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Invariant cubature formulae of the ninth degree of accuracy for the hyperoctahedron

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Abstract

In this paper cubature formulae are obtained for evaluating integrals on the hyperoctahedron, which are exact for any polynomial of degree not exceeding 9, and are invariant with respect to the group of all orthogonal transformations of the hyperoctahedron into itself. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

Let G_n denote the hyperoctahedron in $\mathbb{R}^n$:

$$G_n = \left\{ x = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n \;\middle|\; \sum_{i=1}^{n} |x_i| \leqslant 1 \right\}. \tag{1}$$

The hyperoctahedron (1) is the polyhedron in $\mathbb{R}^n$, with vertices at $2n$ points in $\mathbb{R}^n$:

$$(\pm 1, 0, \ldots, 0),\ (0, \pm 1, 0, \ldots, 0), \ldots, (0, \ldots, 0, \pm 1).$$

The group of all orthogonal transformations of (1) into itself will be denoted by G_nG. It is known (see [2, p. 232]) that the order of the group G_nG is equal to $n!2^n$.

Let C_n denote the hypercube in $\mathbb{R}^n$:

$$C_n = \{x = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n \mid -1 \leqslant x_i \leqslant 1,\ i = 1, 2, \ldots, n\}.$$

The group of all orthogonal transformations of the hypercube C_n into itself will be denoted by C_nG. The group C_nG is congruent with the group G_nG (see [2, p. 232]).

Cubature formulae of the hyperoctahedron G_n which are exact for all polynomials of degree not exceeding m for $m \leqslant 5$ are given by Stroud [8], cubature formulae of the octahedron G_3 for $m = 7$ are

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Table 1

n	3	4	5	6	7	8
N_0	43	91	171	295	477	733
N	53	145	293	529	885	1409
N_1	53	145	341	705	1317	2273
N_2	—	—	292	656	1428	2944
N_3	—	177	373	689	—	—
N_4	—	249	1053	—	—	—

obtained by Mysovskikh [3], cubature formulae of the G_n for $m=5,7,9$ are obtained in [6,7]. Three cubature formulae of the G_n for $m=9$ are obtained in [4]: the first formula exists for $5\leqslant n\leqslant 16$; the second formula exists for $n=4,5,6$; the third formula exists for $n=4,5$.

In this paper, Sobolev's theorem [5] is used to construct cubature formulae for integrals of the hyperoctahedron G_n, which are exact for all polynomials of degree not exceeding 9 and invariant with respect to the group G_nG. The cubature formulae obtained in this paper exist for $3\leqslant n\leqslant 8$.

Let us compare the number of nodes of the formulae obtained in this paper, the number of nodes of formulae obtained in [4,7] and the lower bound for the number of nodes of cubature formulae of the 9th degree of accuracy for central symmetric regions.

The lower bound for the number of nodes of cubature formulae for central symmetric regions has been obtained by Moller [1]. That is Theorem 2 given in [2, p. 220]. According to this theorem, the lower bound for the number of nodes for cubature formulae of the 9th degree of accuracy for central symmetric regions is equal to

$$N_0=(n^4+6n^3+23n^2+18n+12)/12.$$

Let N denote the number of nodes for the cubature formulae obtained in this paper; N_1 the number of nodes for the formulae obtained in [7]; N_2,N_3,N_4 the number of nodes for the first, second and third formulae from [4], respectively.

The number of nodes N_0,N,N_1,N_2,N_3,N_4 at $n=3(1)8$ are given in Table 1.

Table 1 shows that at $n=3$ the number of nodes in the obtained formulae in this paper exceeds the lower bound by 10 units: at $n=3$ and $n=4$, $N=N_1$; at $n=5$, $N=293$, $N_2=292$; while in all other cases the number of nodes for the formulae obtained in this paper is less than those for the cubature formulae in [4,7].

In Sections 2 and 3 we derive the parameters of the cubature formulae for $n\geqslant 4$ and $n=3$, respectively. Numerical results are presented in Section 4.

2. Cubature formula for $n\geqslant 4$

It is known (see [2, p. 232]) that the symmetric polynomials of $x_1^2,x_2^2,\ldots,x_n^2$,

$$\sigma_2=\sum_{i=1}^{n}x_i^2,\quad \sigma_4=\sum_{i<j}x_i^2x_j^2,\ldots,\quad \sigma_{2n}=x_1^2x_2^2\ldots x_n^2, \tag{2}$$

form a set of basis invariant forms of G_nG.

From Theorem 13 (see [2, p. 231]) it follows that any polynomial that is invariant with respect to the group G_nG is a polynomial of the polynomials (2), since the group G_nG is generated by reflections (see [2, p. 231]).

Since the cubature formula must be exact for all polynomials of degree not exceeding 9, according to the Sobolev's theorem ([5] or [2, Theorem 12, p. 230]), for $n \geqslant 4$ it must be exact for 12 invariant polynomials

$$1, \sigma_2, \sigma_2^2, \sigma_2^3, \sigma_2^4, \sigma_4, \sigma_2\sigma_4, \sigma_4^2, \sigma_2^2\sigma_4, \sigma_6, \sigma_2\sigma_6, \sigma_8, \tag{3}$$

where the polynomials $\sigma_{2k},\ k = 1,2,3,4$, are defined by (2).

Accordingly, the nodes of the cubature formula are selected such that the cubature sum depends on 12 parameters at least.

The nodes of the cubature formula are taken as the following seven orbits:

$$(1)\ G_nG(0,0,\dots,0), \quad (2)\ G_nG(a_1,0,\dots,0), \quad (3)\ G_nG(a_2,0,\dots,0),$$

$$(4)\ G_nG(b_1,b_2,0,\dots,0), \quad (5)\ G_nG(c_1,c_1,c_1,0,\dots,0),$$

$$(6)\ G_nG(c_2,c_2,c_2,0,\dots,0), \quad (7)\ G_nG(d,d,\dots,d),$$

where $a_1 \neq 0,\ a_2 \neq 0,\ a_1^2 \neq a_2^2,\ b_1 \neq 0,\ b_2 \neq 0,\ b_1^2 \neq b_2^2,\ c_1 \neq 0,\ c_2 \neq 0,\ c_1^2 \neq c_2^2,\ d \neq 0$.

The first orbit contains only one node $\theta = (0,0,\dots,0)$. For the other orbits only one node is written here, the other nodes being obtained from it by all possible permutations and changes of the sign of the coordinates.

The cubature formula can be written in the form

$$\begin{aligned}\int_{G_n} f(x)\,\mathrm{d}x \simeq{}& Ef(0,0,\dots,0) + A_1 \sum_1^{2n} f(a_1,0,\dots,0)\\
&+ A_2 \sum_1^{2n} f(a_2,0,\dots,0) + B \sum_1^{8C_n^2} f(b_1,b_2,0,\dots,0)\\
&+ C_1 \sum_1^{8C_n^3} f(c_1,c_1,c_1,0,\dots,0) + C_2 \sum_1^{8C_n^3} f(c_2,c_2,c_2,0,\dots,0)\\
&+ D \sum_1^{2^n} f(d,d,,\dots,d),\end{aligned} \tag{4}$$

where the sum is accomplished for all points of the corresponding orbit. The number of nodes is $N = 2^n + (8n^3 - 12n^2 + 16n + 3)/3;\ n \geqslant 4$.

The cubature sum depends on 14 parameters. The parameters $c_2 \neq 0$ and $d \neq 0$ are assigned arbitrarily. The remaining 12 parameters $E,\ A_1,\ A_2,\ B,\ C_1,\ C_2,\ D,\ a_1,\ a_2,\ b_1,\ b_2,\ c_1$ are calculated.

The requirement that formula (4) is exact for polynomials (3) yields the nonlinear system of 12 equations with 12 unknowns $E,\ A_1,\ A_2,\ B,\ C_1,\ C_2,\ D,\ a_1,\ a_2,\ b_1,\ b_2,\ c_1$:

$$(1):\quad E + 2nA_1 + 2nA_2 + 8C_n^2B + 8C_n^3C_1 + 8C_n^3C_2 + 2^nD = 2^n/n!,$$

$$\begin{aligned}
(\sigma_2):\ & 2nA_1a_1^2+2nA_2a_2^2+8C_n^2B(b_1^2+b_2^2)+24C_n^3C_1c_1^2+24C_n^3C_2c_2^2+n2^nDd^2\\
&=n2^{n+1}/(n+2)!,\\
(\sigma_2^2):\ & 2nA_1a_1^4+2nA_2a_2^4+8C_n^2B(b_1^2+b_2^2)^2+72C_n^3C_1c_1^4+72C_n^4C_2c_2^4+n^22^nDd^4\\
&=n(n+5)2^{n+2}/(n+4)!,\\
(\sigma_2^3):\ & 2nA_1a_1^6+2nA_2a_2^6+8C_n^2B(b_1^2+b_2^2)^3+216C_n^3C_1c_1^6+216C_n^3C_2c_2^6+n^32^nDd^6\\
&=n(n^2+15n+74)2^{n+3}/(n+6)!,\\
(\sigma_2^4):\ & 2nA_1a_1^8+2nA_2a_2^8+8C_n^2B(b_1^2+b_2^2)^4+648C_n^3C_1c_1^8+648C_n^3C_2c_2^8+n^42^nDd^8\\
&=n(n^3+30n^2+371n+2118)2^{n+4}/(n+8)!,\\
(\sigma_4):\ & 8C_n^2Bb_1^2b_2^2+24C_n^3C_1c_1^4+72C_n^3C_2c_2^4+n(n-1)2^{n-1}Dd^4\\
&=n(n-1)2^{n+1}/(n+4)!, \qquad (5)\\
(\sigma_2\sigma_4):\ & 8C_n^2B(b_1^2+b_2^2)b_1^2b_2^2+72C_n^3C_1c_1^6+72C_n^3C_2c_2^6+n^2(n-1)2^{n-1}Dd^6\\
&=n(n-1)(n+10)2^{n+2}/(n+6)!,\\
(\sigma_4^2):\ & 8C_n^2Bb_1^4b_2^4+72C_n^3C_1c_1^8+72C_n^3C_2c_2^8+n^2(n-1)^22^{n-2}Dd^8\\
&=n(n-1)(n^2+19n+30)2^{n+2}/(n+8)!,\\
(\sigma_2^2\sigma_4):\ & 8C_n^2B(b_1^2+b_2^2)^2b_1^2b_2^2+216C_n^3C_1c_1^8+216C_n^3C_2c_2^8+n^3(n-1)2^{n-1}Dd^8\\
&=n(n-1)(n^2+25n+198)2^{n+3}/(n+8)!,\\
(\sigma_6):\ & 8C_n^3C_1c_1^6+8C_n^3C_2c_2^6+n(n-1)(n-2)2^{n-1}Dd^6/3\\
&=n(n-1)(n-2)2^{n+2}/[3(n+6)!],\\
(\sigma_2\sigma_6):\ & 24C_n^3C_1c_1^8+24C_n^3C_2c_2^8+n^2(n-1)(n-2)2^{n-1}Dd^8/3\\
&=n(n-1)(n-2)(n+15)2^{n+3}/[3(n+8)!],\\
(\sigma_8):\ & 2^nC_n^4Dd^8=n(n-1)(n-2)(n-3)2^{n+1}/[3(n+8)!].
\end{aligned}$$

System (5) can be solved as follows:
From the equation (σ_8) we find D.

From the equations $(\sigma_2\sigma_6)$ we find

$$C_1c_1^8 + C_2c_2^8 = 5.2^{n+1}/(n+8)!. \tag{6}$$

From the equations (σ_6) we find

$$C_1c_1^6 + C_2c_2^6 = 2^n/(n+6)! - 2^{n+1}/[(n+8)!d^2]. \tag{7}$$

Introducing the notations

$$u = b_1^2 + b_2^2, \quad v = b_1^2b_2^2 \tag{8}$$

from the equations $(\sigma_2\sigma_4)$, (σ_4^2) and $(\sigma_2^2\sigma_4)$ we obtain a nonlinear system of three equations with three unknowns B, u, v, on solving this system and we find b_1^2 and b_2^2 using (8).

From the equation (σ_4) we find

$$C_1c_1^4 + C_2c_2^4 = 2^{n-1}\{1/(n+4)! - (S_1^2/S_2 + 4)/[(n+8)!d^4]\}/(n-2), \tag{9}$$

where

$$S_1 = (8-n)S + 2(n-3), \quad S_2 = 72 - 5n, \quad S = (n+7)(n+8)d^2. \tag{10}$$

From Eqs. (6), (7) and (9) we find C_1, C_2 and c_1 ($c_2 \neq 0$ and $d \neq 0$ are assigned arbitrarily).

Introducing the notations

$$A_1^* = A_1a_1^2, \quad A_2^* = A_2a_2^2 \tag{11}$$

from the equations (σ_2), (σ_2^2), (σ_2^3) and (σ_2^4) we obtain the nonlinear system

$$\begin{aligned} &A_1^* + A_2^* = X_1,\\ &A_1^*a_1^2 + A_2^*a_2^2 = X_2,\\ &A_1^*a_1^4 + A_2^*a_2^4 = X_3,\\ &A_1^*a_1^6 + A_2^*a_2^6 = X_4, \end{aligned} \tag{12}$$

of four equations with four unknowns A_1^*, A_2^*, a_1^2, a_2^2, where

$$\begin{aligned} X_1 &= 2^n/(n+2)! - 2(n-1)[Bu + (n-2)(C_1c_1^2 + C_2c_2^2)] - 2^{n-1}Dd^2,\\ X_2 &= 2^n\{(13-n)/(n+4)! + [3(n-1)S_1^2/S_2 + 4(n-3)\\ &\qquad - 4(n-1)S_1^2/(5S_3)]/[(n+8)!d^4]\},\\ X_3 &= 2^{n+1}[(130+57n-7n^2)S + 14n^2 - 54n + 36\\ &\qquad - 8(n-1)S_1S_2/(5S_3)]/[(n+8)!d^2],\\ X_4 &= 2^{n+2}(261414 - 62679n + 2810n^2 - 25n^3)/[5(n+8)!S_3], \end{aligned} \tag{13}$$

$$S_3 = 9 - n. \tag{14}$$

System (12) can be solved as follows.

Let us find the coefficients p and q of the quadratic equation

$$t^2 + pt + q = 0 \tag{15}$$

with roots a_1^2 and a_2^2.

Pre-multiplying the first equation of system (12) by q, the second equation by p and adding the first three equations of system (12), we obtain

$$qX_1 + pX_2 + X_3 = A_1^*(a_1^4 + pa_1^2 + q) + A_2^*(a_2^4 + pa_2^2 + q) = 0,$$

since a_1^2 and a_2^2 are the roots of Eq. (15).

Pre-multiplying the second equation of system (12) by q, the third equation by p and adding the second, the third and the fourth equations of system (12), we obtain

$$qX_2 + pX_3 + X_4 = A_1^* a_1^2(a_1^4 + pa_1^2 + q) + A_2^* a_2^2(a_2^4 + pa_2^2 + q) = 0.$$

Thus we obtain the linear system

$$\begin{aligned} &qX_1 + pX_2 + X_3 = 0, \\ &qX_2 + pX_3 + X_4 = 0, \end{aligned} \qquad (16)$$

of two equations with two unknowns p and q. We solve system (16) and find p and q. Then we solve Eq. (15) and find its roots a_1^2 and a_2^2.

Afterwards, from the first two equations of system (12) we find unknowns A_1^* and A_2^*. Then using (11) we find the coefficients A_1 and A_2.

From the first equation of system (5) we find the coefficient E.

The solution of system (5) for $n \geqslant 4$ is

$$A_1 = [X_2 - a_2^2 X_1]/[a_1^2(a_1^2 - a_2^2)], \quad a_1^2 = (-r_1 + \sqrt{r_0})/(2r),$$

$$A_2 = [a_1^2 X_1 - X_2]/[a_2^2(a_1^2 - a_2^2)], \quad a_2^2 = (-r_1 + \sqrt{r_0})/(2r),$$

$$B = 2^{n+1} S_1/[(n+8)!uvd^2], \quad b_1^2 = 2d^2(S_2 + 3\sqrt{3S_2})/S_1,$$

$$D = 16/[(n+8)!d^8], \quad b_2^2 = 2d^2(S_2 - 3\sqrt{3S_2})/S_1,$$

$$C_1 = 2^{n-3} q_2^4/[(n+8)! q_1^2 q_3 d^8], \quad c_1^2 = 2q_1 d^2/q_2,$$

$$C_2 = 2^{n-1}\{1/(n+4)! - [S_1^2/S_2 + 4 + (n-2)q_2^2/q_3]/[(n+8)!d^4]\}/[(n-2)c_2^4],$$

$$E = 2^n/n! - 2n(A_1 + A_2) - 4n(n-1)B - 4n(n-1)(n-2)(C_1 + C_2)/3 - 2^n D,$$

$c_2 \neq 0$ and $d \neq 0$ are assigned arbitrarily, where

$$u = 4S_2 d^2/S_1, \quad v = 20 S_2 S_3 d^4/S_1^2, \quad q_1 = 10d^2 + (2 - S)c_2^2,$$

$$q_2 = 2(S-2)d^2 + c_2^2[S_1^2/S_2 + 4 - (n-5)(n+6)Sd^2]/(n-2),$$

$$q_3 = 2q_1 d^2 - q_2 c_2^2, \quad r_1 = X_1 X_4 - X_2 X_3, \quad r_2 = X_3^2 - X_2 X_4,$$

$$r = X_2^2 - X_1 X_3, \quad r_0 = r_1^2 - 4rr_2.$$

$X_1 - X_4$ are found from (13); S_1, S_2, S are found from (10); S_3 is found from (14).

3. Cubature formula for $n = 3$

When $n = 3$ in (3) the number of invariant polynomials of degree not exceeding nine is 11, since the polynomial σ_8 is not a basis one. In this case in system (5) the equation (σ_8) does not participate. To reduce the number of parameters by one, let us suppose that $D = 0$. The cubature sum in formula (4) depends on 12 parameters. The parameter $c_2 \neq 0$ is assigned arbitrary. The remaining 11 parameters are calculated. System (5) in this case has 11 equations with 11 unknowns E, A_1, A_2, B, C_1, C_2, a_1, a_2, b_1, b_2, c_1. The number of nodes is $N = 53$.

The solution of system (5) for $n = 3$ is

$$A_1 = [X_2 - a_2^2 X_1]/[a_1^2(a_1^2 - a_2^2)], \quad a_1^2 = (-r_1 + \sqrt{r_0})/(2r),$$

$$A_2 = [a_1^2 X_1 - X_2]/[a_2^2(a_1^2 - a_2^2)], \quad a_2^2 = (-r_1 - \sqrt{r_0})/(2r),$$

$$B = 4159375/176849568, \quad b_1^2 = (57 + 9\sqrt{19})/275,$$

$$E = 4/3 - 6(A_1 + A_2) - 24B - 8(C_1 + C_2), \quad b_2^2 = (57 - 9\sqrt{19})/275,$$

$$C_1 = 33275\, p_3^4/[517104(57 p_2)^2 p_1], \quad c_1^2 = 57 p_2/(55 p_3),$$

$$C_2 = 103/(5040\, p_1 c_2^4),$$

$c_2 \neq 0$ is assigned arbitrarily, where

$$X_1 = 53651/1939140 - (3025 c_2^2 p_3^3 + 3011823\, p_2)/(36843660\, p_1 p_2 c_2^2),$$

$$X_2 = 787/129276, \quad X_3 = 43/11340, \quad X_4 = 1361/519750,$$

$$p_1 = 342 - 6270 c_2^2 + 37235 c_2^4, \quad p_2 = 6 - 55 c_2^2, \quad p_3 = 57 - 677 c_2^2,$$

$$r_1 = X_1 X_4 - X_2 X_3, \quad r_2 = X_3^2 - X_2 X_4, \quad r = X_2^2 - X_1 X_3, \quad r_0 = r_1^2 - 4 r r_2.$$

4. Numerical results for $n \geqslant 3$

A FORTRAN 77 program written to compute the parameters of formula (4) can be used for any $n \geqslant 3$ if the formula exists, or to establish that the formula does not exist and why.

The program can verify whether the nodes are inside G_n. Since $c_2 \neq 0$ and $d \neq 0$ are assigned arbitrary, we can derive an infinite set of cubature formulae and one may seek such values for c_2 and d for which the derived nodes are inside G_n.

The following results are obtained. Cubature formula (4) exists for $n = 3(1)8$. Formula (4) does not exist for $n \geqslant 9$: for $n = 9$ because $v = 0$, for $n = 10(1)14$ because $v < 0$, for $n \geqslant 15$ because $S_2 < 0$. When $n = 3$ part of the nodes are outside G_n. When $n = 4(1)8$, the nodes are inside G_n.

The results for $n = 3, 4, 5$ are given in Table 2

The results for $n = 6, 7, 8$ are given in Table 3.

Table 2

n	3	4	5
A_1	$0.179782431451 \times 10^{-1}$	$0.620689093680 \times 10^{-3}$	$0.575962925232 \times 10^{-4}$
A_2	$0.139237829260 \times 10^{-2}$	$-0.338096394200 \times 10^{-1}$	$-0.252604877899 \times 10^{-2}$
B	$0.235192827839 \times 10^{-1}$	$0.607433086066 \times 10^{-2}$	$0.151337761639 \times 10^{-2}$
E	$-0.443720294588 \times 10^{-1}$	$0.994050840334 \times 10^{-1}$	$-0.436835515636 \times 10^{-2}$
C_1	$0.672918191342 \times 10^{-2}$	$0.210281781392 \times 10^{-2}$	$0.320806647448 \times 10^{-3}$
C_2	$0.803981740056 \times 10^{-1}$	$0.137153046172 \times 10^{-1}$	$0.146083397384 \times 10^{-2}$
D	0	$0.218908663353 \times 10^{-2}$	$0.100369023980 \times 10^{-2}$
a_1	0.714878539296	0.908849824455	0.936458919599
a_2	0.999987794166	0.176636990487	0.540867961584
b_1	0.591546787489	0.565274863579	0.539375702833
b_2	0.254200418483	0.227800131770	0.200149360944
c_1	0.365780280376	0.333126341417	0.330676365177
c_2	0.20478	0.18	0.21
d	—	0.25	0.2

Table 3

n	6	7	8
A_1	$0.144750236730 \times 10^{-3}$	$0.911527738458 \times 10^{-6}$	$0.112516107581 \times 10^{-3}$
A_2	$-0.235143202827 \times 10^{-2}$	$-0.956174737892 \times 10^{-3}$	$-0.634971759510 \times 10^{-3}$
B	$0.548644846870 \times 10^{-3}$	$0.130505764960 \times 10^{-3}$	$0.501164522329 \times 10^{-4}$
E	$0.533462068168 \times 10^{-3}$	$-0.153545569892 \times 10^{-2}$	$0.386427901528 \times 10^{-3}$
C_1	$0.616068293224 \times 10^{-4}$	$0.128267764358 \times 10^{-4}$	$0.201254287658 \times 10^{-5}$
C_2	$-0.418131127131 \times 10^{-4}$	$0.149188740687 \times 10^{-4}$	$-0.243318625860 \times 10^{-5}$
D	$0.716113000584 \times 10^{-3}$	$0.829079326830 \times 10^{-4}$	$0.128298117716 \times 10^{-4}$
a_1	0.721212771173	0.953724427128	0.530146493517
a_2	0.528425602429	0.475814078165	0.466180649956
b_1	0.489881494755	0.471137304790	0.438013544716
b_2	0.162483534886	0.132093111795	0.090244859386
c_1	0.323820004530	0.305634136000	0.297264803732
c_2	0.2	0.14	0.14
d	0.15	0.14	0.125

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