Some Fifth Degree Integration Formulas for Symmetric Regions

By A. H. Stroud

1. Introduction. Here we discuss some approximate integration formulas of the form

$$(1) \qquad \int \cdots \int_{S_n} f(x_1, \cdots, x_n) \, dx_1 \cdots dx_n \cong \sum_{i=1}^{N} A_i f(\nu_{i1}, \cdots, \nu_{in}).$$

Here S_n is a region in n-dimensional Euclidean space ($n \geq 2$), the A_i are constants and the $(\nu_{i1}, \cdots, \nu_{in})$ are points in the space. We discuss a general class of 5th degree formulas for a class of regions S_n which includes the n-dimensional cube and sphere; a precise description of the regions to which our discussion applies will be given in the next section. Each formula in the class contains no more than $N = 2^n(n + 1)$ points and has all positive coefficients A_i. For the n-sphere we give constants in four useful formulas which contain $2^n(n + 1)$, $2^n n + 1$, $2^{n+1} - 1$ and $2^n + 2n$ points. The $2^n(n + 1)$ point formula has all coefficients equal. The $2^n + 2n$ point formula has fewer points than any other known 5th degree formula in which all coefficients are positive (for the n-sphere, $n \geq 4$). The corresponding formulas for the n-cube are not as useful since, for most values of n, they have some points which lie outside the cube.

Previously, Hammer and Stroud [3] have given formulas of 5th degree for the n-cube and n-sphere which use only $2n^2 + 1$ points. Those formulas, however, have the undesirable feature that, for the n-sphere ($n \geq 5$), some of the coefficients A_i are negative. The only other known general class of 5th degree formulas for the n-sphere, for arbitrary n, are the spherical product formulas; these contain $3^n - 3^{n-1} + 1$ points and have all positive coefficients. (Spherical product formulas were first described, for $n = 2, 3$, by Peirce [6, 7], and for arbitrary n independently by Hetherington [4] and Mysovskih [5]; an alternative description is given by Stroud and Secrest [8].) For the 3-sphere Ditkin [1] gives a 5th degree formula containing 13 points and positive coefficients.

2. A General Class of Formulas. To construct a 5th degree formula let us take the following points and coefficients

$$(2) \qquad (\pm \nu_{i1}, \pm \nu_{i2}, \cdots, \pm \nu_{in}) A_i, \qquad i = 1, \cdots, n + 1$$

where the ν_{ik} and A_i are parameters to be determined. Here we mean that all of the (at most 2^n) points

$$(\pm \nu_{j1}, \pm \nu_{j2}, \cdots, \pm \nu_{jn})$$

are taken with the same coefficient A_j, $j = 1, \cdots, n + 1$. If certain of the ν_{jk} are zero then the number of points with coefficient A_j is less than 2^n.

The regions S_n to which our discussion will apply can be described precisely in

terms of the monomial integrals

$$I(x_1{}^{\alpha_1} \cdots x_n{}^{\alpha_n}) \equiv \int \cdots \int_{S_n} x_1{}^{\alpha_1} x_2{}^{\alpha_2} \cdots x_n{}^{\alpha_n} \, dx_1 \cdots dx_n$$

(where the α_k are all nonnegative integers). We assume S_n has the property that for $0 \leqq \alpha_1 + \cdots + \alpha_n \leqq 5$ the only nonzero monomial integrals are

(3) $$I(1), I(x_i{}^2), I(x_i{}^2 x_j{}^2) \qquad i, j = 1, \cdots, n,$$

and that

$$I(x_1{}^2) = \cdots = I(x_n{}^2),$$

$$I(x_1{}^4) = \cdots = I(x_n{}^4),$$

$$I(x_1{}^2 x_2{}^2) = \cdots = I(x_{n-1}^2 x_n{}^2).$$

Requiring that (1) be exact for the monomials (3) means that a certain system of $(n + 1)(n + 2)/2$ equations must be satisfied. This system can be written in the matrix form

(4) $$\mathbf{X}^T \mathbf{A} \mathbf{X} = \mathbf{C}$$

where $\mathbf{X}^T$ is the transpose of $\mathbf{X}$,

$$\mathbf{X} = \begin{bmatrix} \nu_{11}^2 & \nu_{12}^2 & \cdots & \nu_{1n}^2 & 1 \\ \nu_{21}^2 & \nu_{22}^2 & \cdots & \nu_{2n}^2 & 1 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ \nu_{n+1,1}^2 & \nu_{n+1,2}^2 & \cdots & \nu_{n+1,n}^2 & 1 \end{bmatrix},$$

$$\mathbf{A} = 2^n \begin{bmatrix} A_1 & 0 & \cdots & 0 & 0 \\ 0 & A_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & A_n & 0 \\ 0 & 0 & \cdots & 0 & A_{n+1} \end{bmatrix},$$

$$\mathbf{C} = \begin{bmatrix} c_{40} & c_{22} & \cdots & c_{22} & c_{20} \\ c_{22} & c_{40} & \cdots & c_{22} & c_{20} \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ c_{22} & c_{22} & \cdots & c_{40} & c_{20} \\ c_{20} & c_{20} & \cdots & c_{20} & c_{00} \end{bmatrix},$$

$$c_{\alpha\beta} = \int \cdots \int_{S_n} x_i{}^\alpha x_j{}^\beta \, dx_1 \cdots dx_n, \qquad i, j = 1, \cdots, n.$$

(Here we have assumed all the $\nu_{ij} \neq 0$. If, for a certain i, k of the $\nu_{i1}, \cdots, \nu_{in}$ are zero then the ith diagonal element of the matrix $\mathbf{A}$ must be $2^{n-k} A_i$.)

It is not difficult to see that matrix $\mathbf{C}$ is positive definite. Equation (4) states that matrices $\mathbf{A}$ and $\mathbf{C}$ are congruent. Thus if we can find parameters ν_{ij}, A_i which satisfy (4) with the ν_{ij}^2 all real then, by the law of inertia for quadratic forms (Gantmaher [2]), it must turn out that the A_i are all positive.

3. Formula I: $2^n(n+1)$ Points. For the points (2) let us choose the following

$$(\pm\eta, \pm\eta, \pm\eta, \cdots, \pm\eta, \pm\eta)$$
$$(\pm\nu, \pm\lambda, \pm\lambda, \cdots, \pm\lambda, \pm\lambda)$$
$$(\pm\lambda, \pm\nu, \pm\lambda, \cdots, \pm\lambda, \pm\lambda)$$
$$\vdots \quad\quad \vdots \quad\quad \vdots \quad\quad \cdots \quad\quad \vdots \quad\quad \vdots$$
$$(\pm\lambda, \pm\lambda, \pm\lambda, \cdots, \pm\lambda, \pm\nu)$$

all with the same coefficient A. Then the system (4) reduces to

$$2^n(n+1)A = c_{00},$$

$$\nu^2 + (n-1)\lambda^2 + \eta^2 = \frac{(n+1)c_{20}}{c_{00}},$$

(5)
$$\nu^4 + (n-1)\lambda^4 + \eta^4 = \frac{(n+1)c_{40}}{c_{00}},$$

$$2\nu^2\lambda^2 + (n-2)\lambda^4 + \eta^4 = \frac{(n+1)c_{22}}{c_{00}}.$$

It is not too difficult to show that the solution of this system can be written as

$$\eta^2 = \frac{c_{20}}{c_{00}} \pm \sqrt{\left(\frac{c_{40}}{c_{00}} + \frac{(n-1)c_{22}}{c_{00}} - n\left(\frac{c_{20}}{c_{00}}\right)^2\right)},$$

$$n\lambda^4 - 2\left[\frac{(n+1)c_{20}}{c_{00}} - \eta^2\right]\lambda^2 + \frac{(n+1)c_{22}}{c_{00}} - \eta^4 = 0,$$

$$\nu^2 = \frac{(n+1)c_{20}}{c_{00}} - \eta^2 - (n-1)\lambda^2.$$

For the n-sphere $x_1^2 + x_2^2 + \cdots + x_n^2 \leqq 1$

$$c_{00} = \frac{\pi^{n/2}}{\Gamma\left(\dfrac{n}{2}+1\right)}, \qquad\qquad c_{20} = \frac{1}{n+2}\,c_{00},$$

$$c_{40} = \frac{3}{(n+2)(n+4)}\,c_{00}, \qquad c_{22} = \frac{1}{(n+2)(n+4)}\,c_{00}$$

and there are four solutions to (5). Choosing the negative sign in the expression for η^2 and the smallest of the two corresponding solutions for λ^2 gives the solution

$$\eta^2 = \frac{(n+4) - 2\sqrt{(n+4)}}{(n+2)(n+4)},$$

$$\lambda^2 = \frac{n(n+4) + 2\sqrt{(n+4)} - \sqrt{(2(n+1)(n+2)(n+4))}}{n(n+2)(n+4)},$$

$$\nu^2 = \frac{n(n+4) + 2\sqrt{(n+4)} + (n-1)\sqrt{(2(n+1)(n+2)(n+4))}}{n(n+2)(n+4)}$$

for which all the points in the formula lie inside the n-sphere. In fact, the points $(\pm\eta, \cdots, \pm\eta)$ lie on a sphere of radius

$$r_1 = \sqrt{\left(\frac{n}{n+2} - \frac{2n}{(n+2)\sqrt{(n+4)}}\right)} < 1$$

and the remaining points lie on a sphere of radius

$$r_2 = \sqrt{\left(\frac{n}{n+2} + \frac{2}{(n+2)\sqrt{(n+4)}}\right)} < 1.$$

The other three possible solutions to (5) always give some points which lie outside the sphere for $n > 2$ (or are complex).

For the n-cube, with vertices $(\pm 1, \pm 1, \cdots, \pm 1)$, the solution for which all points are inside the cube for the most values of n $(2 \leq n \leq 6)$ is:

$$\eta^2 = \frac{5 + 2\sqrt{5}}{15},$$

$$\lambda^2 = \frac{5n - 2\sqrt{5} - 2\sqrt{(5(n+1))}}{15n},$$

$$\nu^2 = \frac{5n - 2\sqrt{5} + 2(n-1)\sqrt{(5(n+1))}}{15n}.$$

4. Formula II: $2^n n + 1$ Points. For the points and coefficients (2) we choose

$$
\begin{array}{ll}
(0, \quad 0, \quad 0, \quad \cdots, \quad 0, \quad 0) & A_0 \\
(\pm\nu, \pm\lambda, \pm\lambda, \cdots, \pm\lambda, \pm\lambda) & A_1 \\
(\pm\lambda, \pm\nu, \pm\lambda, \cdots, \pm\lambda, \pm\lambda) & A_1 \\
\quad \vdots \quad\quad \vdots \quad\quad \vdots \quad \cdots \quad\quad \vdots \quad\quad \vdots \quad\quad \vdots & \\
(\pm\lambda, \pm\lambda, \pm\lambda, \cdots, \pm\lambda, \pm\nu) & A_1
\end{array}
$$

System (4) becomes

$$A_0 + 2^n n A_1 = c_{00},$$

$$2^n A_1[\nu^2 + (n-1)\lambda^2] = c_{20},$$

$$2^n A_1[\nu^4 + (n-1)\lambda^4] = c_{40},$$

$$2^n A_1[2\nu^2\lambda^2 + (n-2)\lambda^4] = c_{22}$$

with solution

$$2^n A_1 = \frac{c_{20}^2}{c_{40} + (n-1)c_{22}}, \qquad A_0 = c_{00} - \frac{nc_{20}^2}{c_{40} + (n-1)c_{22}},$$

(6) $\qquad \nu^2 = \frac{c_{40} + (n-1)c_{22} \pm (n-1)\sqrt{(\{c_{40} - c_{22}\}\{c_{40} + (n-1)c_{22}\})}}{nc_{20}},$

$$\lambda^2 = \frac{c_{40} + (n-1)c_{22} \mp \sqrt{(\{c_{40} - c_{22}\}\{c_{40} + (n-1)c_{22}\})}}{nc_{20}}.$$

For the n-sphere, choosing the positive sign in ν^2, gives the solution

$$2^n A_1 = \frac{(n+4)}{(n+2)^2} c_{00}, \qquad A_0 = \frac{4}{(n+2)^2} c_{00},$$

$$\nu^2 = \frac{n + 2 + (n-1)\sqrt{(2(n+2))}}{n(n+4)}, \qquad \lambda^2 = \frac{n + 2 - \sqrt{(2(n+2))}}{n(n+4)}$$

with all points inside the sphere for all n. In fact all points except the origin lie on a sphere of radius

$$r = \sqrt{\left(\frac{n+2}{n+4}\right)}.$$

For the n-cube the solution (6) which gives all points inside the cube for the most values of n $(2 \leqq n \leqq 5)$ is

$$2^n A_1 = \frac{5}{5n+4}\, c_{00}, \qquad A_0 = \frac{4}{5n+4}\, c_{00},$$

$$\nu^2 = \frac{5n+4+2(n-1)\sqrt{(5n+4)}}{15n}, \qquad \lambda^2 = \frac{5n+4-2\sqrt{(5n+4)}}{15n}.$$

5. Formula III: $2^{n+1} - 1$ Points. For the points and coefficients (2) we choose

$$
\begin{array}{cccccll}
(\pm\nu_1, & \pm\lambda, & \pm\lambda, & \cdots, & \pm\lambda, & \pm\lambda) & A_1 \\
(0, & \pm\nu_2, & \pm\lambda, & \cdots, & \pm\lambda, & \pm\lambda) & A_2 \\
\vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots \\
(0, & 0, & 0, & \cdots, & 0, & \pm\nu_n) & A_n \\
(0, & 0, & 0, & \cdots, & 0, & 0) & A_{n+1}.
\end{array}
$$

Equations (4) are

$$2^n A_1 + 2^{n-1} A_2 + \cdots + 2A_n + A_{n+1} = c_{00}$$

(7)
$$[2^n A_1 + \cdots + 2^{n-i+2} A_{i-1}]\lambda^2 + 2^{n-i+1} A_i \nu_i^2 = c_{20}$$
$$[2^n A_1 + \cdots + 2^{n-i+2} A_{i-1}]\lambda^4 + 2^{n-i+1} A_i \nu_i^4 = c_{40} \qquad i = 1, 2, \cdots, n.$$
$$[2^n A_1 + \cdots + 2^{n-i+2} A_{i-1}]\lambda^4 + 2^{n-i+1} A_1 \nu_i^2 \lambda^2 = c_{22}$$

Equations (7) have the unique solution

$$\lambda^2 = \frac{c_{22}}{c_{20}}, \qquad \nu_i^2 = \frac{c_{40}+(i-1)c_{22}}{c_{20}}, \qquad i = 1, \cdots, n,$$

$$2^{n-i+1} A_i = \frac{c_{20}^2[c_{40}-c_{22}]}{[c_{40}+(i-2)c_{22}][c_{40}+(i-1)c_{22}]}, \qquad i = 2, \cdots, n$$

$$2^n A_1 = \frac{c_{20}^2}{c_{40}}, \qquad A_{n+1} = c_{00} - \frac{n c_{20}^2}{c_{40}+(n-1)c_{22}}.$$

For the n-sphere we have

$$\lambda^2 = \frac{1}{n+4}, \qquad \nu_i^2 = \frac{i+2}{n+4}, \qquad i = 1, \cdots, n,$$

$$2^{n-i+1} A_i = \frac{2(n+4)}{(i+1)(i+2)(n+2)}\, c_{00}, \qquad i = 1, \cdots, n,$$

$$A_{n+1} = \left[\frac{2}{n+2}\right]^2 c_{00}$$

and all points except the center lie on a sphere of radius

$$r = \sqrt{\left(\frac{n+2}{n+4}\right)}.$$

For the n-cube some points lie outside the cube for $n \geq 3$.

6. Formula IV: $2^n + 2n$ Points. For the points and coefficients (2) we choose

$$
\begin{array}{llllll}
(\pm\eta, & \pm\eta, & \cdots, & \pm\eta, & \pm\eta) & A_1 \\
(\pm\nu, & 0, & \cdots, & 0, & 0) & A_2 \\
\vdots & \vdots & \cdots & \vdots & \vdots & \vdots \\
(0, & 0, & \cdots, & 0, & \pm\nu) & A_2.
\end{array}
$$

System (4) is

(8)

$$2^n A_1 + 2n A_2 = c_{00},$$

$$2^n A_1 \nu^2 + 2 A_2 \eta^2 = c_{20},$$

$$2^n A_1 \nu^4 + 2 A_2 \eta^4 = c_{40},$$

$$2^n A_1 \eta^4 = c_{22}.$$

The values of ν^2, η^2 satisfy

$$(c_{20}^2 - c_{00}c_{22})\nu^4 - 2c_{20}(c_{40} - c_{22})\nu^2 + (c_{40} - c_{22})^2 + nc_{22}(c_{40} - c_{22}) = 0,$$

$$[nc_{20}^2 - c_{00}(c_{40} - c_{22})]\eta^4 - 2nc_{20}c_{22}\eta^2 + nc_{22}^2 + c_{22}(c_{40} - c_{22}) = 0,$$

where corresponding to the largest value of ν^2 we must use the smallest value of η^2 and vice versa.

For the n-sphere the solution

$$\nu^2 = \frac{n+4 - \sqrt{(2(n+4))}}{n+4}, \qquad \eta^2 = \frac{n(n+4) + 2\sqrt{(2(n+4))}}{(n^2 + 2n - 4)(n+4)},$$

$$2^n A_1 = \frac{1}{(n+2)(n+4)\eta^4} c_{00}, \qquad 2A_2 = \frac{2}{(n+2)(n+4)\nu^4} c_{00}$$

gives all points inside the n-sphere for $n \geq 4$.

For the n-cube, $n \geq 2$, there is no solution for which all the points are inside.

7. Concluding Remarks and Examples. For the n-sphere the above $2^{n+1} - 1$ point formula can be constructed in another way which is rather interesting.

As mentioned above, the spherical product of n, 3-point one-dimensional formulas contains $3^n - 3^{n-1} + 1$ points. A 5th degree spherical product formula can be constructed, however, using fewer points than this. Let us take, as in the usual spherical product, the 3-point one-dimensional Gauss formula for the radial component. For each of the $n - 1$ angular components let us take 5th degree, 4-point one-dimensional Lobatto formulas (which include the end points among the four points). By a somewhat tedious counting argument, which we will not carry out here, it can be shown that the resulting formula contains only $2^{n+1} - 1$ distinct

TABLE 1. *Approximate values of integrals*

Number of points	J_4	J_8
$2n^2 + 1$	3.4854745	2.6958484
$2^n + 2n$	3.4767683	2.6759335
$2^{n+1} - 1$	3.4823309	2.6807257
$2^n n + 1$	3.4827397	2.6815415
$2^n(n + 1)$	3.4824007	2.6812335
$3^n - 3^{n-1} + 1$	3.4836193	2.6827835

points and, in fact, coincides with the above Formula III. To our knowledge, however, Formula III has never been constructed by this technique. The advantage of using Lobatto formulas in constructing spherical product formulas was first pointed out to us by R. A. Sack; to our knowledge he was the first to propose this. The number of points in spherical product formulas of degree $2m - 1$, for general m, constructed from Lobatto formulas is given by Stroud and Secrest [8].

To illustrate the use of the formulas we have derived we numerically evaluate the integral

$$J_n \equiv \int \cdots \int_{S_n} \cos(x_1 + \cdots + x_n)\, dx_1 \cdots dx_n \,,$$

where S_n is the unit n-sphere ($n \geq 2$). The exact value of this integral is given by

$$J_n = c_{00}\left[1 - \frac{1}{k_1} + \frac{1}{k_1 k_2} - \cdots + \frac{(-1)^m}{k_1 k_2 \cdots k_m} + \cdots\right],$$

where, as before, c_{00} is the volume of the n-sphere and

$$k_\alpha = \frac{4}{n}\alpha^2 + 2\alpha, \qquad \alpha = 1, 2, \cdots.$$

The approximate values obtained from our four formulas, and also the formulas containing $2n^2 + 1$ and $3^n - 3^{n-1} + 1$ points, are given in Table 1 for $n = 4, 8$. The exact values, correct to 8 decimals, are

$$J_4 = 0.705668057\,\frac{\pi^2}{2} = 3.48233228,$$

$$J_8 = 0.660697220\,\frac{\pi^4}{24} = 2.68157983.$$

It should be noted that in 4 dimensions certain coefficients in the $2n^2 + 1$ point formula are zero so, in effect, that formula uses only 5 points.

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