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On the Existence of Regions with Minimal Third Degree Integration Formulas*

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Abstract. A. H. Stroud has shown that $n + 1$ is the minimum possible number of nodes in an integration formula of degree three for any region in E_n. In this paper, in answer to the question of the attainability of this minimal number, we exhibit for each n a region that possesses a third degree formula with $n + 1$ nodes. This is accomplished by first deriving an $(n + 2)$-point formula of degree three for an arbitrary region that is invariant under the group of affine transformations that leave an n-simplex fixed. The formula is then applied to a one-parameter family of such regions, and a value of the parameter is determined for which the weight at the centroid vanishes.

1. Introduction. An approximate N-point integration formula of the form

$$I(f) \equiv \int_R f \, d\mu = \sum_{k=1}^{N} A_k f(\mathbf{x}_k) + E(f),$$

with *nodes* $\mathbf{x}_k$ and *weights* A_k for a region R in n-dimensional Euclidean space E_n, where $d\mu$ is ordinary n-dimensional Lebesgue measure, is said to be of *degree* m if $E(f) = 0$ whenever f is a polynomial of degree at most m in the n variables $\mathbf{x} = (x_1, \cdots, x_n)$. Such a formula is said to be *positive* if $A_k > 0$ for $k = 1, \cdots, N$; *self-contained* if $\mathbf{x}_k \in R$ for $k = 1, \cdots, N$.

Let S_n be the n-simplex with vertices $\mathbf{v}_0, \mathbf{v}_1, \cdots, \mathbf{v}_n$ and let $\mathbf{c}$ be the centroid of S_n. Let R be any subset of E_n with positive Lebesgue measure which is invariant under the group of affine transformations that map S_n onto itself. A region that possesses this property for some S_n will be called *simplicially-symmetric*. We assume that all polynomials of degree at most three in the n variables are integrable over R. We shall consider third degree $(n + 2)$-point formulas of the form

$$\int_R f \, d\mu = A \sum_{k=0}^{n} f(\mathbf{x}_k) + Bf(\mathbf{c}) + E(f), \tag{1}$$

where

$$\mathbf{x}_k = r\mathbf{v}_k + (1 - r)\mathbf{c} \qquad (k = 0, 1, \cdots, n).$$

In this paper we obtain a condition on the simplicially-symmetric region R for the existence of a formula of form (1) which is of degree three. We derive general expressions for the unknowns A, B and r, and show that the weight A must be positive, while B is unrestricted in sign. We exhibit a region for which $B = 0$, so that the formula actually involves only $n + 1$ points. Stroud [6] has shown that $n + 1$ is the smallest number of nodes possible in an integration formula of degree three

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for any region, but it was not known in general prior to the publication of this example whether this minimal number was attained by any region. In fact a conjecture to the contrary was made by Hammer and Stroud [3].

Specifically, a one-parameter family of star-shaped simplicially-symmetric regions $S_n(d)$ is studied. There is a unique value $d = d_n^*$ for which the formula fails to exist. A result due to Mysovskikh [5] enables us to explain the failure for $n = 2$ and 3, but the significance of $S_n(d_n^*)$ is still unexplained for $n > 3$. A unique value $d = d_n \neq d_n^*$ is determined for which the number of nodes reduces to $n + 1$. The formula is positive for $d \geqq d_n$. It is further shown that the formula is self-contained for all d. We have proved [2, pp. 96–104] that $S_2(d_2)$ is an isolated example, in the sense that any three-point third degree formula for a member $S_2(d)$ of the family must be of form (1) with $B = 0$. It is not known whether the same is true for $n > 2$.

The results reported here provide further evidence in support of the concluding remark of Stroud [7]: ". . . the minimal point formulas of degree 3 for a region are related to the group of symmetries of the region."

2. Derivation of Formulas for the Unknowns. As discussed by Hammer and Wymore [4], we may identify any two regions that are affine-equivalent for the purpose of deriving approximate integration formulas. We may accordingly take S_n to be the n-simplex

$$\{x \in E_n : x_i \geqq 0, x_1 + x_2 + \cdots + x_n \leqq 1\}. \tag{2}$$

THEOREM. *If we determine A, B, and r so that formula* (1) *is exact for the three monomials* 1, x_1^2, x_1^3, *then the formula is of degree three.*

This theorem is proved in Stroud [8]. His proof is based on a special case of the following lemma.

LEMMA. *Let L be a linear functional which is invariant under the symmetries of S_n; that is, if T is an affine transformation for which $TS_n = S_n$ and if $g(\mathrm{x}) = f(T\mathrm{x})$, then $L(g) = L(f)$. If $0 \leqq k < n$ and $\{\alpha_i\}_{i=1}^k$ is a sequence of positive integers, then $L(x_1^{\alpha_1} \cdots x_k^{\alpha_k} x_{k+1})$ can be expressed as a linear combination of the values of L on the $k + 1$ monomials*

$$\prod_{i \leqq k} x_i^{\alpha_i}, \qquad \prod_{i \leqq k} x_i^{\alpha_i + \delta_{ij}} \qquad (j = 1, 2, \cdots, k),$$

where δ_{ij} is the Kronecker delta symbol, and the empty product

$$\prod_{i \leqq 0} x_i^{\alpha_i} = 1.$$

The proof depends mainly on the invariance of L under the affine transformation which interchanges vertices v_0 (= **0**) and v_{k+1} (= $(k + 1)$th unit vector) of S_n. Use of the Lemma allows us to express $L(f)$, where f is any polynomial of degree at most three, as a linear combination of $L(1)$, $L(x_1^2)$, $L(x_1^3)$. Noting that both sides of (1) have the required invariance proves the Theorem.

By application of the Theorem, a necessary and sufficient condition for (1) to be a formula of degree three for the simplicially-symmetric region R is that A, B, and r be solutions of the following system of nonlinear equations:

$$(n + 1)A + B = I_0 \equiv I(1); \tag{3}$$

(4) $$\frac{1 + nr^2}{n + 1} A + \frac{1}{(n + 1)^2} B = I_2 \equiv I(x_1^2);$$

(5) $$\frac{1 + 3nr^2 + n(n - 1)r^3}{(n + 1)^2} A + \frac{1}{(n + 1)^3} B = I_3 \equiv I(x_1^3).$$

We may use Eq. (3) to eliminate B from the other two equations

(4′) $$n(n + 1)Ar^2 = J_2 \equiv (n + 1)^2 I_2 - I_0;$$

(5′) $$n(n + 1)[(n - 1)r + 3]Ar^2 = J_3 \equiv (n + 1)^3 I_3 - I_0.$$

Since

$$J_2 = \int_R [(n + 1)x_1 - 1]^2 \, d\mu > 0,$$

necessary conditions for the existence of a solution are $A > 0$ and $r \neq 0$. Substituting Eq. (4′) into (5′) and solving for r, we obtain

(6) $$r = \frac{J_3 - 3J_2}{(n - 1)J_2} \equiv \frac{D}{(n - 1)J_2}.$$

Thus *a necessary and sufficient condition on the region R for the existence of a third degree formula of form* (1) *is that*

(7) $$D = \int_R [(n + 1)x_1 - 1]^3 \, d\mu \neq 0.$$

If R satisfies Eq. (7), then there exists a unique formula (1) given by Eq. (6),

(8) $$A = \frac{J_2}{n(n + 1)r^2} = \frac{(n - 1)^2 J_2^3}{n(n + 1)D^2},$$

and

(9) $$B = I_0 - (n + 1)A = \frac{nI_0D^2 - (n - 1)^2 J_2^3}{nD^2} \equiv \frac{P}{nD^2}.$$

While A is always positive, the sign of B is determined by that of P. We observe that, since $J_2 > 0$, $P = 0$ implies $D \neq 0$. Thus if we can find a region R for which $P = 0$ we will have an example of a region that possesses a positive formula of degree three with the minimum possible number of nodes.

3. A Family of Star-Shaped Simplicially-Symmetric Regions. In the remainder of this paper we shall apply these formulas to a family of star-shaped simplicially-symmetric regions $S_n(d)$ over which the necessary integrals can be computed, in order to prove the existence of a region for which this minimal number of nodes is attained. For notational clarity, if Q is one of the quantitites introduced in the preceding section, then $Q_n(d)$ will denote the value of this quantity for $S_n(d)$. The order of presentation will be as follows:

1. Derive formulas for $A_n(d)$, $B_n(d)$, and $r_n(d)$ as rational functions of the parameter d, with coefficients which are polynomials in the dimension n.

2. Prove the existence of a unique value d_n of d for which $P_n(d_n) = 0$, so that $S_n(d_n)$ possess a formula of form (1) with $B = 0$.

3. Prove that there exists a unique value d_n^* of d for which $D_n(d_n^*) = 0$, and consequently formula (1) fails to exist for $S_n(d_n^*)$.

4. Finally, show that the formula is self-contained for all $d > 0$, $d \neq d_n^*$. (Note that formula (1) need not be self-contained, in general.)

The regions $S_n(d)$ are defined as follows. Let S_n be the n-simplex with vertices $\mathbf{v}_0, \mathbf{v}_1, \cdots, \mathbf{v}_n$. Let F_k be the face of S_n that does *not* contain the vertex $\mathbf{v}_k$ and let $\mathbf{c}_k$ be the centroid of F_k. Let $d > 0$ and define the points $\mathbf{u}_k(d)$ by:

$$\mathbf{u}_k(d) = d\mathbf{c}_k + (1 - d)\mathbf{c} \qquad (k = 0, 1, \cdots, n).$$

Let $S_{nk}(d)$ be the pyramid (simplex) with base F_k and vertex $\mathbf{u}_k(d)$. ($S_{nk}(d)$ degenerates to the face F_k when $d = 1$.) Define

$$\begin{aligned} S_n(d) &= S_n \cup \left(\bigcup_{k=0}^{n} S_{nk}(d) \right) \quad \text{if } d \geqq 1; \\ &= S_n - \left(\bigcup_{k=0}^{n} S_{nk}(d) \right) \quad \text{if } 0 < d < 1. \end{aligned}$$

Clearly, $S_n(1) = S_n$. For $d > 1$, this star-shaped polyhedral region can be visualized as the result of "pushing out" the center of each face of S_n. This family of regions was previously studied for $n = 2$ by De Vogelaere [1], who knew of the existence of $S_2(d_2)$. Since $\mathbf{u}_k(d)$ lies on the line determined by $\mathbf{v}_k$ and $\mathbf{c}$, the set $\{\mathbf{u}_0(d), \mathbf{u}_1(d), \cdots, \mathbf{u}_n(d)\}$ is invariant under any affine transformation that leaves S_n invariant, and $S_n(d)$ is simplicially-symmetric.

4. Application of the Formulas to $S_n(d)$. Let us now specialize S_n to the simplex (2). If we use the natural simplicial decomposition of $S_n(d)$, a straightforward but extremely tedious computation [2, pp. 72–75, 151–159] yields the following values for the needed monomial integrals:

$$I_{0n}(d) = \frac{d}{n!},$$

$$I_{2n}(d) = \frac{2d}{n(n+1)^2(n+2)!} [d^2 + (n-1)d + n^2(n+2)],$$

$$I_{3n}(d) = \frac{6d}{n^2(n+1)^3(n+3)!} [(1-n)d^3 + (5n-1)d^2 + n(n-1)(n+4)d + n^2(n^3 + 3n^2 + 2n - 2)].$$

We may now compute $A_n(d)$, $B_n(d)$, and $r_n(d)$.

$$J_{2n}(d) = (n+1)^2 I_{2n}(d) - I_{0n}(d) = \frac{d}{n(n+2)!} \psi_n(d),$$

where

(10) $$\psi_n(d) = 2d^2 + 2(n-1)d + n(n-1)(n+2).$$

$$J_{3n}(d) = (n+1)^3 I_{3n}(d) - I_{0n}(d) = \frac{d}{n^2(n+3)!} \chi_n(d),$$

where

$$\chi_n(d) = 6(1 - n)d^3 + 6(5n - 1)d^2 + 6n(n - 1)(n + 4)d + n^2(n - 1)(5n^2 + 17n + 18).$$

(11) $$D_n(d) = J_{3n}(d) - 3J_{2n}(d) = \frac{2(n-1)d}{n(n^2+3)!}\phi_n(d),$$

where

(12) $$\phi_n(d) = 3d^3 + 3(n - 1)d^2 - 3nd - n^3(n + 1).$$

From Eq. (6) we obtain:

(13) $$r_n(d) = \frac{D_n(d)}{(n-1)J_{2n}(d)} = \frac{-2}{n(n+3)}\frac{\phi_n(d)}{\psi_n(d)}.$$

Provided $D_n(d) \neq 0$, we similarly obtain from Eqs. (8) and (9) the following:

(14) $$A_n(d) = \frac{(n+3)^2 d}{4(n+1)(n+2)!}\frac{[\psi_n(d)]^3}{[\phi_n(d)]^2}.$$

(15) $$B_n(d) = \frac{P_n(d)}{n[D_n(d)]^2} = \frac{d}{4(n+2)!}\frac{F_n(d)}{[\phi_n(d)]^2},$$

where

(16) $$F_n(d) = 4(n + 1)(n + 2)[\phi_n(d)]^2 - (n + 3)^2[\psi_n(d)]^3.$$

5. A Region that Possesses an $(n + 1)$-Point Formula of Degree Three. We have seen that, whenever $D_n(d) \neq 0$, $S_n(d)$ possesses a third degree formula of the form (1) with $r = r_n(d)$, $A = A_n(d)$, and $B = B_n(d)$ given by Eqs. (13), (14), and (15), respectively. From Eq. (15) we see that $B_n(d)$, the weight at the centroid, is negative, zero, or positive according as the polynomial $F_n(d)$ is negative, zero, or positive. Hammer and Stroud [3] showed that $B_n(1)$ is negative, while the leading coefficient of $F_n(d)$ is $4n(7n + 15) > 0$. Hence there exists a $d_n > 1$ such that $F_n(d_n) = 0$. As remarked above, $D_n(d_n) \neq 0$. Thus, $S_n(d_n)$ *possesses a positive* $(n + 1)$*-point formula of degree three*, providing the first known example of a region with the minimal number of nodes.

A consideration based on the Descartes rule of signs and the use of a polynomial root finder to compute the real and complex roots of the polynomials in n that appear in the coefficients of $F_n(d)$ in Eq. (16) enables us to conclude [2, pp. 77–80] that $F_n(d)$ possesses a single positive root and d_n *is uniquely determined for* $n \geqq 3$. The case $n = 2$ deserves special attention. $F_2(d)$ has two positive roots, one between 0 and 1 and the other greater than 1. One may easily verify that $F_2(4/d) = (2/d)^6 F_2(d)$, so that F_2 is "reciprocal" in the sense that if d is a root, so is $4/d$. The geometrical significance of this property of F_2 is that $S_2(4/d)$ is similar to $S_2(d)$. Thus, the two positive roots of F_2 must result in similar figures, and d_2 *is essentially unique*. The two reciprocal figures $S_2(d_2)$ and $S_2(4/d_2)$, based on an equilateral triangle, are depicted in Fig. 1.

6. The Exceptional Member of the Family. From Eq. (12) we see by the Descartes rule of signs that ϕ_n has exactly one positive root, which we shall call d_n^*.

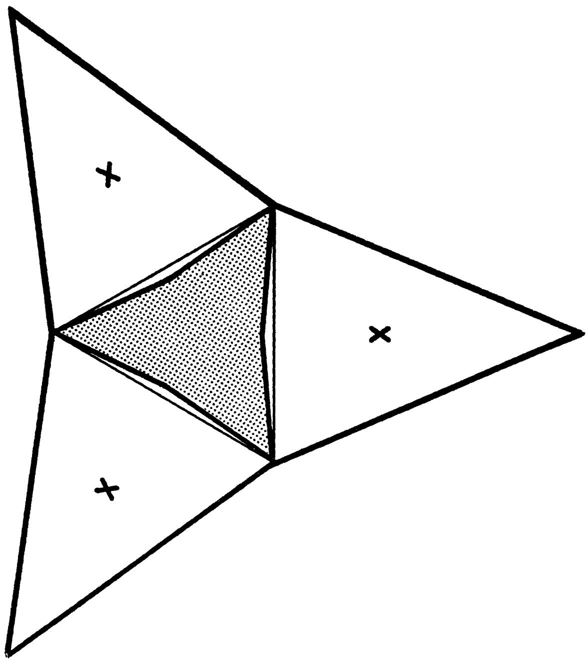

FIGURE 1. $S_2(d_2)$ *and (shaded)* $S_2(4/d_2)$, *two planar regions which possess three-point formulas of degree three. The x's locate the nodes for* $S_2(d_2)$.

From Eq. (11) we see that $D_n(d_n^*) = 0$ and $D_n(d) \neq 0$ for $d \neq d_n^*$. In other words, there is only one member $S_n(d_n^*)$ of the family for which a formula of the desired form fails to exist. Since $J_{2n}(d) > 0$ for all $d > 0$, Eq. (13) shows that the sign of $r_n(d)$ is the same as that of $D_n(d)$, and that $r_n(d_n^*) = 0$. Thus, the formula fails to exist because all $n + 2$ nodes coincide, and their associated weights become infinite.

For $n = 2$, $d_2^* = 2$ is the unique positive value of d for which $4/d = d$. When based on an equilateral triangle, $S_2(2)$ is a regular hexagon. It is the only centrally-symmetric member of the family. As Mysovskikh [5] shows, there exist infinitely many third degree four-point formulas for $S_2(2)$, but none of them has **c** as one of its nodes. A formula of form (1) *must* fail to exist, because the four nodes are not centrally-symmetric with respect to **c**. For $n = 3$, $d_3^* = 3$. Again, $S_3(3)$ is the only centrally-symmetric member of the family. (When based on a regular tetrahedron, it is a cube.) In this case, since the Mysovskikh result shows that six is the minimal number of nodes for third degree formulas on $S_3(3)$, a 5-point formula *must* fail to exist. For $n > 3$, $d_n^* > n$. We remark that in this case there is no centrally-symmetric member of the family, and the significance of the nonexistence of such a formula for $S_n(d_n^*)$ is still not known for $n > 3$.

We know from the general theory of Section 2 that $d_n \neq d_n^*$. In fact, one can show [2, pp. 82–85] that for all $n \geqq 2$,

$$d_n^* < n^{4/3} < d_n.$$

This separation property is illustrated in Fig. 5-1 of [2, p. 95].

7. Self-Containment of the Formulas. We show further that *the formula is self-contained for all* $d > 0$ $(d \neq d_n^*)$ *and all* $n \geqq 2$. Note that this does not follow from the general theory. It is evident that $\mathbf{u}_k(d)$ and $\mathbf{x}_k$ both lie on the line determined by $\mathbf{v}_k$ and $\mathbf{c}$. $\mathbf{u}_k(d)$ is on the opposite side of $\mathbf{c}$ from $\mathbf{v}_k$. If $r_n(d) > 0$, $\mathbf{x}_k$ is on the same side as $\mathbf{v}_k$, and the condition for self-containment in this case is

$$r_n(d) \leqq 1 \quad \text{for } 0 < d < d_n^*. \tag{17}$$

If $r_n(d) < 0$, $\mathbf{x}_k$ is on the same side as $\mathbf{u}_k(d)$, and the condition for self-containment is

$$\rho_n(d) \equiv -\frac{n}{d}\, r_n(d) \leqq 1 \quad \text{for } d > d_n^*. \tag{18}$$

Condition (17) can be verified by differentiating Eq. (13) and observing that $r_n'(d) < 0$ for all $d > 0$, $n \geqq 2$. Since one can easily see that $r_n(0) < 1$, (17) holds with strict inequality. From Eqs. (10), (12), (13), condition (18) can be shown to hold with strict inequality by observing that $2\phi_n(d) < (n + 3)\, d\psi_n(d)$ for all $d > d_n^*$, $n \geqq 2$. We remark that numerical computations have shown that $\rho_n(d_n) < .5$ for $n = 2(1)50$, and indicate that $\rho_n(d_n)$ decreases monotonically to zero as $n \to \infty$.

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