Symmetric Quadrature Formulae for Simplexes

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Abstract. Symmetric interpolation polynomials are defined for N-dimensional simplexes with the aid of a symmetric coordinate notation. These polynomials are used to produce symmetric interpolatory quadrature formulae of arbitrary degree of precision over simplexes of arbitrary dimensionality. Tabulated values of weight coefficients are given for triangles and tetrahedra.

1. Introduction. Interpolative quadrature formulae for N-dimensional simplexes have been given by various authors, e.g., Stroud [1] or Hammer and Stroud [2]. Their principal attraction in applications lies in the fact that multidimensional regions of integration can often be closely approximated by unions of simplexes. The object of this paper is to show that, for any N, it is possible to define quadrature formulae of any degree of precision n, symmetric in the sense of Hammer, Marlowe, and Stroud [3]; and to give a straightforward procedure for finding the weights and node locations. Although the resulting quadrature formulae are not *efficient* in the sense of [3], they possess the advantage of being very convenient computationally, and can be generated easily for any reasonable values of N and n. They represent a natural generalization of the Newton-Cotes formulae to the N-dimensional case, and include the latter for $N = 1$.

2. Notation for Simplexes. A simplex is defined by its $N + 1$ vertices in the N-space spanned by the coordinates $x^{(1)}, x^{(2)}, \cdots, x^{(N)}$. Let S be the N-dimensional simplex whose kth vertex coordinates are $x_k^{(i)}$, $i = 1, 2, \cdots, N$. Let the *size* of the simplex S be denoted by $\sigma(S)$ and defined as

$$\sigma(S) = \frac{1}{N!}\begin{vmatrix} 1 & x_1^{(1)} & \cdots & x_1^{(N)} \\ & \cdots & \cdots & \\ 1 & x_{N+1}^{(1)} & \cdots & x_{N+1}^{(N)} \end{vmatrix} . \tag{1}$$

Under this definition, the size of a 1-simplex is its length, that of a 2-simplex its area, and so on.

Let a point P be located within the simplex S. Let S_m denote the simplex defined by P and the vertices of S other than the mth, i.e., by vertices $1, 2, \cdots, m - 1, m + 1, \cdots, N, N + 1$ of S, and the point P. S_m is contained entirely within S. Any interior point P thus defines a unique partitioning of S into $N + 1$ subsimplexes S_k, $k = 1, 2, \cdots, N + 1$. Using Eq. (1), it is readily verified that

$$\sum_{k=1}^{N+1} \sigma(S_k) = \sigma(S) . \tag{2}$$

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Let

$$\zeta_m = \sigma(S_m)/\sigma(S) . \tag{3}$$

These numbers may be termed *simplex coordinates,* alluding to the fact that S forms the portion $0 \leqq \zeta_m \leqq 1$, $m = 1, \cdots, N+1$, of the hyperplane

$$\sum_{m=1}^{N+1} \zeta_m = 1 \tag{4}$$

in the Cartesian $N + 1$-space spanned by $\zeta_1, \zeta_2, \cdots, \zeta_{N+1}$, by virtue of (2). Geometrically, the simplex coordinate ζ_m measures normalized distance toward the mth vertex orthogonally from the $N - 1$-dimensional simplex defined by all vertices of S other than the mth.

3. Interpolation Polynomials. Let polynomials $R_m(z)$ be defined by

$$\begin{aligned} R_m(z) &= \prod_{k=0}^{m-1} \frac{z - z_k}{z_m - z_k}, \qquad m > 0 \\ R_0(z) &= 1 , \end{aligned} \tag{5}$$

where the z_k are arbitrary distinct numbers, $0 \leqq z_k \leqq 1$. An interpolation polynomial in 1-space, of degree n, is then given by

$$\alpha_{ij} = R_i(\zeta_1)R_j(\zeta_2) , \qquad i + j = n \tag{6}$$

provided the numbers z_k are chosen symmetrically, that is, provided that

$$z_p + z_q = 1 \quad \text{whenever } p + q = n . \tag{7}$$

Choosing $z_k = k/n$, the polynomials α_{ij} turn out to be the conventional closed Newton-Cotes interpolation polynomials, while the choice $z_k = (k + 1)/(n + 2)$ produces the open Newton-Cotes polynomials, expressed in terms of ζ_1 and ζ_2.

Equations (6) and (7) suggest a direct generalization for the N-dimensional case. Let

$$\alpha_{k_1 k_2 \cdots k_{N+1}} = \prod_{i=1}^{N+1} R_{k_i}(\zeta_i) , \quad \sum_{i=1}^{N+1} k_i = n \tag{8}$$

subject to the proviso

$$\sum_{i=1}^{N+1} z_{l_i} = 1 \quad \text{whenever } \sum_{i=1}^{N+1} l_i = n . \tag{9}$$

A solution, valid for any N and n, of (9) is

$$z_k = \frac{k + \mu}{n + \mu(N + 1)} , \tag{10}$$

where μ is a nonnegative parameter. The specific choices $\mu = 0$ and $\mu = 1$ lead to equispaced point lattices over the simplex, with the boundary nodes included and not included, respectively. When $N = 1$, these correspond to the closed and open Newton-Cotes interpolation nodes. In the closed case $\mu = 0$ the auxiliary polynomials $R_m(z)$ become

$$R_m(z) = \frac{1}{m!} \prod_{k=0}^{m-1} (Nz - k), \qquad m > 0 \tag{11}$$

and in the open case, $\mu = 1$, there is obtained

$$R_m(z) = \frac{1}{m!} \prod_{k=1}^{m} [(n + N + 1)z - k], \qquad m > 0. \tag{12}$$

Clearly, other polynomials and corresponding node placements will result from other choices of μ.

4. Quadrature Formulae. In general, all interpolatory quadrature formulae may be written in the form [4]

$$\int_S f(x^{(1)}, \cdots)dU \simeq \sigma(S) \sum_i c_i f_i \tag{13}$$

where the summation extends over all the interpolation nodes in S. The weights c_i are given by

$$c_i = \frac{1}{\sigma(S)} \int_S \alpha_i(\zeta_1, \cdots, \zeta_{N+1})dU \tag{14}$$

where α_i is the polynomial associated with the ith interpolation node. The integrals of monomials over a simplex are well known [5],

$$\int \zeta_1^{p_1} \cdots \zeta_{N+1}^{p_{N+1}} dU = \frac{p_1!p_2! \cdots p_{N+1}!N!}{(p_1 + \cdots + p_{N+1} + N)!} \sigma(S). \tag{15}$$

The quadrature weights c_i are therefore readily evaluated by expanding the polynomials and integrating term by term. All required arithmetic steps are direct, and can be coded for evaluation by computer. There is no essential difficulty in obtaining formulae for any reasonable N and n.

5. Quadrature Weights for $N = 2$ and $N = 3$. For $N = 1$, (14) gives the well-known and extensively tabulated Newton-Cotes quadrature weights for one-dimensional integration. For $N = 2$ and $N = 3$, corresponding tabulations appear below. To economize on the extent of the tables, the weights have been numbered with $N + 1$ subscripts corresponding to those of the interpolation polynomials; e.g., for $N = 2$,

$$c_{ijk} = \frac{1}{\sigma(S)} \int \alpha_{ijk}(\zeta_1, \zeta_2, \zeta_3)dU. \tag{16}$$

From (8) and (15), it is readily seen that the formulae are symmetric, and the weights the same for any permutation of i, j, k:

$$c_{ijk} = c_{ikj} = c_{kij} = \cdots. \tag{17}$$

Only one of these weights needs to be tabulated. In the tables, the weights are expressed exactly as integer quotients, the numerators being tabulated individually and one common denominator being shown for each of the open and closed forms.

Application of the tabulated data to a specific simplex is made as follows. Let the vertices of the triangle (or tetrahedron) be X_0, X_1, X_2 (or X_0, X_1, X_2, X_3),

TABLE I

Newton-Cotes Quadrature Weights for Triangles

Degree n	Point index	WEIGHTS: Numerators, closed	Numerators, open	Denominators, closed	Denominators, open	Number of points ν
1	100	1	1	3	3	3
2	200	0	7	3	12	3
	110	1	−3			3
3	300	4	8			3
	210	9	3	120	30	6
	111	54	−12			1
4	400	0	307			3
	310	4	−316			6
	220	−1	629	45	720	3
	211	8	−64			3
5	500	11	71			3
	410	25	−13			6
	320	25	57	1008	315	6
	311	200	−167			3
	221	25	113			3
6	600	0	767			3
	510	36	−1257			6
	420	−27	2901			6
	411	72	387	840	2240	3
	330	64	−3035			3
	321	72	−915			6
	222	−54	3509			1
7	700	1336	898			3
	610	2989	−662			6
	520	3577	1573			6
	511	32242	−2522			3
	430	2695	−191	259200	4536	6
	421	−6860	2989			6
	331	44590	−5726			3
	322	3430	1444			3
8	800	0	1051445			3
	710	368	−2366706			6
	620	−468	6493915			6
	611	704	1818134			3
	530	1136	−9986439			6
	521	832	3757007	14175	3628800	6
	440	−1083	12368047			3
	431	672	478257			6
	422	−1448	10685542			3
	332	1472	−6437608			3

where X_i denotes a two (or three) component vector. For a quadrature formula of precision n, each node is designated by three (or four) integers z_i such that $\sum z_i = n$; these nodes will be located at the points $\sum_{i=0}^{2} (z_i + \mu)X_i/(n + 3\mu)$ on the triangle, or the points $\sum_{i=0}^{3} (z_i + \mu) X_i/(n + 4\mu)$ in the tetrahedron. Formulae of open type are obtained by taking $\mu = 1$, of closed type by taking $\mu = 0$. Each of the ν distinct points obtained by permuting the point indices z_i is to be assigned a weight $N(\mu) \sigma/D(\mu)$, σ being the area (or volume) of the simplex, $N(\mu)$ and $D(\mu)$ the tabulated numerator and denominator. As an example of this procedure, the node index numbers and quadrature weights are given in Fig. 1 for the closed formula with $n = 3$, $N = 2$.

The tabulated figures have been verified by computing integrals of monomials, and some polynomials, up to and including degree $n + 2$. Their degree of precision has been verified as n.

TABLE II

Newton-Cotes Quadrature Weights for Tetrahedra

		WEIGHTS				
Degree n	*Point index*	*Numerators closed*	*Numerators open*	*Denominators closed*	*Denominators open*	*Number of points ν*
1	1000	1	1	4	4	4
2	2000	−1	11			4
	1100	4	−4	20	20	6
3	3000	1	20			4
	2100	0	13	40	120	12
	1110	9	−29			4
4	4000	−5	79			4
	3100	16	−68			12
	2200	−12	142	420	210	6
	2110	16	−12			12
	1111	128	2			1
5	5000	33	277			4
	4100	−35	97			12
	3200	35	223	4032	2240	12
	3110	275	−713			12
	2210	−75	505			12
	2111	375	−53			4
6	6000	−7	430			4
	5100	24	−587			12
	4200	−30	1327			12
	4110	0	187			12
	3300	40	−1298	1400	1512	6
	3210	30	−398			24
	3111	180	22			4
	2220	−45	1537			4
	2211	0	−38			6

6. Conclusion. The Newton-Cotes quadrature formulae, well known for one-dimensional integration, lend themselves to direct generalisation in N-dimensional simplexes. For the most important two- and three-dimensional cases, weight coefficients for open and closed forms have been computed and tabulated.

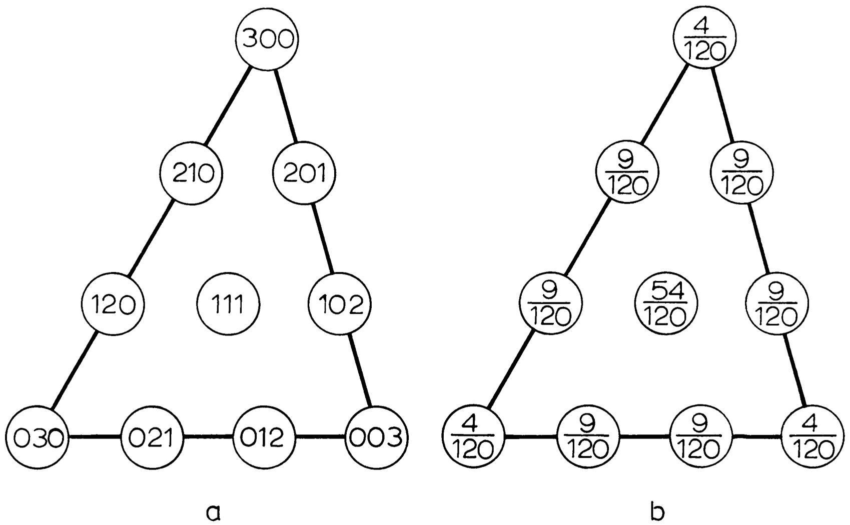

FIGURE 1. *Cubic Quadrature over a Triangle.* (a) *Index Numbering of Quadrature Nodes,* (b) *Quadrature Weights at the Nodes.*

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