Numerical Integration Formulas of Degree Two

By A. H. Stroud

1. Introduction. Here we discuss numerical integration formulas of the form

$$\int_R f(x)w(x)\,dx \cong \sum_i a_i f(\nu_i)$$

where R is a region in n-dimensional, real, euclidean space; $x = (x_1, x_2, \cdots, x_n)$; the a_i are constants; and the ν_i are points in the space. Most previous authors have given formulas for special regions (for a bibliography see [4]). Thacher [7] has given a method for constructing formulas of degree 2 with $n + 1$ points for general regions and of degree 3 with $2n$ points for certain symmetric regions; with his method, however, each region must also be treated separately. Our main results are to obtain specific formulas of degree 2 with $n + 1$ points for a general region satisfying a certain condition of non-degeneracy, and to show that for these regions such formulas cannot be obtained with fewer points. We also give a specific $2n$ point formula of degree 3 for a general centrally symmetric region. These results are a generalization of those of Georgiev [1, 2, 3] who has obtained similar results (but gives no general formulas) for $n = 2, 3$ with $w(x) \equiv 1$. Our results are obtained by a different method which was developed without knowledge of Georgiev's work.

2. Formulas of degree 2. We assume at first that an integration formula of degree 2 for R with respect to $w(x)$ can be obtained with $n + 1$ points

$$\nu_i = (\nu_{i1}, \cdots, \nu_{in}), \qquad i = 0, 1, \cdots, n.$$

Then the equations

$$\begin{aligned} &a_0 + a_1 + \cdots + a_n = c_0 \\ (1)\qquad &a_0\nu_{0j} + a_1\nu_{1j} + \cdots + a_n\nu_{nj} = c_{0j} \\ &a_0\nu_{0j}\nu_{0k} + a_1\nu_{1j}\nu_{1k} + \cdots + a_n\nu_{nj}\nu_{nk} = c_{jk} \qquad j, k = 1, 2, \cdots, n \end{aligned}$$

must be solved for both the a_i and the ν_i, where

$$c_0 = \int_R w(x)\,dx, \qquad c_{0j} = \int_R x_j\, w(x)\,dx, \qquad c_{jk} = \int_R x_j\, x_k\, w(x)\,dx.$$

We begin by writing (1) as the matrix equation

$$U^T A U = C \tag{2}$$

where

$$U = \begin{bmatrix} 1 & \nu_{01} & \cdots & \nu_{0n} \\ 1 & \nu_{11} & \cdots & \nu_{1n} \\ & & \cdots & \\ 1 & \nu_{n1} & \cdots & \nu_{nn} \end{bmatrix} \quad A = \begin{bmatrix} a_0 & 0 & \cdots & 0 \\ 0 & a_1 & \cdots & 0 \\ & & \cdots & \\ 0 & 0 & \cdots & a_n \end{bmatrix} \quad C = \begin{bmatrix} c_0 & c_{01} & \cdots & c_{0n} \\ c_{01} & c_{11} & \cdots & c_{1n} \\ & & \cdots & \\ c_{0n} & c_{1n} & \cdots & c_{nn} \end{bmatrix}$$

and where we assume $0 < c_0 < \infty$ and $0 < |\det C| < \infty$.

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Since C is non-singular we can find a matrix T such that

$$T^T U^T A U T = T^T C T = c_0 E \tag{3}$$

where E is a diagonal matrix with elements ± 1. The method for finding T is well known (see [5], p. 56); we illustrate it using $n = 3$.

Since $c_0 \neq 0$ we define $t_{0i} = -c_{0i}/c_0$, $i = 1, 2, 3$, and form

$$T_1 = \begin{bmatrix} 1 & t_{01} & t_{02} & t_{03} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \qquad C_1 = T_1^T C T_1 = \begin{bmatrix} c_0 & 0 & 0 & 0 \\ 0 & c_{11}^{(1)*} & c_{12}^{(1)} & c_{13}^{(1)} \\ 0 & c_{12}^{(1)} & c_{22}^{(1)} & c_{23}^{(1)} \\ 0 & c_{13}^{(1)} & c_{23}^{(1)} & c_{33}^{(1)} \end{bmatrix}.$$

Now if $c_{11}^{(1)*} = 0$ some $c_{1i}^{(1)} \neq 0$ since $\det C \neq 0$. Assuming $c_{12}^{(1)} \neq 0$ we form

$$T_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & h & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \qquad C_2 = T_2^T C_1 T_2 = \begin{bmatrix} c_0 & 0 & 0 & 0 \\ 0 & 2hc_{12}^{(1)} + h^2 c_{22}^{(1)} & c_{12}^{(1)} + hc_{22}^{(1)} & c_{13}^{(1)} + hc_{23}^{(1)} \\ 0 & c_{12}^{(1)} + hc_{22}^{(1)} & c_{22}^{(1)} & c_{23}^{(1)} \\ 0 & c_{13}^{(1)} + hc_{23}^{(1)} & c_{23}^{(1)} & c_{33}^{(1)} \end{bmatrix}$$

and choose h so that $c_{11}^{(1)} = 2hc_{12}^{(1)} + h^2 c_{22}^{(1)} \neq 0$; if $c_{11}^{(1)*} \neq 0$ we take $h = 0$ so that $c_{11}^{(1)} = c_{11}^{(1)*}$. In this way we are assured that the element in the 1, 1 position is $\neq 0$.

Similarly we may find matrices T_3, T_4 and T_5 such that

$$C_3 = T_4^T T_3^T C_2 T_3 T_4 = \begin{bmatrix} c_0 & 0 & 0 & 0 \\ 0 & c_{11}^{(1)} & 0 & 0 \\ 0 & 0 & c_{22}^{(2)} & c_{23}^{(2)} \\ 0 & 0 & c_{22}^{(2)} & c_{33}^{(2)} \end{bmatrix} \qquad T_5^T C_3 T_5 = \begin{bmatrix} c_0 & 0 & 0 & 0 \\ 0 & c_{11}^{(1)} & 0 & 0 \\ 0 & 0 & c_{22}^{(2)} & 0 \\ 0 & 0 & 0 & c_{33}^{(3)} \end{bmatrix},$$

where $c_{22}^{(2)}$ and $c_{33}^{(3)}$ are $\neq 0$. Defining T_6 as the diagonal matrix

$$[1, [c_0/|c_{11}^{(1)}|]^{\frac{1}{2}}, [c_0/|c_{22}^{(2)}|]^{\frac{1}{2}}, [c_0/|c_{33}^{(3)}|]^{\frac{1}{2}}]$$

we have finally $T = T_1 T_2 T_3 T_4 T_5 T_6$.

We can assume E has the form $[1, 1, \cdots, 1, -1, \cdots, -1]$ since any other arrangement of $+1$'s and -1's can be put into this form by a suitable interchange of the rows of UT and the corresponding columns of $T^T U^T$. If C is positive definite (for example if $w(x)$ is of constant sign on R) E will be the identity. It should be noted that the first element of E will always be positive.

In the following we write

$$UT = \begin{bmatrix} 1 & \xi_{01} & \cdots & \xi_{0n} \\ 1 & \xi_{11} & \cdots & \xi_{1n} \\ & & \cdots & \\ 1 & \xi_{n1} & \cdots & \xi_{nn} \end{bmatrix} = \begin{bmatrix} 1 & \nu_{01} & \cdots & \nu_{0n} \\ 1 & \nu_{11} & \cdots & \nu_{1n} \\ & & \cdots & \\ 1 & \nu_{n1} & \cdots & \nu_{nn} \end{bmatrix} \begin{bmatrix} 1 & \tau_{01} & \cdots & \tau_{0n} \\ 0 & \tau_{11} & \cdots & \tau_{1n} \\ & & \cdots & \\ 0 & \tau_{n1} & \cdots & \tau_{nn} \end{bmatrix}.$$

Because UT is non-singular and $E^{-1} = E$ we easily obtain from (3)

$$(UT)E(UT)^T = c_0 A^{-1}.$$

In terms of the ξ_i this equation is

$$1 + \xi_{i1}\xi_{j1} + \cdots + \xi_{ip}\xi_{jp} - \xi_{i,p+1}\xi_{j,p+1} - \cdots - \xi_{in}\xi_{jn} = \frac{c_0}{a_1}\delta_{ij} \tag{4}$$

$$i, j, = 0, 1, \cdots, n.$$

where $p + 1$, $0 \leqq p \leqq n$, is the number of $+1$'s in E. We discuss the solution of (4); the ν_i are obtained from the ξ_i by $\nu_{ij} = \tau'_{0j} + \xi_{i1}\tau'_{1j} + \cdots + \xi_{in}\tau'_{nj}$, $i = 0, 1, \cdots, n$, $j = 1, \cdots, n$, where

$$T^{-1} = \begin{bmatrix} 1 & \tau'_{01} & \cdots & \tau'_{0n} \\ 0 & \tau'_{11} & \cdots & \tau'_{1n} \\ & & \cdots & \\ 0 & \tau'_{n1} & \cdots & \tau'_{nn} \end{bmatrix}.$$

We are only interested in real solutions of (1) and therefore precisely $n - p + 1$ of the a_i must be negative by Sylvester's "law of inertia" ([5], p. 56). If E is the identity ($p = n$) clearly we must have $0 < a_i < c_0$; if $p < n$ the only condition for the a_i is that they be non-zero.

Table 1 gives a particular solution of (4); we have assumed $a_0, \cdots, a_{n-p}$ negative and $a_{n-p+1}, \cdots, a_n$ positive. In the places where a double sign occurs we mean to use the lower sign for the last $n - p$ components of each vector and the upper sign for the first p components. Each ξ_i is real.

TABLE 1

$$\xi_0 = \left(0, 0, \cdots, 0, 0, \left[\frac{c_0 - a_0}{\pm a_0}\right]^{1/2}\right)$$

$$\xi_1 = \left(0, 0, \cdots, 0, \left[\frac{c_0(c_0 - a_0 - a_1)}{\pm(c_0 - a_0)a_1}\right]^{1/2}, \mp\left[\frac{\pm a_0}{c_0 - a_0}\right]^{1/2}\right)$$

$$\xi_2 = \left(0, 0, \cdots, \left[\frac{c_0(c_0 - a_0 - a_1 - a_2)}{\pm(c_0 - a_0 - a_1)a_2}\right]^{1/2}, \mp\left[\frac{\pm c_0 a_1}{(c_0 - a_0)(c_0 - a_0 - a_1)}\right]^{1/2}, \mp\left[\frac{\pm a_0}{c_0 - a_0}\right]^{1/2}\right)$$

$$\cdots\cdots$$

$$\xi_{n-2} = \left(0, \left[\frac{\pm c_0(c_0 - a_0 - \cdots - a_{n-2})}{(c_0 - a_0 - \cdots - a_{n-3})a_{n-2}}\right]^{1/2}, \cdots\right.$$
$$\left.\cdots, \mp\left[\frac{\pm c_0 a_2}{(c_0 - a_0 - a_1)(c_0 - a_0 - a_1 - a_2)}\right]^{1/2}, \left[\frac{\pm c_0 a_1}{(c_0 - a_0)(c_0 - a_0 - a_1)}\right]^{1/2}, \mp\left[\frac{\pm a_0}{c_0 - a_0}\right]^{1/2}\right)$$

$$\xi_{n-1} = \left(\left[\frac{\pm c_0(c_0 - a_0 - \cdots - a_{n-1})}{(c_0 - a_0 - \cdots - a_{n-2})a_{n-1}}\right]^{1/2}, \mp\left[\frac{\pm c_0 a_{n-2}}{(c_0 - a_0 - \cdots - a_{n-3})(c_0 - a_0 - \cdots - a_{n-2})}\right]^{1/2}, \cdots\right.$$
$$\left.\cdots, \mp\left[\frac{\pm c_0 a_2}{(c_0 - a_0 - a_1)(c_0 - a_0 - a_1 - a_2)}\right]^{1/2}, \mp\left[\frac{\pm c_0 a_1}{(c_0 - a_0)(c_0 - a_0 - a_1)}\right]^{1/2}, \mp\left[\frac{\pm a_0}{c_0 - a_0}\right]^{1/2}\right)$$

$$\xi_n = \left(\mp\left[\frac{\pm c_0 a_{n-1}}{(c_0 - a_0 - \cdots - a_{n-2})a_n}\right]^{1/2}, \mp\left[\frac{\pm c_0 a_{n-2}}{(c_0 - a_0 - \cdots - a_{n-3})(c_0 - a_0 - \cdots - a_{n-2})}\right]^{1/2}, \cdots\right.$$
$$\left.\cdots, \mp\left[\frac{\pm c_0 a_2}{(c_0 - a_0 - a_1)(c_0 - a_0 - a_1 - a_2)}\right]^{1/2}, \mp\left[\frac{\pm c_0 a_1}{(c_0 - a_0)(c_0 - a_0 - a_1)}\right]^{1/2}, \mp\left[\frac{\pm a_0}{c_0 - a_0}\right]^{1/2}\right)$$

From a particular solution ξ_{ij} of (4) other solutions may be obtained as follows. If

$$S = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & \sigma_{11} & \cdots & \sigma_{1n} \\ & & \cdots & \\ 0 & \sigma_{n1} & \cdots & \sigma_{nn} \end{bmatrix}$$

is a cogredient automorph of E, that is if $SES^{\mathsf{T}} = E$, then

$$\xi'_{ij} = \xi_{i1}\sigma_{1j} + \cdots + \xi_{in}\sigma_{rj}$$

is also a solution. If Q is an arbitrary skew matrix of order $n + 1$, with first row and column entirely zero, such that det $(E + Q)(E - Q) \neq 0$, then

$$S = (E + Q)^{-1}(E - Q)$$

is a cogredient automorph of E (see [5], p. 65) of the above form. If E is the identity S is orthogonal. We remark that in this latter case (4) determines the distances $d(\xi_i, 0)$ and $d(\xi_i, \xi_j)$, $i, j = 0, 1, \cdots, n$, $i \neq j$,

$$d(\xi_i, 0) = [(c_0 - a_i)/a_i]^{\frac{1}{2}} \qquad d(\xi_i, \xi_j) = [c_0(a_i + a_j)/a_ia_j]^{\frac{1}{2}}$$

The formulas discussed above are minimal; that is, similar formulas cannot be obtained with fewer points. For if a formula could be obtained with $m + 1$ points ν_i, $i = 0, 1, \cdots, m$, $m < n$, then equation (2) would still hold, where C is the same as before and

$$U = \begin{bmatrix} 1 & \nu_{01} & \cdots & \nu_{0n} \\ 1 & \nu_{11} & \cdots & \nu_{1n} \\ & & \cdots & \\ 1 & \nu_{m1} & \cdots & \nu_{mn} \end{bmatrix} \qquad A = \begin{bmatrix} a_0 & 0 & \cdots & 0 \\ 0 & a_1 & \cdots & 0 \\ & & \cdots & \\ 0 & 0 & \cdots & a_m \end{bmatrix};$$

that is, U is a rectangular matrix. Since U and A have rank at most $m + 1$, then $U^{\mathsf{T}}AU$ has rank at most $m + 1$ and therefore det $(U^{\mathsf{T}}AU) = 0$. By assumption det $C \neq 0$ and thus (2) cannot hold for $m < n$.

3. Formulas of degree 3 for centrally symmetric regions. We assume R to be centrally symmetric with respect to the origin; then if x is in R, $-x$ is also in R. Let us further assume $w(-x) = w(x)$ for x in R. Then

$$\int_R x_i w(x)\, dx = \int_R x_i x_j x_k w(x)\, dx = 0, \qquad i, j, k = 1, \cdots, n.$$

We may obtain an integration formula of degree 3 for R with respect to $w(x)$ with $2n$ points as follows. Take the points to be ν_i, $-\nu_i$, $i = 1, \cdots, n$, and take ν_k, $-\nu_k$ to have common weight a_k. Any $2n$ points chosen in this way integrate exactly the monomials x_i, $x_ix_jx_k$ with respect to $w(x)$ over R. In addition we must solve

$$\begin{aligned} a_1 + a_2 + \cdots + a_n &= \tfrac{1}{2}c_0 \\ a_1\nu_{1j}\nu_{1k} + a_2\nu_{2j}\nu_{2k} + \cdots + a_n\nu_{nj}\nu_{nk} &= \tfrac{1}{2}c_{jk} \qquad j, k = 1, \cdots, n. \end{aligned}$$

The second of these may be written as the matrix equation (2) where now

$$U = \begin{bmatrix} \nu_{11} & \nu_{12} & \cdots & \nu_{1n} \\ \nu_{21} & \nu_{22} & \cdots & \nu_{2n} \\ & \cdots & & \\ \nu_{n1} & \nu_{n2} & \cdots & \nu_{nn} \end{bmatrix} \quad A = \begin{bmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \cdots & 0 \\ & & \cdots & \\ 0 & 0 & \cdots & a_n \end{bmatrix} \quad C = \frac{1}{2} \begin{bmatrix} c_{11} & c_{12} & \cdots & c_{1n} \\ c_{12} & c_{22} & \cdots & c_{2n} \\ & & \cdots & \\ c_{1n} & c_{2n} & \cdots & c_{nn} \end{bmatrix}$$

and where we assume $-\infty < c_0 < \infty$ and $0 < |\det C| < \infty$.

We solve this equation by a method similar to that of the preceding section. We find a non-singular matrix T such that

$$T^{\tau} U^{\tau} A U T = T^{\tau} C T = E$$

where E is diagonal with elements ± 1. Again it is convenient to assume

$$E = [1, \cdots, 1, -1, \cdots, -1]$$

where the first p elements are $+1$, $0 \leqq p \leqq n$. Now writing

$$UT = \begin{bmatrix} \xi_{11} & \xi_{12} & \cdots & \xi_{1n} \\ \xi_{21} & \xi_{22} & \cdots & \xi_{2n} \\ & \cdots & & \\ \xi_{n1} & \xi_{n2} & \cdots & \xi_{nn} \end{bmatrix} = \begin{bmatrix} \nu_{11} & \nu_{12} & \cdots & \nu_{1n} \\ \nu_{21} & \nu_{22} & \cdots & \nu_{2n} \\ & & \cdots & \\ \nu_{n1} & \nu_{n2} & \cdots & \nu_{nn} \end{bmatrix} \begin{bmatrix} \tau_{11} & \tau_{12} & \cdots & \tau_{1n} \\ \tau_{21} & \tau_{22} & \cdots & \tau_{2n} \\ & & \cdots & \\ \tau_{n1} & \tau_{n2} & \cdots & \tau_{nn} \end{bmatrix}$$

the ξ_{ij} may be solved for in terms of the a_i. This gives

$$(5) \quad \xi_{i1}\xi_{j1} + \cdots + \xi_{ip}\xi_{jp} - \xi_{i,p+1}\xi_{j,p+1} - \cdots - \xi_{in}\xi_{jn} = \frac{1}{a_i}\delta_{ij} \quad i, j = 1, \cdots, n$$

precisely $n - p$ of the a_i must be negative in order that the ξ_i be real.

If $a_1, \cdots, a_p$ are positive and $a_{p+1}, \cdots, a_n$ negative a particular solution of (5) is

$$\xi_i = (0, \cdots, 0, \sqrt{1/|a_i|}, 0, \cdots, 0) \qquad i = 1, \cdots, n$$

where the ith component of ξ_i is non-zero. If $S = (\sigma_{ij})$ is any cogredient automorph of E then $\xi'_{ij} = \xi_{i1}\sigma_{1j} + \cdots + \xi_{in}\sigma_{nj}$ is also a solution of (5). If E is the identity, that is, C is positive-definite, the solutions of (5) correspond to the sets of n orthogonal vectors in the space having the property that the ith vector of each set is a distance $\sqrt{1/a_i}$ from the origin.

4. Concluding remarks. The importance of the result given in this paper for formulas of degree 2 is that it is the first result (other than the trivial one point formula, the centroid of R, which integrates any linear function) which holds for an arbitrary region in n-dimensional space and which gives all such formulas containing the minimum number of points.

A question, which may have some practical importance, which may be asked about the above formulas of degree 2 concerns the conditions R must satisfy, say for $w(x) \equiv 1$, in order that such a formula will exist with all of its points interior to R. For example, can a formula interior to R be found if R is convex? if R is star-like about its centroid?

The error bound of von Mises [6] for n-dimensional integration formulas is very well suited for use with the formulas developed in this paper. In a later paper we will give specific values of this error bound for various known formulas.

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University of Wisconsin
Madison, Wisconsin

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