and fast rules for doing so. In the above example, for instance, if we substitute some other number, k say, for 2.507, the desired effect does not occur for all values of k. An integral power of ten will not work (since we are assuming rounding-off is done in the decimal system). Also one finds experimentally in this case that $k = 1.001$ and $k = 2$ are unsatisfactory choices.

In our present study we might use a transformation of the type

$$(64) \qquad\qquad s = ks'$$

and re-evaluate the α_j in equation (2) by expanding the function

$$(65) \qquad\qquad \phi(s') = f(ks')$$

around the point

$$(66) \qquad\qquad a' = \frac{a}{k},$$

obtaining quantities α_j' as coefficients of $(s' - a')^i$, from which, theoretically

$$(67) \qquad\qquad \alpha_j = \frac{\alpha_j'}{k^i}.$$

Then by comparing the original quantities α_j, with those obtained from (67), as j increases, one could estimate the cumulative building up of round-off errors.

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Numerical Integration over Simplexes and Cones

1. Introduction. In this paper we develop numerical integration formulas for simplexes and cones in n-space for $n \geq 2$. While several papers have been written on numerical integration in higher spaces, most of these have dealt with hyper-rectangular regions. For certain exceptions see [3]. Hammer and Wymore [1] have given a first general type theory designed through systematic use of cartesian product regions and affine transformations to extend the possible usefulness of formulas for each region.

Particular formulas were developed by Hammer and Wymore for certain symmetrical type regions including spheres and hyperspheres, cubes and hypercubes. The methods they have used make it possible to obtain numerical integration formulas for a much larger class of regions than heretofore. However, it is not practical to obtain specific integration formulas for all regions of interest. Hence, in this paper we develop methods for obtaining numerical integration formulas over simplexes which may be used, in principle, to approximate other regions. Since one of the methods is applicable to cones in general if a formula is given for the base, we include that in the development.

While we have calculated certain formulas in specific cases for $n = 2, 3,$ and 4, we use these as illustrations and hope to build a more complete table later. Inductively we give integration formulas holding exactly for the k-th degree polynomial in n variables over the n-simplex. Another method which may be more valuable in some applications requires affine symmetry of the evaluation points. Here the general theory is missing, but a general type of method is proposed for which illustrations are provided.

2. Approximate integration formulas for cones. In the following a theorem of Hammer and Wymore will be used which we state as follows:

THEOREM 1. *If*

$$\sum_i a_j f(\xi_j) - \int_R f(\xi) dV = E(f),$$

then

$$\sum_i W a_j g(\eta_j) - \int_{TR} g(\eta) dV = WE(f),$$

where T is an affine transformation, $\eta = A\xi + \eta_0$, of E_n onto itself; $g(\eta) = f(\xi)$; W is the absolute value of the determinant of A; R is an n-dimensional region included in the domain of f and $\xi_1, \cdots, \xi_k, \cdots$, are points in the domain of f.

This theorem permits us to consider convenient, specific regions R to develop formulas for the class of all their affine transforms.

We want integration formulas of the form

$$(1) \qquad \int_R f dV \doteq \sum_1^k a_j f(\xi_j),$$

where the numbers a_j are constants; $\xi_1, \cdots, \xi_k$ are points in the domain of f; R is a bounded closure of an open set in E_n. From this standpoint the most interesting simple regions are the simplexes, which are special cones, since every polyhedron is composed of a finite number of simplexes.

Let an n-dimensional region R be embedded in the hyperplane $x = 1$ in E_{n+1} where we represent the points in E_{n+1} by (ξ, x), where ξ is a point in E_n. Then the set of all points xR, where $0 \leq x \leq 1$, is a cone C with base R and vertex at the origin in E_{n+1}.

Let $f(\xi, x)$ be a function defined over C and suppose that a suitable numerical integration formula is given over the base R of C. If, for example,

$$(2) \qquad \int_R f(\xi, 1) dV_n \doteq \sum_j a_j f(\xi_j, 1),$$

then

$$(3) \qquad \int_C f(\xi, x)dV = \int_0^1 dx \int_{xR} f(\xi, x)dV_n \doteq \int_0^1 x^n \sum_j a_j f(x\xi_j, x)dx,$$

since the Jacobian of the affine transformation from R to xR is x^{-n}. Define a function

$$g(x) = \sum_j a_j f(x\xi_j, x)$$

and then we have

$$\int_C f dv \doteq \int_0^1 x^n g(x)dx.$$

Now we ask for numerical integration formulas of the form

$$(4) \qquad \int_0^1 x^n g(x)dx \doteq \sum_i b_i g(x_i).$$

Since such formulas may certainly be found we then have

$$(5) \qquad \int_C f dv \doteq \sum_i \sum_j b_i a_j f(x_i\xi_j, x_i),$$

which is of the form required, that is, a weighted sum of integrand values.

THEOREM·2. *If a formula* (2) *holds precisely for polynomials f of n variables of at most degree m over a region R and if a formula* (4) *holds precisely for polynomials g of at most degree m in x, then* (5) *holds over C for all polynomial functions f containing terms of at most degree m in its n + 1 variables.*

We will forego a formal proof of Theorem 2 since it follows from the affine invariance of the class of polynomials of at most a certain degree, so that

$$x^n \sum a_j f(x\xi_j, x) = \int_{xR} f(\xi, x)dV_n.$$

In order to develop specific formulas one may start with any of the numerous formulas for a line segment integration and proceed to obtain a formula for a triangle; using this obtain a formula for a tetrahedron and so on. This is the type we consider now. In higher spaces, to keep the number of points smaller, the integration formulas we choose for $\int_0^1 x^n g(x)dx$ are based on orthogonal polynomials with weight function x^n so that with m values of x_j the formula holds precisely for a polynomial of degree at most $2m - 1$ by formula (3). For $n = 0$ this gives the Gauss integration formula on the line with points of evaluation the roots of the m-th Legendre polynomial. Then if the formula (2) for the base is exact for polynomials of at most degree $2m - 1$ in the first n variables, the final formula holds for polynomials of degree $2m - 1$ at most. Thus by this means we obtain with m^n points a formula valid for all $(2m - 1)$-degree polynomials over a simplex in n-space. While we have discussed a range from 0 to 1, the affine invariance permits us to give the formulas as valid for all simplexes, the necessary

adjustment of coefficients and points being given by the transformation as in Theorem 1.

The orthogonal polynomials, $q_m(x)$, over the interval $(0, 1)$ with weight functions x^n are given by Christoffel's formula in terms of the Legendre polynomials, $P_m(x)$, on the interval $(0, 1)$:

$$
(6) \qquad x^n q_m(x) =
\begin{vmatrix}
P_m(x) & P_{m+1}(x) & \cdots & P_{m+n}(x) \\
P_m(0) & P_{m+1}(0) & \cdots & P_{m+n}(0) \\
P'_m(0) & P'_{m+1}(0) & \cdots & P'_{m+n}(0) \\
\cdot & \cdot \cdot & \cdots & \cdot \\
P_m^{(n-1)}(0) & P_{m+1}^{(n-1)}(0) & \cdots & P_{m+n}^{(n-1)}(0)
\end{vmatrix} .
$$

In this formula and in the tables the value of n is one less than the dimension of the space—for the line, $n = 0$; for the plane, $n = 1$; and so on. The resulting

TABLE I. $n = 1$

m	j	x_j	b_j	$q_m(x)$
1	1	0.66666 66666 66666 667	0.50000 00000 00000 000	$\sqrt{4}(2 - 3x)$
2	1	0.35505 10257 21682 190	0.18195 86182 56022 831	$\sqrt{6}(3 - 12x + 10x^2)$
	2	0.84494 89742 78317 810	0.31804 13817 43977 169	
3	1	0.21234 05382 39152 944	0.06982 69799 01454 1224	$\sqrt{8}(4 - 30x + 60x^2 - 35x^3)$
	2	0.59053 31355 59265 287	0.22924 11063 59586 248	
	3	0.91141 20404 87296 044	0.20093 19137 38959 648	
4	1	0.13975 98643 43780 552	0.03118 09709 50008 0822	$\sqrt{10}(5 - 60x + 210x^2 - 280x^3$
	2	0.41640 95676 31083 175	0.12984 75476 08232 439	$+ 126x^4)$
	3	0.72315 69863 61876 278	0.20346 45680 10271 322	
	4	0.94289 58038 85482 299	0.13550 69134 31488 149	
5	1	0.09853 50857 98826 4273	0.01574 79145 21692 2766	$\sqrt{12}(6 - 105x + 560x^2 - 1260x^3$
	2	0.30453 57266 46363 885	0.07390 88700 72616 6584	$+ 1260x^4 - 462x^5)$
	3	0.56202 51897 52613 862	0.14638 69870 84669 768	
	4	0.80198 65821 26391 897	0.16717 46380 94369 395	
	5	0.96019 01429 48531 218	0.09678 15902 26651 7818	

TABLE II. $n = 2$

m	j	x_j	b_j	$q_m(x)$
1	1	0.75000 00000 00000 000	0.33333 33333 33333 333	$\sqrt{5}(4x - 3)$
2	1	0.45584 81559 88774 713	0.10078 58820 79825 431	$\sqrt{7}(15x^2 - 20x + 6)$
	2	0.87748 51773 44558 620	0.23254 74512 53507 905	
3	1	0.29499 77901 11501 618	0.02995 07030 08580 6981	$\sqrt{9}(56x^3 - 105x^2 + 60x - 10)$
	2	0.65299 62339 61648 121	0.14624 62692 59866 020	
	3	0.92700 59759 26850 269	0.15713 63610 64886 615	
4	1	0.20414 85821 03227 136	0.01035 22407 49918 0652	$\sqrt{11}(210x^4 - 504x^3$
	2	0.48295 27048 95632 480	0.06863 38871 72923 0663	$+ 420x^2 - 140x + 15)$
	3	0.76139 92624 48137 593	0.14345 87897 99214 191	
	4	0.95149 94505 53002 709	0.11088 84156 11277 894	
5	1	0.14894 57870 52983 580	0.00411 38252 03099 00782	$\sqrt{13}(792x^5 - 2310x^4$
	2	0.36566 65273 69113 217	0.03205 56007 22961 9169	$+ 2520x^3 - 1260x^2 + 280x - 21)$
	3	0.61011 36129 34480 701	0.08920 01612 21590 0168	
	4	0.82651 96792 28304 566	0.12619 89618 99911 440	
	5	0.96542 10600 81784 870	0.08176 47842 85770 9715	

TABLE III. $n = 3$

m	j	x_j	b_j	$q_m(x)$
1	1	0.80000 00000 00000 000	0.25000 00000 00000 000	$\sqrt{6}(4-5x)$
2	1	0.52985 79358 94884 910	0.06690 52498 06888 7467	$\sqrt{8}(10-30x+21x^2)$
	2	0.89871 34926 76543 662	0.18309 47501 93111 252	
3	1	0.36326 46302 16511 947	0.01647 90592 82671 7230	$\sqrt{10}(20-105x+168x^2-84x^3)$
	2	0.69881 12691 63613 535	0.10459 98975 56806 681	
	3	0.93792 41006 19874 523	0.12892 10431 60521 608	
4	1	0.26147 77888 30889 686	0.00465 83670 60069 48897	$\sqrt{12}(35-280x+756x^2-840x^3$
	2	0.53584 64460 88250 229	0.04254 17241 42766 6674	$+330x^4)$
	3	0.79028 32299 69286 800	0.10900 43689 38641 000	
	4	0.95784 70805 66118 662	0.09379 55398 58522 9295	

TABLE IV. *Integration Formula over Triangle Exact for 7th Degree Polynomial*

k	y_k	a_k
1	0.86113 63115 94052 580	0.34785 48451 37453 860
2	0.33998 10435 84856 264	0.65214 51548 62546 143
3	−0.33998 10435 84856 264	0.65214 51548 62546 143
4	−0.86113 63115 94052 580	0.34785 48451 37453 860

Points of evaluation $(x_j, x_j y_k)$

j	x_j	$x_j y_1 = -x_j y_4$	$x_j y_2 = -x_j y_3$
1	0.13975 98643 43780 552	0.12035 22940 89888 328	0.04751 57045 30876 4547
2	0.41640 95676 31083 175	0.35858 53991 82305 152	0.14157 13593 61934 441
3	0.72315 69863 61876 278	0.62273 67399 39136 723	0.24585 96668 98990 366
4	0.94289 58038 85482 299	0.81196 18147 75453 378	0.32056 66993 96768 242

$w_{jk} = b_j a_k = $ *weights for points* $(x_j, x_j y_k)$

j	$k = 1, 4$	$k = 2, 3$
1	0.01084 64518 21050 5090	0.02033 45191 28957 5733
2	0.04516 80985 64739 8624	0.08467 94490 43492 5770
3	0.07077 61357 96171 8794	0.13268 84322 14099 443
4	0.04713 67363 86764 6765	0.08837 01770 44723 4729

$q_m(x)$ are orthogonal, but not necessarily normal. The roots are the values of x_j required. Normalization of the $q_m(x)$ gives the weights b_j by:

$$(7) \qquad b_j^{-1} = \sum_{i=0}^{m-1} [q_i(x_j)]^2$$

where x_j is a zero of $q_m(x)$.

    The orthogonal polynomials, $q_m(x)$, over the interval $(0, 1)$ with weight function x^n are the Jacobi polynomials under the linear transformation $x' = \frac{1}{2}(1 + x)$. The standard definition of the Jacobi polynomials gives the weight function as $(1 - x)^\alpha (1 + x)^\beta$ and the interval of orthogonality as $(-1, 1)$. In this case, $\alpha = 0, \beta = n$ and the linear transformation given above takes $(1 + x)^n$ into $(2x')^n$ and $(-1, 1)$ onto $(0, 1)$. From this fact, explicit representations of $q_m(x)$ are available.

    We consider an example of how to combine a formula for $n = 0$ (the Gauss formula on the line) and one for $n = 1$, to obtain a formula for the triangle. In the following discussion we consider a plane triangle with vertices $(0, 0), (1, 1)$

and $(1, -1)$. Use of the formulas may be made for arbitrary triangles by applying theorem 1. If we take, in each of the above cases, $m = 4$, a formula is obtained which is exact for the general polynomial of degree $2m - 1 = 7$. For $n = 1$, x_j shall denote the roots of $q_4(x)$, and b_j the corresponding weight. The roots of the Legendre polynomial, P_4, shall be denoted by y_k, and the corresponding weights by a_k. Table IV gives the values of x_j, b_j, and y_k, a_k; the points, (x_j, x_jy_k), at which the integrand is to be evaluated, and the weights, w_{jk}, at these points.

The first three tables give: 1) the polynomials $q_m(x)$ obtained from equation (6) for $n = 1, 2, 3$ respectively, and values of m indicated in each table, 2) the roots x_j of $q_m(x)$, and 3) the values of b_j obtained from equation (7). The calculations were made at the University of Wisconsin Numerical Analysis Laboratory using a CPC with Eugene Albright's 18-digit floating decimal board. The approximate error in the x_j's is no more than 1 in the seventeenth significant figure; the approximate error in the b_j's is no more than 1 in the sixteenth significant figure. The sum of the b_j's is $1/(n + 1)$ where n is defined as in equation (6).

3. Symmetrical formulas. While the foregoing development makes it possible, in principle, to obtain numerical integration formulas for the n-simplex to hold exactly for polynomials of at most degree k, we do not mean to suggest that such formulas are the most desirable. One feature of these formulas is that they are unsymmetrical—i.e., in a given simplex the particular points of evaluation are not an invariant set under affine transformations taking the simplex onto itself.

In this section we give the preliminary results of our investigations resulting from a *requirement* of affine symmetry. We give these results since we believe that formulas for triangle and tetrahedron will be most useful and we have certain specific formulas for these regions.

The requirement of affine symmetry we make is simply this: If an integration formula involves calculation of the integrand at a certain point P to be multiplied by a weight, w, then all images of P under all affine transformations of the region onto itself will appear in the formula with the *same* weight, w. While such a requirement would appear to increase the number of points, in dealing with polynomials this is not the case; actually we have obtained fewer points than with the other method.

Let us represent points in the space as vectors and write the vertices of a triangle as V_1, V_2, V_3, and the centroid as $C = \frac{1}{3} \sum_1^3 V_i$. The first affine invariant formula for the triangle is to use the centroid as the sole evaluation point with weight equal to the area. This method works for all bounded regions in all finite dimensional spaces to give a formula for the general linear function over the region. For simplexes or for hypersquares, this is likely to be useful.

The quadratic function over the triangle we have shown to be integrated exactly by evaluations at $rV_i + (1 - r)C$, where $i = 1, 2, 3$. Since this is an affinely symmetric set, we find that the weight (for each point) is one-third the area, and $r = \pm \frac{1}{2}$. For $r = +\frac{1}{2}$ the evaluation points are the distinct trisection points of the median chords and for $r = -\frac{1}{2}$ the evaluation points are the midpoints of the sides. These formulas we consider to offer prospects of extensive usefulness, especially the latter. Since the general quadratic function has 6 terms, we have used three fewer points than an arbitrary specification of evaluation points would have permitted.

The cubic polynomial is integrated over the triangle with $rV_i + (1 - r)C$ and C as evaluation points where $r = \frac{2}{5}$; the weight associated with the centroid is $(-\frac{9}{16})\Delta$ and the weight with each of the other three points is $(25/48)\Delta$, where Δ is the area of the triangle.

The quintic polynomial is integrated precisely with seven points in the triangle using $rV_i + (1 - r)C$, weight a; $sV_i + (1 - s)C$, weight b; and C, weight c. We find $r = \dfrac{1 + \sqrt{15}}{7}$, $s = \dfrac{1 - \sqrt{15}}{7}$, and $a = \left(\dfrac{155 - \sqrt{15}}{1200}\right)\Delta$, $b = \left(\dfrac{155 + \sqrt{15}}{1200}\right)\Delta$, $c = (9/40)\Delta$. Since the general quintic polynomial in two variables has 21 terms this formula appears to be a type we call *efficient* noting that one might not hope to accomplish a formula with fewer than $7 = 21/3$ points. Here the "3" is the number of degrees of freedom for each point due to coordinates and weight. However, there are known *hyperefficient* formulas (cf. [1]), which use fewer points than indicated by this argument. While we will not reproduce the argument here, we used a triangle with vertices $(0, 0)$, $(1, -1)$, $(1, 1)$. Then the requirements of the affine symmetry of the formula with the form of the region assured that all monomials with odd powers of y could be omitted. This left 12 equations. We chose five of these and solved them for a, b, c, r, and s, and verified that the remaining 7 were satisfied.

Over the tetrahedron we have a formula for the general quadratic in three variables involving $rV_i + (1 - r)C$, $i = 1, 2, 3, 4$, and weight a. We calculate $r = 1/\sqrt{5}$ and the weight $a = (\frac{1}{4})\Delta$, where Δ is the volume of the tetrahedron. Another formula with points outside the tetrahedron results if $r = -1/\sqrt{5}$. This type of formula will generally be less used than one with points inside.

For the cubic polynomial over the tetrahedron we have $r = \frac{1}{3}$, $a = (9/20)\Delta$, and $c = (-\frac{4}{5})\Delta$; the centroid C must now be included and c is its weight. This formula is efficient since it involves 5 points and the number of terms in the general cubic is 20.

Generalization and extension of the affinely symmetric methods is now being carried out. However, these specific results seem sufficiently useful to include now.

4. Conclusion. In this paper we have taken a step towards obtaining reasonable numerical integration formulas over simplexes and cones. The cones which are not simplexes have not been emphasized. However, the method devised for cones permits obtaining a formula for integration over a cone (finite) provided a formula is at hand for the base. Thus later on we hope to obtain other formulas for the solid sphere which is a special cone based on its surface.

Error analysis has not been attempted. Experimental calculations on simple regions indicated that for "reasonable" functions there is a decisive factor in favor of the classical formulas here presented over Monte Carlo methods.

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Numerical Integration over Simplexes

1. Introduction. Integration formulae for numerical evaluation of integrals over the simplex in n-space have been given inductively by Hammer, Marlowe, and Stroud [1] so that it is possible in principle to determine a formula holding exactly for the kth degree polynomial in n variables. In the same paper certain affinely symmetric integration formulae are given for the triangle and tetrahedron. Using the theory proposed by Hammer and Wymore [2], it is possible to extend the usefulness of methods developed by transformations of the regions and by use of Cartesian products.

In this paper we give two integration formulae of affinely symmetric type for the simplex in n-space which respectively hold exactly for the quadratic polynomial and the cubic polynomial in n variables. The method for establishing the exact values of integrals needed we believe is new in that the "numerical" formulae are used for the purpose.

2. The formula for cubic polynomials. Let the vertices of the n-simplex, S_n, be $V_0, \cdots, V_n$ and then its centroid is given by $C = \sum_1^n V_i/(n+1)$. Let Δ_n be the hypervolume of S_n.

THEOREM 1: *An integration formula exact for the general cubic polynomial over S_n for $n \geq 1$ is given by*

$$(1) \qquad \int_{S_n} f dv_n = a_n \sum_0^n f(U_i) + c_n f(C)$$

where

$$a_n = \frac{(n+3)^2}{4(n+1)(n+2)} \Delta_n \quad c_n = \frac{-(n+1)^2}{4(n+2)} \Delta_n$$

and

$$U_i = \frac{2}{n+3} V_i + \frac{n+1}{n+3} C \quad i = 0, \cdots, n.$$

Proof: It may first be remarked that the points U_i are on the median lines of S_n and that the statement of the theorem is in symmetric form. In particular, under an affine transformation taking S_n onto itself, the set of points $\{U_i\}$ is invariant and the centroid C is fixed. Since there exists an affine transformation mapping any simplex in E_n onto any other we may choose any particular simplex S_n to carry out the proof. Our choice is specified by vertices as follows:

$$V_0 = (0, \cdots, 0), \qquad V_1 = (1, 0, \cdots, 0),$$
$$V_2 = (1, 1, 0, \cdots, 0), \cdots, \quad V_n = (1, 0, \cdots, 0, 1).$$