - 2)] - (n+1)^{3-i-j-k} n^i \}.$$

Now it may then be directly verified that (4) gives the same result as the right of (3) for $0 \leq i + j + k \leq 3$, $0 \leq i \leq 3$ and $j \geq k$. Hence in view of the symmetry with which the last $n - 1$ coordinates appear in the set of vertices $V_0, \cdots, V_n$, (4) is verified as correct for all monomials of form $x_1^i x^j_{i_1} x^k_{i_2}$ for $0 \leq i + j + k \leq 3$, $i_1 \neq i_2$ where i_1 and i_2 are taken from $2, \cdots, n$. The only monomial type thus omitted is $x_2 x_3 x_4$ provided $n \geq 4$. Using formula (2) for this monomial, we find

$$(5) \quad \int_{S_n} x_2 x_3 x_4 dv_n = \frac{\Delta_n}{4(n + 1)(n + 2)(n + 3)}$$

which coincides with the value obtained on substituting $f = x_2 x_3 x_4$ in (1). Hence the formula (1) holds for all required monomials and for the cubic polynomials provided it holds on S_{n-1}. Hence by complete induction the formula (1) holds.

3. A formula for the quadratic polynomial.

THEOREM 2: *The formula*

$$(6) \quad \int_{S_n} f dv_n = \frac{\Delta_n}{n + 1} \sum_0^n f(U_i)$$

holds for the quadratic polynomial over S_n, $n \geq 1$ *provided* $U_i = rV_i + (1 - r)C$ *where either* $r = 1/\sqrt{n+2}$ *or* $r = -1/\sqrt{n+2}$. *The choice of the positive sign for* r *gives points* U_i *inside* S_n *for all* n. *If the negative sign is chosen, the points* U_i *are outside* S_n *for* $n > 2$.

The proof of this theorem may be made along the same lines as that of theorem 1, by induction.

4. Remarks. The formulae given are affinely symmetrical. Those for the cubic polynomial are based on rational combinations of the vertices whereas the formulae for the quadratic function are based on irrational combinations unless $n + 2$ is a perfect square. The weight of the centroid is negative and increases numerically with n for the cubic case. The formula for the cubic polynomial may well be used as an exact integration formula for any polynomial of degree at most three. Since the general cubic polynomial has $(n + 1)(n + 2)(n + 3)/6$ terms, the formula (1) is hyperefficient (see [1] or [2]) for $n > 3$ since it is based on $n + 2$ evaluation points.

The practicality of using simplicial decompositions of regions decreases rapidly with increasing n. For $n = 1$, the formula (1) is based on three evaluation points whereas Gauss' formula uses only two. We conjecture that for no region of bounded volume in E_n for $n \geq 2$ will it be possible to obtain a numerical integration formula exact for the cubic polynomial based on fewer than $n + 2$ points. Over the hypercube, Tyler [3] has shown that the cubic polynomial may be integrated exactly by a formula using $2n$ points. Hammer and Wymore have extended this result to certain symmetrical regions.

Extension of affinely symmetric formulae for integration over the simplex to higher degree polynomials promises to offer significantly greater complexity. In the tetrahedron, for example, we have shown that evaluation points to obtain a formula exact for the fourth degree polynomial cannot all be taken on the median lines. However, the methods used here may be of use for higher degree polynomials.

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1. P. C. HAMMER, O. J. MARLOWE, & A. H. STROUD, "Numerical integration over simplexes and cones" [see p. 130 this issue].

2. P. C. HAMMER & A. W. WYMORE, "Numerical evaluation of multiple integrals." Unpublished manuscript.

3. G. W. TYLER, "Numerical integration of functions of several variables," *Canadian Jn. Math.*, v. 5, 1953, p. 393–412.