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A Quadrature Formula of Degree Three

LEOPOLD FLATTO

Department of Mathematics, Yeshiva University, New York, New York 10033

AND

SEYMOUR HABER

National Bureau of Standards, Washington, D. C. 20234
and Department of Mathematics, University of Maryland, Catonsville, Maryland 21228

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Let R be a region in n-space and Q a linear quadrature formula for R of the form

$$Q(f) = \sum_{r=1}^{k} a_r f(x_r).$$

It is known that if $Q(f) = \int_R f$ whenever f is a polynomial of degree 3 or lower, then $k \geqslant n + 1$. It is known that the minimum possible value of k depends on the region R, being $2n$ for the n-cube and $n + 2$ for the n-simplex ($n > 1$). In 1956 Hammer and Stroud conjectured that $k \geqslant n + 2$ for every R, when $n > 1$. In this paper we construct an R, and a Q with the required property, with $k = n + 1$.

An important problem in the theory of numerical quadrature has been the extension, to integration of functions of several variables, of the idea of the "Gaussian" quadrature formulas for functions of one variable. The latter are families of l-point linear formulas

$$\int_a^b f(x)\, dx \approx Q(f) = \sum_{r=1}^{l} a_r f(x_r) \qquad (l = 1, 2, \ldots)$$

which integrate exactly all polynomials of degree $2l - 1$ or lower. It is known that they are "most efficient"—that is, if we let the "degree of precision" of a linear quadrature formula be the highest integer d such that

$$\int_a^b P(x)\, dx = Q(P)$$

whenever P is a polynomial of degree d or lower, then l, the number of points used in Q, must be at least $1 + [d/2]$ (where "$[x]$" denotes the greatest integer less than or equal to x). Gaussian formulas are known to exist for all intervals on the real line, whether finite, semiinfinite, or infinite, for integration with respect to any nonnegative weight function $\omega(x)$ for which

$$\int_a^b \omega(x)x^m\,dx < \infty, \qquad m = 0, 1, 2, \ldots .$$

For multiple integrals the situation is quite different. The number of linearly independent polynomials of degree d or lower—in n variables—is

$$\binom{n+d}{d}.$$

It is known [1] that if R is any n-dimensional region then a formula

$$\int_R f \approx Q(f) = \sum_{r=1}^{l} a_r f(\mathbf{x}_r)$$

that is of degree d must have

$$l \geqslant \binom{n+[d/2]}{[d/2]}, \tag{1}$$

but it is definitely not the case that the lower bound in (1) can be attained for every d and for every region R. A survey of some of the recent work on this problem may be found in [2, pp. 488–497]; here we shall mention only a few of the known results. For $d = 0$ or 1, the lower bound in (1) is 1, and the 1-point formula in which $\mathbf{x}_1$ is the centroid of R and a_1 the volume of R is indeed of degree 1. For $d = 2$ the minimum number of points needed is $n + 1$, and Thacher [3] and Stroud [4] have found $(n + 1)$-point formulas of degree 2 for all finite regions R. For $d \geqslant 3$ the situation for $n \geqslant 2$ becomes different from the one-dimensional situation. With $d = 3$, the lower bound in (1) is $n+1$; however, Mysovskih [5] has shown that if R is the n-cube the lowest possible number of points in a degree-3 formula is $2n$. On the other hand, Stroud and Hammer [6] found a formula of degree 3 for the n-simplex using $n + 2$ points. Stroud and Hammer conjectured that there is no bounded region R in n-space, $n > 1$, for which there exists a degree-3 quadrature formula using only $n + 1$ points. Stroud [11] conjectured further that the lower bound in (1) is not attainable for any odd $d > 1$, with $n > 1$. In this paper we shall show that these conjectures are incorrect, so that the lower bound in (1) is attainable for some regions when $d = 3$.[1]

THEOREM. *Let n be an integer* $\geqslant 2$. *Let* σ *be a regular n-simplex in Euclidean n-space* E^n, *having its center of mass at the origin and having one vertex at* $(1, 0, 0,..., 0)$. *Let* $p_0, p_1, p_2, ..., p_n$ *be the vertices of* σ, *and, for any function f defined on* σ, *set*

$$Q(f) = 1/(n+1) \sum_{i=0}^{n} f(p_i).$$

Then there is a region R_n *such that*

$$1/|R_n| \int_{R_n} P = Q(P), \tag{2}$$

whenever P is a polynomial of degree 3 *or lower.*

(Here " $| R |$ " denotes the volume of R, when R is a region in E^n; later on we shall also use $| R |$ to denote the "area" of R when R is a region on the unit n-sphere.)

Proof. Let G_n be the symmetry group of the simplex σ—i.e., the group of all isometries of E^n taking σ onto itself. It is known [7, p. 130] that G_n is isomorphic to the symmetric group on $n + 1$ letters (in fact the elements of G_n, acting on the vertices of σ, are just all the permutations of those vertices). We first specify that the region R_n be invariant under G_n—i.e., that $g(R_n) = R_n$ for every $g \in G_n$. The center of mass of R_n will, thus, be at the origin, and (2) will certainly hold whenever P is of degree 0 or 1.

A function f is called "invariant under G_n" if $f(g(\mathbf{x})) = f(\mathbf{x})$ for every $g \in G_n$. If f is any function, set

$$\hat{f}(\mathbf{x}) = 1/(n+1)! \sum_{g \in G_n} f(g(\mathbf{x})).$$

For any $h \in G_n$,

$$\begin{aligned} \hat{f}(h(\mathbf{x})) &= 1/(n+1)! \sum_{g \in G_n} f(g(h(\mathbf{x}))) = 1/(n+1)! \sum_{g \in G_n} f((g \cdot h)(\mathbf{x})) \\ &= 1/(n+1)! \sum_{g \in G_n} f(g(\mathbf{x})) = \hat{f}(\mathbf{x}), \end{aligned}$$

[1] After this paper was written, we were informed by Stroud that the theorem below had already been found by F. N. Fritsch in a paper which has since appeared as [12]. The region R_n that we construct is different from that found by Fritsch, but the methods of the present paper and of [12] are closely related. However, where Fritsch bases his work on an apparently very special algebraic theorem due to Stroud [13], we use the Hilbert basis theorem in a manner which, we feel, makes the underlying algebraic situation clearer. In part as a result, the algebraic and analytic manipulations in this paper are somewhat simpler than Fritsch's.

since, as g runs through the elements of G_n, so does $g \cdot h$. (Here $g \cdot h$ is the product, in G_n, of g and h—i.e., their composition.) Thus, $\hat{f}$ is always invariant under G_n. Furthermore, as can easily be seen,

$$1/| R_n | \int_{R_n} \hat{f}(\mathbf{x})\, d\mathbf{x} = 1/| R_n | \int_{R_n} f(\mathbf{x})\, d\mathbf{x}$$

and

$$Q(\hat{f}) = Q(f).$$

It follows that a n.a.s.c. for (2) to hold for a function f is that it hold for $\hat{f}$. Now when f is a polynomial, $\hat{f}$ is a polynomial of the same degree, and so a n.a.s.c. for (2) to hold for all polynomials of degrees 2 and 3 is that it holds for all polynomials of degrees 2 and 3 that are invariant under G_n. Polynomials invariant under a group G of linear transformations are known, simply, as "invariants" of G.

It is a classical theorem of Hilbert (see, e.g. [8, pp. 274–276]) that the set of all invariants of a finite[2] group G has a finite "integrity basis"—i.e., that there is a finite collection of invariants $\{P_1, P_2, ..., P_k\}$ such that every invariant is a polynomial in $P_1, P_2, ..., P_k$. The particular group G_n with which we are dealing is one generated by those of its members which are reflections [7, p. 187]. For such groups it was shown by Chevalley [9] that their invariants have an integrity basis consisting of n algebraically independent homogeneous invariant polynomials, of certain degrees $m_1, m_2, ..., m_n$. For the group G_n, Coxeter (who denotes this group by "$[3^{n-1}]$") gives the numbers $m_1, m_2, ..., m_n$ as $2, 3, 4, ..., n+1$ [10, Table 3].

Now we observe that the polynomial

$$I_2(\mathbf{x}) = (x^1)^2 + (x^2)^2 + \cdots + (x^n)^2$$

is invariant under G_n. If $\{\pi_2, \pi_3, ..., \pi_{n+1}\}$ ($\deg \pi_r = r$) is an integrity basis for the invariants of G_n, of the kind described by Chevalley, and $I_2 = P(\pi_2, \pi_3, ..., \pi_{n+1})$, then indeed $P(\pi_2, \pi_3, ..., \pi_{n+1})$ is just $c\pi_2$, for some nonzero constant c. Otherwise $P(\pi_2, ..., \pi_{n+1})$ would contain terms of degree higher than 2, and the sum of all those terms—which would itself be a polynomial in $\pi_2, \pi_3, ..., \pi_{n+1}$—would be identically zero, contradicting the algebraic independence of the π_i. By the same reasoning, any other invariant of G_n of degree 2 is a constant multiple of π_2 and thus of I_2. Similarly,

$$I_3(\mathbf{x}) = \sum_{r=0}^{n} (\mathbf{x} \cdot \mathbf{p}_r)^3$$

[2] Hilbert's theorem is not restricted to finite groups.

(where "$\mathbf{x} \cdot \mathbf{p}_r$" is the inner product of $\mathbf{x}$ and $\mathbf{p}_r$) is a homogeneous invariant of degree 3, and any other homogeneous invariant of G_n of degree 3 is a constant multiple of I_3. Any invariant of G_n of degree 3 is then a linear combination of I_2 and I_3.

It follows that (2) will hold for all P's of degree 2 and 3 if and only if it holds for I_2 and I_3. To calculate $Q(I_2)$ and $Q(I_3)$, we note that if f is invariant under G_n,

$$Q(f) = 1/(n+1) \sum_{r=0}^{n} f(\mathbf{p}_r) = f(\mathbf{p}_0);$$

and we may take $\mathbf{p}_0$ to be the vertex $(1, 0, 0,..., 0)$. So $Q(I_2) = 1$; and since the first coordinate of each of the vertices $\mathbf{p}_1, \mathbf{p}_2, ..., \mathbf{p}_n$ is $-1/n$,

$$Q(I_3) = \sum_{r=0}^{n} (\mathbf{p}_r^1)^3 = 1 - 1/n^2.$$

Call this last quantity, for convenience, "b". To complete the proof of the theorem, it is now necessary and sufficient to find a region R_n (invariant under G_n) such that

$$1/|R_n| \int_{R_n} I_2 = 1 \tag{3}$$

and

$$1/|R_n| \int_{R_n} I_3 = b. \tag{4}$$

We first introduce polar coordinates, representing any point $\mathbf{x}$ in E^n by (r, φ), where r is the distance of $\mathbf{x}$ from the origin, and φ the point in which the ray from the origin through $\mathbf{x}$ meets the unit sphere S_n.[3] G_n, acting on S_n, partitions it into $(n+1)!$ congruent "fundamental regions" [7, p. 63 and Chapter XI] which are spherical simplexes and which are interchanged under the elements of G_n. Choose one of them, containing the point $\mathbf{p}_0$ (as a vertex); call it F. In the cone $C_F = \{r, \varphi \mid \varphi \in F\}$ we shall construct a region R_F; R_n shall consist of R_F together with all its images under the transformations $g \in G_n$, which guarantees that R_n will be invariant under G_n. It is clear that

$$1/|R_n| \int_{R_n} I_r = 1/|R_F| \int_{R_F} I_r, \qquad r = 2, 3.$$

Thus, conditions (3) and (4) must be satisfied with R_F in place of R_n.

[3] Here S_n is the set of all x satisfying $(x^1)^2 + (x^2)^2 + \cdots + (x^n)^2 = 1$. Below we shall refer to the "unit ball" B_n, defined by $(x^1)^2 + (x^2)^2 + \cdots + (x^n)^2 \leqslant 1$.

Let F_ϵ be the intersection of F with an ϵ-neighborhood of p_0, ϵ to be specified later. Let ρ be a number $\geqslant 1$, also to be specified later, and set

$$\begin{aligned} R_F &= R \cup R', \\ R &= \{(r, \varphi) |\, 0 \leqslant r \leqslant 1, \varphi \in F\}, \\ R' &= \{(r, \varphi) |\, 1 \leqslant r \leqslant \rho, \varphi \in F_\epsilon\}. \end{aligned}$$

Now

$$| R | = | B_n |/(n+1)!, \tag{5}$$

where B_n is the unit n-ball. Also

$$| R' | = \int_1^\rho dr \int_{rF_\epsilon} d\mu,$$

where rF_ϵ is the set of all (r, φ) with $\varphi \in F_\epsilon$, and $d\mu$ is the area measure on the appropriate n-sphere (that of radius r). Thus,

$$| R' | = \int_1^\rho dr \left(r^{n-1} \int_{F_\epsilon} d\mu \right) = ((\rho^n - 1)/n) \, | F_\epsilon |. \tag{6}$$

We now integrate I_2 and I_3 over R and R':

$$\begin{aligned} \int_R I_2 &= \int_0^1 dr \int_{rF} r^2 \, d\mu = \int_0^1 r^{n+1} \, dr \int_F d\mu \\ &= (1/(n+2))(| S_n |/(n+1)!). \end{aligned} \tag{7}$$

$$\begin{aligned} \int_R I_3 &= 1/(n+1)! \int_{B_n} I_3 = 1/(n+1)! \sum_{i=0}^{n} \int_{B_n} (\mathbf{x} \cdot \mathbf{p}_i)^3 \\ &= 1/n! \int_{B_n} (\mathbf{x} \cdot \mathbf{p}_0)^3 = 1/n! \int_{B_n} (x^1)^3 = 0. \end{aligned} \tag{8}$$

In a manner similar to the calculation of (6) we obtain

$$\int_{R'} I_2 = ((\rho^{n+2} - 1)/(n+2)) \, | F_\epsilon |. \tag{9}$$

Since $I_3(a\mathbf{x}) = a^3 I_3(\mathbf{x})$,

$$\int_{R'} I_3 = \int_1^\rho dr \int_{rF} I_3 \, d\mu = \int_1^\rho r^{n+2} \, dr \int_{F_\epsilon} I_3 \, d\mu.$$

For ϵ near zero, $I_3(\mathbf{x})$ is very near $I_3(\mathbf{p}_0) = b$ throughout F_ϵ; thus,

$$\int_{R'} I_3 = ((\rho^{n+3} - 1)/(n+3)) b \, | F_\epsilon | \, (1 + O(\epsilon)), \qquad \text{as} \quad \epsilon \to 0. \tag{10}$$

Now let ϵ_0 be the least ϵ for which $F_\epsilon = F$. We will show that for any ϵ in $[0, \epsilon_0]$ we may choose a $\rho = \rho^*(\epsilon)$ for which R' will be such that

$$\int_{R_F} I_2 = | R_F |;$$

i.e., so that (2) will hold for I_2 : First take $\epsilon = \epsilon_0$. Then R_F is just the region $\{(r, \varphi) | \, 0 \leqslant r \leqslant \rho, \varphi \in F\}$. In the same manner as we obtained (5) and (7), we obtain

$$| R_F | = (| B_n |/(n+1)!) \, \rho^n, \qquad \int_{R_F} I_2 = (\rho^{n+2}/(n+2))(| S_n |/(n+1)!).$$

Thus,

$$1/| R_F | \int_{R_F} I_2 = (n/(n+2)) \, \rho^2,$$

and we take

$$\rho^*(\epsilon_0) = ((n+2)/n)^{1/2}.$$

For $\epsilon < \epsilon_0$, we note that

$$1/| R | \int_R I_2 = n/(n+2) < 1$$

and

$$1/| R' | \int_{R'} I_2 = (n/(n+2))((\rho^{n+2} - 1)/(\rho^n - 1)). \tag{11}$$

The right side of (11) is an increasing function of ρ, that goes from 1 to ∞ as ρ goes from 1 to ∞. Thus,

$$\int_{R'} I_2 - | R' |$$

increases from zero to infinity, and we set $\rho^*(\epsilon)$ to be that value of ρ for which it is equal to $| R | - \int_R I_2$.

By (6) and (9) we see that for any fixed ρ the quantity $\int_{R'} I_2 - | R' |$ will go to zero as $\epsilon \to 0$, since $| F_\epsilon |$ goes to zero. On the other hand, $| R | - \int_R I_2$ is independent of ϵ. Thus, $\rho^*(\epsilon)$ must go to infinity as $\epsilon \to 0$, and it is easy to see that ρ^* is continuous in ϵ.

We now, for each ϵ, take $\rho = \rho^*(\epsilon)$, specifying R' and R_F as functions of ϵ. Set

$$\Delta(\epsilon) = 1/| R_F | \int_{R_F} I_3 - b.$$

By the same reasoning as was used for (8) we see that $\int_{\rho B_n} I_3 = 0$ and so $\Delta(\epsilon_0) = -b$. By (10) and (9), as $\epsilon \to 0$, $\int_{R'} I_3 / \int_{R'} I_2 \to \infty$. Since, by (11), $| R' | = o(\int_{R'} I_2)$,

$$\left(\int_{R'} I_3 - | R' |\right) \Big/ \left(\int_{R'} I_2 - | R' |\right) \to \infty.$$

However,

$$\int_{R'} I_2 - | R' | = | R | - \int_R I_2,$$

which is independent of ϵ; so

$$\int_{R'} I_3 - | R' | \to \infty$$

as $\epsilon \to 0$. Thus, for ϵ sufficiently near zero, $\int_{R'} I_3 - | R' |$, and a fortiori $\int_{R'} I_3 - b \, | R' |$, is greater than $b \, | R |$. Therefore,

$$(1/| R_F |) \int_{R_F} I_3 = (1/(| R | + | R' |)) \int_{R'} I_3 > b$$

and so $\Delta(\epsilon) > 0$. Thus, Δ is negative at ϵ_0 and positive near 0 and is continuous in ϵ; setting ϵ equal to a zero of Δ completes the definition of R_F and the proof of the theorem.

R_F is made up of a cone consisting of all the radii from the origin to the fundamental region F on S_n, together with a radial spike sticking out from part of F, to some distance $\rho > 1$. The line from the origin to $\mathbf{p}_0$ lies on one edge of this spike. $n!$ fundamental regions meet at $\mathbf{p}_0$—F is one of them—and the $n!$ corresponding spikes meet along the line from the origin to $\mathbf{p}_0$ to form a single spike. Thus, the shape of the final region R_n is that of an n-ball with $n + 1$ radial spikes sticking out of it.

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