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CUBATURE FORMULAS ON THE SPHERE THAT ARE INVARIANT UNDER THE TRANSFORMATIONS OF THE DIHEDRAL GROUPS OF ROTATIONS WITH INVERSION

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Abstract. An algorithm for finding the best cubature formulas (in a sense) on the sphere that are invariant under the transformations of the dihedral groups of rotations with inversion is described. This algorithm is applied for finding parameters of all the best cubature formulas of this symmetry type up to the 35th order of accuracy.

Keywords: numerical integration, invariant cubature formulas, invariant polynomials, dihedral group of rotations.

1. Introduction

Cubature formulas on the sphere that are invariant under the transformations of various dihedral groups of symmetries were considered in [1–8]. In particular, in [3], we proposed an algorithm for constructing the best cubature formulas (in a sense) on the sphere that are invariant under the dihedral group of rotations with inversion D_{6h}, in [4] – under the group D_{4h}, in [5] – under the group D_{2h}, in [6] – under the group D_{5d}, and in [7] – under the group D_{3d}. All cubature formulas invariant under these groups possess central symmetry and hence are accurate for all odd functions.

In the present article, we describe an analogous general algorithm for constructing the best cubature formulas invariant under the dihedral groups of rotations with inversion. We carry out computations by this algorithm with the purpose of finding the parameters of all the best cubature formulas of this symmetry type up to the

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35th order of accuracy n. We give the parameters of new cubature formula with 16 significant digits for $n = 17$.

2. An algorithm for finding the best cubature formulas

Let S be the unit sphere centered at the origin, i. e., the set of the points $(x, y, z) \in R_3$ for which $x^2 + y^2 + z^2 = 1$. On S, we consider the integral

$$U(f) = \frac{1}{4\pi} \int_S f(s)\, ds, \tag{1}$$

where $s \in S$, ds is the surface element of the sphere, $U(1) = 1$.

For finding integral (1), we construct a numerical cubature formula

$$V(f) = \sum_{i=1}^{N} w_i f(s_i), \tag{2}$$

where N is the number of the nodes, w_i are the weights, and s_i are the nodes.

The quantity $P(f) = U(f) - V(f)$ is referred to as the error of the cubature formula (2) at the function f. If the cubature formula is accurate for the function f then $P(f) = 0$.

Let $\{Z_{kj}(x, y, z);\ k = 0, 1, \ldots, n;\ j = 1, 2, \ldots, 2k+1\}$ be an orthonormal system of polynomials of degree at most n for which $U(Z_{kj} Z_{lm}) = \delta_{kl}\delta_{jm}$. Here the index k enumerates the degrees of the basis polynomials and the index j enumerates the polynomials at the given k; δ_{kl} is the Kronecker symbol. We note that the polynomials Z_{kj} are bound with the usual spherical harmonics Y_{kj} by the relation $Z_{kj} = \sqrt{4\pi} Y_{kj}$.

We say that the given cubature formula has algebraic accuracy order n (or simply order n) if it is accurate for all polynomials of degree at most n and is not accurate at least for one polynomial of degree $n+1$. Refer as the error of the cubature formula (2) at the polynomials of degree k to the quantity (see [9])

$$E_k = \left(\sum_{j=1}^{2k+1} P^2(Z_{kj}) \right)^{1/2}.$$

For a cubature formula of order n, all the quantities $E_k = 0$ for $k \le n$ and $E_{n+1} > 0$. The quantity E_{n+1} characterizes the degree of proximity of the given cubature formula of order n to the cubature formula of order $n+1$.

In the present article, we attempt to construct all the best cubature formulas on the sphere for $n \le 35$ that are invariant under the transformations of the dihedral groups of rotations with inversion. Moreover, as the best among all cubature formulas of this form having a given order n, we regard cubature formulas satisfying the following four conditions (see [9]):

1) the nodes belong to the integration domain;
2) the weights are positive;
3) the number of nodes is minimal;
4) the quantity E_{n+1} is minimal.

Cubature formulas that are invariant under the dihedral groups of rotations with inversion D_k may be of two types depending on if k is even or odd. If k is even then this type of symmetry is denoted as the group D_{kh}, and if k is odd then this type is denoted as the group D_{kd} (see [10]).

Cubature formulas of the group D_{kh} are of the form

$$V(f) = A_0\sum_{j=1}^{2} f(a_{0j}) + B_0\sum_{j=1}^{k} f(b_{0j}) + C_0\sum_{j=1}^{k} f(c_{0j}) + \sum_{i=1}^{J} A_i\sum_{j=1}^{2k} f(a_{ij}) + \sum_{i=1}^{K} B_i\sum_{j=1}^{2k} f(b_{ij}) + \sum_{i=1}^{L} C_i\sum_{j=1}^{2k} f(c_{ij}) + \sum_{i=1}^{M} D_i\sum_{j=1}^{4k} f(d_{ij}), \tag{3}$$

where 2 points a_{0j} lie at the poles of the dihedron (bipyramid) inscribed in the sphere and have coordinates $(0, 0, \pm 1)$; k points b_{0j} lie at the vertices of the base of the dihedron and are generated by the point $(1, 0, 0)$ of the group C_k; k points c_{0j} correspond to the midpoints of the base of the dihedron and are generated by the point $(\cos(\pi/k), \sin(\pi/k), 0)$ of the group C_k; $2k$ points a_{ij} lie at the base of the dihedron and are generated by the points $(a_i, \pm b_i, 0)$ of the group C_k; $2k$ points b_{ij} lie at $k/2$ vertical planes passing through the vertices of the dihedron and are generated by the points $(c_i, 0, \pm d_i)$ of the group C_k; $2k$ points c_{ij} lie at $k/2$ vertical planes passing through the midpoints of the dihedron and are generated by the points $(g_i \cos(\pi/k), g_i \sin(\pi/k), \pm h_i)$, $g_i = \sqrt{1 - h_i^2}$ of the group C_k; $4k$ points d_{ij} are the points of general position of the group D_{kh} and are generated by the points $(p_i, \pm q_i, \pm r_i)$ of the group C_k.

We remind that one point (a, b, c) of the group C_k generates k points:

$$(x_1 = a,\ y_1 = b,\ z_1 = c), \quad (x_{l+1} = ux_l - vy_l,\ y_{l+1} = vx_l + uy_l,\ z_{l+1} = c),$$

where $u = \cos(2\pi/k)$, $v = \sin(2\pi/k)$, $l = 1, 2, \ldots, k-1$.

Observe that we associate our dihedron with the right bipyramid inscribed in the sphere whose poles lie at the axis z and whose common bases, which are the regular k-sided polygons, lie in the equator plane $z = 0$ (see, for example, [11]). Our dihedron is taken to itself under rotations by an angle that is a multiple of $2\pi/k$ around the k-order axis z. These rotations constitute the cyclic symmetry group C_k. Moreover, the dihedron goes to itself under the rotation by the angle π around any of the second-order axes lying in the plane $z = 0$ and joining the origin to the vertices or to the midpoints of the dihedron [11]. The family of all these transformations forms the symmetry group called the group D_k [10]. This group contains $2k$ elements: k rotations around the kth order axis z and k rotations around the second-order horizontal axes. In formula (3), one of the second-order axes coincides with the axis x. Therefore, the cubature formula is invariant under the change of the point (x, y, z) by $(x, -y, -z)$. Adding to the group D_k the symmetry operation with respect to the plane $z = 0$, we get our group D_{kh} which contains $4k$ elements (see [10]).

Cubature formulas of the group D_{kd} are of the form

$$V(f) = A_0\sum_{j=1}^{2} f(a_{0j}) + B_0\sum_{j=1}^{2k} f(b_{0j}) + \sum_{i=1}^{L} A_i\sum_{j=1}^{2k} f(a_{ij}) + \sum_{i=1}^{M} B_i\sum_{j=1}^{4k} f(b_{ij}), \tag{4}$$

where 2 points a_{0j} lie at the poles of the dihedron and have coordinates $(0, 0, \pm 1)$; $2k$ points b_{0j} correspond to the vertices and midpoints of the base of the dihedron and are generated by the point $(1, 0, 0)$ of the group C_{2k}; $2k$ points a_{ij} lie at k vertical symmetry planes [10]; $4k$ points b_{ij} are the points of general position of the group D_{kd}. In our case of odd k, one of the symmetry planes coincides with the plane $x = 0$. Hence, $2k$ points a_{ij} are generated by the points $(0, a_i, b_i)$ and

$(0, -a_i, -b_i)$ of the group C_k; $4k$ points b_{ij} are generated by the points $(\pm c_i, d_i, e_i)$ and $(\pm c_i, -d_i, -e_i)$ of the group C_k.

When k is even, the cubature formula (3) is invariant under the reflections in the planes $x = 0$, $y = 0$ and $z = 0$. When k is odd, the cubature formula (4) is invariant under the reflection in the plane $x = 0$. Hence, cubature formulas (3) and (4) are invariant under the change of the point (x, y, z) by $(-x, -y, -z)$.

In application to our case, Theorem 1 in [12] sounds as follows:

Theorem 1. *For cubature formula (3) (or (4)) to have order n, it is necessary and sufficient that it be accurate for all polynomials of degree at most n that are invariant under the group D_{kh} (or D_{kd}).*

It is known (see, for instance, [8]) that every polynomial invariant under the dihedral group D_k is representable on the unit sphere as a polynomial of basis invariant forms

$$u = \sin^2\theta, \quad v = \sin^k\theta\cos k\varphi, \quad w = \cos\theta\sin^k\theta\sin k\varphi,$$

where θ and φ are the angular coordinates of the spherical coordinate system. The forms u, v and w have degrees 2, k and $k+1$ respectively. Since $w^2 = (1-u)(u^k - v^2)$, the polynomial w occur in the basis at most in degree 1.

The cubature formulas of the group D_{kh} are invariant to the reflections in $k+1$ planes for which the form $w = 0$. The cubature formulas of the group D_{kd} are invariant to the reflections in k planes for which the form $v = 0$. Hence, for the group D_{kh}, the basis polynomials are of the form $u^i v^j$ where $i, j = 0, 1, \ldots$; $2i + kj \le n$. For the group D_{kd}, the basis polynomials are of the form $u^i v^{2j} w^l$ where $i, j = 0, 1, \ldots$; $l = 0, 1$; $2i + 2kj + (k+1)l \le n$.

The algorithms in detail for constructing the best cubature formulas of the group D_{kh} for $k = 2$, 4, 6 were given in [3–5], and algorithms of the group D_{kd} for $k = 3$, 5 were given in [6, 7].

3. Construction of the concrete best cubature formulas

When constructing the best cubature formulas for a given n, we wish to get formula (2) with positive weights w_i and minimal number of nodes N. To achieve this purpose for the dihedral groups with inversion D_{kh} for even k and D_{kd} for odd k, we keep the following rules.

All groups D_{kh} for even k contain the subgroup D_{2h}. Thus, the best cubature formulas of the group D_{2h} are also the best cubature formulas for all groups D_{kh} with even k. Construction of the best cubature formulas invariant under the group D_{2h} was performed for $n \le 35$ in [5].

In analogy, to construct the best cubature formulas for all dihedral groups with inversion D_{kd} for odd k, it is sufficient to treat the cases of primitive $k = 3$, 5, 7, ... The cases $k = 3$, 5 were examined in [6, 7]. Here, we describe an analogous case $k = 7$.

So, we put in (4) $k = 7$. The parameters of cubature formula (4) are the weights A_0, B_0, A_i, B_i and the coordinates of the nodes a_{ij}, b_{ij}. With account taken of the constraint equations

$$a_i^2 + b_i^2 = 1, \quad c_i^2 + d_i^2 + e_i^2 = 1,$$

it is easy to see that the nodes a_{0j} and b_{0j} have one free parameter each (their weights A_0 and B_0), the nodes a_{ij} – two free parameters each, and the nodes b_{ij}

– three free parameters each. As a result, for one free parameter, we have: 2 nodes a_{0j}, 7 nodes a_{ij}, $28/3$ nodes b_{ij}, 14 nodes b_{0j}.

Denote the total number of basis polynomials of degree at most n by m. Since the total number of free parameters in a cubature formula of order n must be m, for obtaining a formula with minimal number of nodes N for given n, it is the most economic to use first the nodes a_{0j}, then – a_{ij}, and only in the last place, the nodes b_{ij} and b_{0j}.

However, one essential restriction is available here. The matter is in the fact that the basis polynomials of degree $n \geq 14$ contain the polynomials of the form $u^i v^{2j} w^l$ with $j \geq 1$. These polynomials are equal to zero at the nodes a_{0j} and a_{ij}, but the integral $U(u^i v^{2j}) > 0$. Therefore, correct integration of these polynomials is possible only in the case when the nodes b_{0j} and b_{ij} are used. For a cubature formula of order n, the number of basis functions that require to use the nodes b_{0j} and b_{ij} is the value m_0 which is equal to the total number of basis functions m for a cubature of order $n - 14$. Thus, for value M in (4), the condition $3M \geq m_0$ must perform when $B_0 = 0$, and the condition $3M + 1 \geq m_0$ must perform when $B_0 > 0$.

Then, we take the value L в (4) in such a way that the total number of free parameters of the cubature formula is equal to m. Here, if it is necessary, we can put $A_0 = 0$ or $B_0 = 0$.

After this, we substitute m basis functions for f in formula (4) and solve the system of m nonlinear algebraic equations for m unknown free parameters of the cubature formula. In analogy with the groups D_{3d} and D_{5d} (see [6, 7]), here we can not be sure that the system of nonlinear equations is solvable. Moreover, we can not be sure that all the weights of the cubature formula are positive. Therefore, as a rule, we need perform a number of attempts with different sets of parameters of the cubature formula to get for given n the formula with minimal N and with positive weights. As it was written in section 2, if we have several such formulas with equal N, then the formula with minimal quantity E_{n+1} is regarded as the best of them.

Let us now give a summary table containing the main characteristics of the best cubature formulas within the framework of all dihedral groups of rotations with inversion D_k ($k \geq 2$) to date up to the 35th accuracy order.

n	N	η	E_{n+1}	G	L	n	N	η	E_{n+1}	G	L
1	2	0.6667	2.2361	$D_{\infty h}$	[13]	19	132	1.0101	1.8019	D_{2h}	[5]
3	6	0.8889	2.2913	O_h	[13]	21	158	1.0211	1.7500	D_{3d}	[7]
5	12	1.0000	2.3917	Y_h	[13]	23	190	1.0105	1.6144	D_{2h}	[5]
7	22	0.9697	2.1112	D_{5d}	[2]	25	222	1.0150	1.7239	D_{2h}	[5]
9	32	1.0417	2.2441	Y_h	[14]	27	258	1.0129	1.5206	D_{3d}	[7]
11	48	1.0000	1.9700	T_h	[15]	29	296	1.0135	1.4910	D_{2h}	[5]
13	64	1.0208	1.9977	D_{2h}	[5]	31	336	1.0159	1.4782	D_{2h}	[5]
15	84	1.0159	2.0117	T_h	[15]	33	380	1.0140	1.3583	D_{3d}	[7]
17	104	1.0385	1.9269	D_{3d}	[7]	35	424	1.0189	1.6075	D_{2h}	[5]

Here $\eta = (n+1)^2/(3N)$ is the so called efficiency coefficient [16], G is the symmetry group of the cubature formula, L is a reference to the original source. The names of symmetry groups were taken from [10].

The table shows that the best cubature formulas have $\eta < 1$ for $n = 1$, 3, 7; they have $\eta = 1$ for $n = 5$, 11; and they have $\eta > 1$ for other n. We can also notice that, in principle, as n grows, the quantity E_{n+1} weakly decreases for the best cubature formulas while remaining a quantity of order 1. The analogous situation also holds for other symmetry groups (see, for example, [8]).

We note that all cubature formulas given in this table (excepting $n = 11$, 19) are the best to date not only for the dihedral groups with inversion but also for all symmetry groups.

Let us give the parameters of the best cubature formula for $n = 17$. This formula has lesser quantity E_{n+1} in comparison with analogous formula from [2].

The cubature formula $n = 17$, $N = 104$, group D_{3d}. Thus, we put in (4) $k = 3$, $L = 7$, $M = 5$, $B_0 = 0$,

$A_0 = +0.9342573892324555E-2,$

$A_1 = +0.8762068908226539E-2,$ $A_2 = +0.8855993970587790E-2,$

$A_3 = +0.9402668447457946E-2,$ $A_4 = +0.9486978920795083E-2,$

$A_5 = +0.9490118031206573E-2,$ $A_6 = +0.1015111348140314E-1,$

$A_7 = +0.1035117203236427E-1,$ $B_1 = +0.8629021193920530E-2,$

$B_2 = +0.9697570733637392E-2,$ $B_3 = +0.9830473398652804E-2,$

$B_4 = +0.1003707532918216E-1,$ $B_5 = +0.1033204013319902E-1,$

$a_1 = +0.6447995692562899E+0,$ $b_1 = +0.7643516962020187E+0,$

$a_2 = +0.3496613824025354E+0,$ $b_2 = -0.9368761485150254E+0,$

$a_3 = +0.3700255991533820E+0,$ $b_3 = +0.9290215583995781E+0,$

$a_4 = +0.8998157520076080E+0,$ $b_4 = +0.4362701140795492E+0,$

$a_5 = +0.7634062452930442E+0,$ $b_5 = -0.6459186517260331E+0,$

$a_6 = +0.9552419487254085E+0,$ $b_6 = -0.2958256570943162E+0,$

$a_7 = +0.9970600721887599E+0,$ $b_7 = +0.7662383732850336E-1,$

$c_1 = +0.2667352251743902E+0,$ $d_1 = +0.7524694835340987E+0,$

$c_2 = +0.3027438514086927E+0,$ $d_2 = +0.8288535933119254E+0,$

$c_3 = +0.2341522729013902E+0,$ $d_3 = +0.5539667298995539E+0,$

$c_4 = +0.3311052409749708E+0,$ $d_4 = +0.9064290885886043E+0,$

$c_5 = +0.3394158177994734E+0,$ $d_5 = +0.9344847952285059E+0,$

$e_1 = +0.6021976386545318E+0,$ $e_2 = -0.4704762281860166E+0,$

$e_3 = -0.7989327726783447E+0,$ $e_4 = +0.2622129416320609E+0,$

$e_5 = -0.1074014437251755E+0.$

The calculation of the parameters of this cubature formula was carried out with the use of high-precision arithmetic (more than 30 decimal digits in the mantissa) on the computers of the Siberian Supercomputer Center. The systems of nonlinear algebraic equations were solved by a Newton-type method.

4. Conclusion

We have presented an algorithm for finding the best cubature formulas on the sphere that are invariant under the transformations of the dihedral groups of rotations with inversion D_{kh} for even k and D_{kd} for odd k. The cases $k \geq 2$ were investigated. The case $k = 1$ was not treated because it is more natural to treat this special case of the group D_{1d} as the case of the cyclic group C_{2h} (see, for example, [10]). Computations by this algorithm were carried out with the aim to find the parameters of all the best cubature formulas of the given symmetry type up to the 35th accuracy order n. The parameters of new cubature formula of the group D_{3d} for $n = 17$ were given with 16 significant digits. The numerical method used in the article does not guarantee that all possible solutions have been found to the system of nonlinear equations from which the parameters of the cubature formula are determined. Therefore, it is not impossible that the results obtained in the article can be improved for some n.

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