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 \( \mathbb{E}^n \). 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

\[
I(f) = \int_R f \, d\mu = \sum_{k=1}^N A_k f(x_k) + E(f),
\]

with nodes \( x_k \) and weights \( A_k \) for a region \( R \) in \( n \)-dimensional Euclidean space \( \mathbb{E}^n \), 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 \( x = (x_1, \ldots, x_n) \). Such a formula is said to be positive if \( A_k > 0 \) for \( k = 1, \ldots, N \); self-contained if \( x_k \in R \) for \( k = 1, \ldots, N \).

Let \( S_n \) be the \( n \)-simplex with vertices \( v_0, v_1, \ldots, v_n \) and let \( c \) be the centroid of \( S_n \). Let \( R \) be any subset of \( \mathbb{E}^n \) 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

\[
(1) \quad \int_R f \, d\mu = A \sum_{k=0}^n f(x_k) + Bf(c) + E(f),
\]

where

\[
x_k = rv_k + (1 - r)c \quad (k = 0, 1, \ldots, n).
\]

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...
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 $d = d_n$ is determined for which the number of nodes reduces to $n + 1$. The formula is positive for $d = d_n$. 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

\[ \{x \in \mathbb{R}^n: x_i \geq 0, x_1 + x_2 + \cdots + x_n \leq 1 \}. \]

**Theorem.** If we determine $A$, $B$, and $r$ so that formula (1) is exact for the three monomials $1$, $x_1^j$, $x_2^j$, 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 $g(x) = f(Tx)$, then $L(g) = L(f)$. If $0 \leq k < n$ and $\{\alpha_i\}_{i=1}^k$ is a sequence of positive integers, then $L(x_{i_1}^{\alpha_1} \cdots x_{i_j}^{\alpha_j} x_{i_{j+1}}^{\alpha_{j+1}})$ can be expressed as a linear combination of the values of $L$ on the $k + 1$ monomials

\[ \prod_{i \leq k} x_i^{\alpha_i}, \quad \prod_{i \geq k} x_i^{\alpha_i+1} \quad (j = 1, 2, \ldots, k), \]

where $\delta_{ij}$ is the Kronecker delta symbol, and the empty product

\[ \prod_{i \geq 0} x_i^{\alpha_i} = 1. \]

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 $L(1)$, $L(x_1^3)$, $L(x_2^3)$. 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:

\[(n + 1)A + B = I_0 \equiv I(1);\]
REGIONS WITH MINIMAL THIRD DEGREE FORMULAS

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

\begin{align*}
(4') & \quad n(n + 1)A_1 = J_2 \equiv (n + 1)^2 I_2 - I_0; \\
(5') & \quad n(n + 1)((n - 1)r + 3)A_2 = J_3 \equiv (n + 1)^3 I_3 - I_0.
\end{align*}

Since

\[ J_2 = \int_{\mathcal{R}} [(n + 1)x_1 - 1] d\mu > 0, \]

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

\[ r = \frac{J_3 - 3 J_2}{(n - 1)J_2} = \frac{D}{(n - 1)J_2}. \]

Thus a necessary and sufficient condition on the region $\mathcal{R}$ for the existence of a third degree formula of form (1) is that

\[ D = \int_{\mathcal{R}} [(n + 1)x_1 - 1]^2 d\mu \neq 0. \]

If $\mathcal{R}$ satisfies Eq. (7), then there exists a unique formula (1) given by Eq. (6),

\[ A = \frac{J_2}{n(n + 1)r^2} = \frac{(n - 1)^2 J_2^2}{n(n + 1)D^2}, \]

and

\[ B = I_0 - (n + 1)A = \frac{n I_0 D^2 - (n - 1)^2 J_2^2}{n D^2} = \frac{P}{n D^2}. \]

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 $\mathcal{R}$ 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 quantities 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 $n$. 

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2. Prove the existence of a unique value \( d_0 \) of \( d \) for which \( P_0(d_0) = 0 \), so that \( S_0(d_0) \) possess a formula of form (1) with \( B = 0 \).

3. Prove that there exists a unique value \( d^* \) of \( d \) for which \( D_0(d^*) = 0 \), and consequently formula (1) fails to exist for \( S_0(d^*) \).

4. Finally, show that the formula is self-contained for all \( d > 0, d \neq d^* \). (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 \( v_0, v_1, \ldots, v_n \). Let \( F_k \) be the face of \( S_n \) that does not contain the vertex \( v_k \) and let \( c_k \) be the centroid of \( F_k \). Let \( d > 0 \) and define the points \( u_k(d) \) by:

\[
u_k(d) = d c_k + (1 - d) c \quad (k = 0, 1, \ldots, n).
\]

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

\[
S_n(d) = \begin{cases} 
S_n \cup \left( \bigcup_{k=0}^n S_{nk}(d) \right) & \text{if } d \geq 1; \\
S_n - \left( \bigcup_{k=0}^n S_{nk}(d) \right) & \text{if } 0 < d < 1.
\end{cases}
\]

Clearly, \( S_0(1) = S_n \). 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 \( u_k(d) \) lies on the line determined by \( v_k \) and \( c \), the set \( \{u_0(d), u_1(d), \ldots, u_n(d)\} \) 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:

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

\[
I_{2n}(d) = \frac{2d}{n(n + 1)^2(n + 2)!} \left[ d^2 + (n - 1)d + n^3(n + 2) \right],
\]

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

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

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

where

\[
(10) \quad \psi_n(d) = 2d^2 + 2(n - 1)d + n(n - 1)(n + 2).
\]

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

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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) \[ D_n(d) = J_{2n}(d) - 3J_{2n}(d) = \frac{2(n - 1)d}{n(n + 3)!} \phi_n(d), \]

where

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

From Eq. (6) we obtain:

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

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

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

(15) \[ B_n(d) = \frac{P_n(d)}{n[D_n(d)]^3} = \frac{d}{4(n + 2)!} \left[ \frac{F_n(d)}{[\phi_n(d)]^3} \right]^2, \]

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 \( n \geq 3 \). 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 \( F_2(4/d) = (2/d)^2F_2(d) \), 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 \( \phi_n \) has exactly one positive root, which we shall call \( d^*_n \).
Figure 1. $S_3(d_3)$ and (shaded) $S_4(4/d_4)$, two planar regions which possess three-point formulas of degree three. The x's locate the nodes for $S_3(d_3)$.

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 $d_4 \neq d^*_4$. In fact, one can show [2, pp. 82–85] that for all $n \geq 2$,

$$d^*_n < n^{4/3} < d_4.$$

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 \( n \geq 2 \). Note that this does not follow from the general theory. It is evident that \( u_k(d) \) and \( x_k \) both lie on the line determined by \( v_k \) and \( c \). \( u_k(d) \) is on the opposite side of \( c \) from \( v_k \). If \( r_n(d) > 0 \), \( x_k \) is on the same side as \( v_k \), and the condition for self-containment in this case is

\[
(17) \quad r_n(d) \leq 1 \quad \text{for} \quad 0 < d < d^*_n.
\]

If \( r_n(d) < 0 \), \( x_k \) is on the same side as \( u_k(d) \), and the condition for self-containment is

\[
(18) \quad \frac{n}{d} r_n(d) \leq 1 \quad \text{for} \quad d > d^*_n.
\]

Condition (17) can be verified by differentiating Eq. (13) and observing that \( r_n'(d) < 0 \) for all \( d > 0 \), \( n \geq 2 \). 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 \( 2 \phi_n(d) < (n + 3) d \phi_n(d) \) for all \( d > d^*_n \), \( n \geq 2 \). 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 \( n \to \infty \).

Acknowledgments. The author wishes to express his deep gratitude to Professor R. Sherman Lehman for the direction of his thesis research and to A. C. Hindmarsh and R. E. von Holdt for their suggestions concerning the organization of this paper.

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1. R. J. De Vogelaere, Private communication.