

Some Fourth Degree Integration Formulas for Simplexes

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Abstract. A fourth degree integration formula is given for the n -dimensional simplex for $n = 3, 4, 5, 6, 7, 8, 10, 11, 12$. The formula contains $(n^2 + 3n + 4)/2$ points.

1. Introduction. We consider integration formulas

$$(1) \quad \int \cdots \int_{T_n} f(x_1, \dots, x_n) dx_1 \cdots dx_n \approx \sum_{k=1}^N A_k f(x_{k1}, \dots, x_{kn}).$$

Here T_n is the n -simplex whose $n + 1$ vertices are

$$\begin{aligned} &(0, 0, 0, \dots, 0, 0), \\ &(1, 0, 0, \dots, 0, 0), \\ &(0, 1, 0, \dots, 0, 0), \\ &\quad \dots \\ &(0, 0, 0, \dots, 0, 1). \end{aligned}$$

A formula (1) is said to have degree d if it is exact for all polynomials of degree $\leq d$ and if there is at least one polynomial of degree $d + 1$ for which it is not exact.

A number of formulas (1) are given by Stroud [4, pp. 306–315]. Other than product formulas there is only one formula of degree four known for all $n \geq 3$. This formula (denoted in [4] as $T_n : 4 - 1$) contains $(n + 4)/(4!n!)$ points; it was first given by Lauffer [2]. A fourth degree formula for T_2 is known with six points [3].

The purpose of this note is to give a fourth degree formula (1) for $n = 3, 4, 5, 6, 7, 8, 10, 11, 12$ which contains $N = (n + 1)(n + 2)/2 + 1$ points. For an arbitrary n -dimensional region R_n it is known that a fourth degree formula must contain at least $(n + 1)(n + 2)/2$ points (see [4, p. 118]). For T_n , $n \geq 3$, we believe that no fourth degree formula exists with $(n + 1)(n + 2)/2$ points; if this is true, the formulas given below contain the minimal number of points for fourth degree.

2. Construction of the Formulas. The formulas to be described are invariant under all affine transformations of T_n onto itself. We use the notation of [4, p. 307] to describe the points in these formulas. The notation

$$(2) \quad (u_1, u_2, \dots, u_n; u_{n+1})$$

denotes the set of points consisting of the point (u_1, u_2, \dots, u_n) and all points which this point maps into under the set of all $(n + 1)!$ affine transformations of T_n onto itself. (It will always be true that $u_1 + u_2 + \dots + u_{n+1} = 1$.) The coefficients A_k in formula (1) which correspond to the points in a set (2) will all have the same value. We seek formulas with points and coefficients as follows:

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	set of points	coeff.	number of points in set
(3)	$(r, r, \dots, r, r; r)$	A	1
(4)	$(s, s, \dots, s, s; t)$	B	$n + 1$
(5)	$(u, u, \dots, u, v; v)$	C	$n(n + 1)/2$

Here $r = 1/(n + 1)$ and the point (3) is the centroid of T_n . Unless $s = t = r$ or $u = v = r$ the union of the sets (3), (4), (5) contains $(n^2 + 3n + 4)/2$ distinct points. There are five free parameters t, v, A, B, C to be determined.

THEOREM 1. *If formula (1) consists of the points and coefficients (3), (4), (5), and if this formula is exact for the monomials*

$$(6) \quad 1, x_1^2, x_1^3, x_1^4, x_1^2x_2^2,$$

then the formula is exact for all polynomials of degree ≤ 4 .

Proof. The proof is an application of Theorem 3.14-1 of [4, p. 115]. The fact that the formula is exact for all polynomials of degree ≤ 3 is the same as the proof of Theorem 3.14-2 of [4, p. 116]. To complete the proof we must only yet show that the formula is exact for $x_1^3x_2, x_1^2x_2x_3$ and $x_1x_2x_3x_4$. Since the formula is known to be exact for x_1^3 and x_1^4 , Theorem 3.14-1 shows it is exact for $x_1^3x_2$. Since it is exact for $x_1^2x_2, x_1^3x_2$ and $x_1^2x_2^2$, Theorem 3.14-1 shows it is exact for $x_1^2x_2x_3$. Since it is exact for $x_1x_2x_3, x_1^2x_2x_3, x_1x_2^2x_3$ and $x_1x_2x_3^2$, Theorem 3.14-1 shows it is exact for $x_1x_2x_3x_4$. This completes the proof.

The equations which must be satisfied if the points and coefficients (3), (4), (5) are to be a formula which is exact for the monomials (6) are the following:

$$(7-1) \quad A + (n + 1)B + n(n + 1)C/2 = I[1],$$

$$(7-2) \quad Ar^2 + B[ns^2 + t^2] + nC \left[\frac{(n-1)}{2} u^2 + v^2 \right] = I[x_1^2],$$

$$(7-3) \quad Ar^3 + B[ns^3 + t^3] + nC \left[\frac{(n-1)}{2} u^3 + v^3 \right] = I[x_1^3],$$

$$(7-4) \quad Ar^4 + B[ns^4 + t^4] + nC \left[\frac{(n-1)}{2} u^4 + v^4 \right] = I[x_1^4],$$

$$(7-5) \quad Ar^4 + B[(n-1)s^4 + 2s^2t^2] + C \left[\frac{(n-1)(n-2)}{2} u^4 + 2(n-1)u^2v^2 + v^4 \right] = I[x_1^2x_2^2],$$

$$I[x_1^\alpha x_2^\beta] \equiv \int_{T_n} \dots \int x_1^\alpha x_2^\beta dx_1 \dots dx_n.$$

TABLE 1. Parameters in fourth degree formulas for T_n .

n	N	t	v	A	B	C
3	11	0.785714285714	0.399403576167	-(-1) 0.789333333333	(-1) 0.457333333333	0.149333333333
4	16	0.780733498587	0.366579388086	-(-1) 0.983302480775	(-1) 0.192923735600	0.100186838028
5	22	0.811215900283	0.340802583309	-0.109943825884	(-2) 0.739194676530	(-1) 0.710394763528
6	29	0.900166058447	0.320286968058	-0.110339568956	(-2) 0.227922954713	(-1) 0.521135696251
7	37	1.128449432395	0.303911709407	-(-1) 0.952531177701	(-3) 0.438002222641	(-1) 0.389910392853
8	46	1.977701277860	0.290994448736	-(-1) 0.593130083305	(-4) 0.216445010761	(-1) 0.294199502172
10	67	-0.765469225444	0.274565829532	(-1) 0.964993209382	(-3) 0.158577857342	(-1) 0.163955695024
11	79	-0.257655788561	0.271782267706	0.191367778454	(-2) 0.318837768540	(-1) 0.116722983230
12	92	-(-1) 0.684931506849	0.275510204082	-(-1) 0.718169212074	(-1) 0.371721301760	(-2) 0.754588755025

We solve equations (7-1), (7-2), (7-3) for A, B, C in terms of r, s, t, u, v . Substituting these expressions into (7-4) and (7-5) and using the fact that

$$ns + t = 1, \quad (n - 1)u + 2v = 1,$$

gives two simultaneous equations

$$(8) \quad g_1(n, t, v) = 0, \quad g_2(n, t, v) = 0,$$

for t and v . For a given n , if values of t and v can be found to satisfy (8), and if these values are such that the determinant of the linear system for A, B, C (obtained from (7-1), (7-2), (7-3)) is nonzero, then t, v, A, B, C give the desired formula. Table 1 contains numerical values of the parameters for the formulas we found in this way. No formulas were found for $n = 9$ and $n \geq 13$.

A graph of $1/t$ as a function of n , for the t values of Table 1, shows that for $n = 9$, $1/t \approx 0$. This is an indication that for $n = 9$ no formula exists. For $n = 3, 4, 5, 6$ all the points in the formula lie inside T_n , but the coefficient A for the centroid is negative. For $n = 7, 8, 10, 11, 12$ the $n + 1$ points with coefficient B lie outside T_n . For $n = 10, 11$ all the coefficients are positive.

3. Concluding Remarks. Bykova [1] has given an eleven point fourth degree formula for three dimensional regions which are symmetric with respect to the coordinate planes. T_3 does not have this symmetry; as far as we know, all the formulas given above are new.

The above calculations were carried out in Fortran double precision (about sixteen significant digits) on the IBM 360/65 at the Data Processing Center at Texas A & M University. We wish to thank the Department of Mathematics at Texas A & M University for the computing time for this work.

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