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CUBATURE FORMULAS ON THE SPHERE THAT ARE INVARIANT UNDER THE TRANSFORMATIONS OF THE DIHEDRAL GROUP OF ROTATIONS $\mathbf{D_4}$

A.S. POPOV

Abstract. An algorithm for finding the best cubature formulas (in a sense) on the sphere that are invariant under the transformations of the dihedral group of rotations D_4 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 invariant under the transformations of various dihedral groups of symmetries were considered in [1–7]. In particular, in [3], we proposed an algorithm for constructing the best cubatures (in a sense) on the sphere 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] — with respect to the group D_{5d}, and in [7] — with respect to the group D_{3d}. All cubatures invariant under these groups have central symmetry and hence are accurate for all odd functions.

In the present article, we describe an analogous algorithm for constructing the best cubatures invariant under the general dihedral group of rotations D_4. We carry out computations by this algorithm with the purpose of finding the parameters of all the best cubatures of this symmetry group up to 35th order of accuracy n. We give the parameters of new cubatures with 16 significant digits for $n = 10, 12$.

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2. An Algorithm for Finding the Best Cubatures of the Group D_4

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, 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), construct a numerical cubature formula invariant under the transformation of the group D_4 in the form

$$V(f) = A_0 \sum_{j=1}^{2} f(a_{0j}) + B_0 \sum_{j=1}^{4} f(b_{0j}) + C_0 \sum_{j=1}^{4} f(c_{0j}) + \sum_{i=1}^{M} A_i \sum_{j=1}^{8} f(a_{ij}), \tag{2}$$

where the 2 points a_{0j} lie at the poles of the dihedron (bipyramid) inscribed in the sphere and have coordinates $(0, 0, \pm 1)$; the 4 points b_{0j} lie at the vertices of the base of the dihedron with coordinates $(\pm 1, 0, 0)$, $(0, \pm 1, 0)$; the 4 points c_{0j} correspond to the midpoints of the base of the dihedron with coordinates $(\pm 1/\sqrt{2}, \pm 1/\sqrt{2}, 0)$; the 8 points a_{ij} correspond to points of general position on the lateral faces of the dihedron with coordinates (a_i, b_i, c_i), $(a_i, -b_i, -c_i)$, $(-a_i, b_i, -c_i)$, $(-a_i, -b_i, c_i)$, $(b_i, a_i, -c_i)$, $(b_i, -a_i, c_i)$, $(-b_i, a_i, c_i)$, $(-b_i, -a_i, -c_i)$.

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 squares, lie in the equator plane $z = 0$ (see, for example, [8]). Our dihedron is taken to itself under rotations by an angle that is a multiple of $\pi/2$ around the fourth-order axis z. These rotations constitute a cyclic symmetry group C_4. 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 edges of the dihedron [8]. The family of all these transformations forms a symmetry group called the group D_4 [9, Chapter 12]. This group contains 8 elements: 4 rotations around the fourth order axis z and 4 rotations around the second-order horizontal axes. In (2), one of the second-order axes coincides with the axis x; therefore, the cubature is invariant under the change of the point (x, y, z) by $(x, -y, -z)$.

Denote the total number of the nodes in the cubature formula (2) by N.

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 a given k; δ_{kl} is the Kronecker symbol.

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 [10])

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

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 this cubature of order n to the cubature of order $n + 1$.

In the present article, we attempt at constructing all the best cubature formulas of the form (2) on the sphere for $n \leq 35$. Moreover, as the best among all cubature formulas of this form having a given order n, we regard cubatures satisfying the following four conditions (see [10]): (1) the nodes belong to the integration domain; (2) the weights are positive; (3) the number of the nodes is minimal; (4) the quantity E_{n+1} is minimal.

In application to our case, Theorem 1 in [11] sounds as follows:

Theorem 1. *For cubature (2) to have order n, it is necessary and sufficient that it be accurate for all polynomials of degree at most n invariant under the group D_4.*

It is known (see, for instance, [11]) that every polynomial invariant under the cyclic group C_k is representable on the unit sphere as a polynomial of the basis invariant forms $z = \cos\theta$, $p = \sin^k\theta\cos k\varphi$, and $q = \sin^k\theta\sin k\varphi$, where θ and φ are the angular coordinates of the spherical coordinate system.

In the case of the dihedral group D_k, to the invariant transformations of the group C_k, the requirement of invariance under the replacement of the point (x, y, z) by the point $(x, -y, -z)$. Obviously, after such replacement, the basis form p does not change, and the basis forms z and q change sign. Consequently, z^2, p, and zq are invariant forms for D_k.

Thus, every polynomial invariant under D_4 is representable on the unit sphere as a polynomial of the basis invariant forms

$$u = \sin^2\theta = x^2 + y^2, \quad v = \sin^4\theta\cos 4\varphi = (x^4 - 6x^2y^2 + y^4),$$
$$w = \cos\theta\sin^4\theta\sin 4\varphi = 4(x^2 - y^2)xyz,$$

which are polynomials of degrees 2, 4, and 5 respectively. Here $x = \sin\theta\cos\varphi$, $y = \sin\theta\sin\varphi$, $z = \cos\theta$.

Note that $u = v = w = 0$ at the nodes a_{0j}; $u = v = 1$, $w = 0$ at the nodes b_{0j}; $u = 1$, $v = -1$, $w = 0$ at the nodes c_{0j} .

Write down all the polynomials constituting the basis in the space of polynomials invariant under D_4 up to degree 12:

$$1, u, u^2, v, w, u^3, uv, uw, u^4, u^2v, v^2, u^2w, vw, u^5, u^3v, uv^2, u^3w, uvw, u^6, u^4v, u^2v^2, v^3.$$

Since $w^2 = (1 - u)(u^4 - v^2)$, the polynomials w occur in the basis at most in degree 1.

The parameters of cubature (2) are the weights A_0, B_0, C_0, A_i and the coordinates of the nodes a_{ij}. With account taken of the constraint equations $a_i^2 + b_i^2 + c_i^2 = 1$, it is easy to see that the nodes a_{0j}, b_{0j}, and c_{0j} have one free parameter each (their weights A_0, B_0, and C_0), and the nodes a_{ij} — three free parameters each. As a result, for one free parameter, we have: 2 nodes a_{0j}, 4 nodes b_{0j} or c_{0j}, $8/3$ nodes a_{ij}.

Denote the total number of basis polynomials of degree at most n by m. Since the total number of free parameters in a cubature of order n must be m, for obtaining a formula with the 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_{0j} and c_{0j}.

Three cases are possible:

(1) $m = 3M$, put $A_0 = B_0 = C_0 = 0$ in (2);

(2) $m = 3M + 1$, put $B_0 = C_0 = 0$;

(3) $m = 3M + 2$, put $C_0 = 0$.

In considering these cases, we departured from the conjecture that such parametrizations lead to solvable systems of nonlinear equations and, as a result, give cubatures with positive weights and nodes lying on the sphere. Our experience of practical computations speaks in favor of this conjecture (see the next section).

By analogy with [2–7], in implementing practical computations with the purpose of finding the parameters of concrete cubatures, it is more convenient to use not the parameters a_i, b_i, c_i but the parameters u_i, v_i, w_i, which are equal to the value of the functions u, v, w at the nodes a_{ij} respectively. The equations

$$w_i^2 = (1 - u_i)(u_i^4 - v_i^2),$$

of te constraints imposed on the parameters of each of the M groups of points a_{ij} will not be solved explicitly but added to the initial system of m equations that arise after substituting all the basic functions for f in (2). Thus, in total, we will have $m + M$ equations defining the parameters of our cubature. Solving this system, we obtain M sets of parameters u_i, v_i, w_i. For finding the parameters a_i, b_i, c_i through the found quantities u_i, v_i, w_i, we can use the following algorithm:

1. Let $x_i \geq y_i \geq 0$ be the roots of the quadratic equation

$$x^2 - u_i x + (u_i^2 - v_i)/8 = 0.$$

2. If $w_i \geq 0$ then we put $a_i = \sqrt{x_i}$, $b_i = \sqrt{y_i}$; otherwise, $a_i = \sqrt{y_i}$, $b_i = \sqrt{x_i}$.
3. Put $c_i = \sqrt{1 - u_i}$.

Since the group D_4 is a subgroup of the previously studied dihedral group of rotations D_{4h} [4] and also a subgroup in the octahedral group of rotations O [10] and the octahedral group of rotations with inversion O_h [12], we infer that, for some n, the best cubatures of the group D_4 may coincide with the best cubatures of the groups D_{4h}, O, or O_h.

3. Construction of Concrete Cubatures of the Group D_4

Applying the above-described algorithm to searching for the best cubatures of different accuracy orders $n \leq 35$, we find that, for all odd $n \geq 3$ and also for even $n = 6k + 2$ ($k = 1, 2, \dots$), the best cubatures of the group D_4 either coincide with the best cubatures of the groups D_{4h}, O, or O_h, or have the same number of nodes with them but lesser E_{n+1}. And for all even $n = 6k, 6k - 2$, the best cubatures of D_4 contain less nodes compared to the best cubatures of the above-mentioned groups of greater symmetry.

Let us give parameters of these cubatures for $n = 4$, 6, 10, 12.

The cubature $n = 4$, $N = 10$, $M = 1$, $A_0 = 1/12$, $B_0 = C_0 = 0$, $A_1 = 5/48$, $a_1^2 = (2 + \sqrt{2})/5$, $b_1^2 = (2 - \sqrt{2})/5$, $c_1^2 = 1/5$.

This formula has symmetry of the group D_{4d} (see [9]) and was first obtained in [13].

The cubature $n = 6$, $N = 18$, $M = 2$, $A_0 = 2/45$, $B_0 = C_0 = 0$,

$$\begin{aligned} A_1 &= (410 - \sqrt{30})/7200, & A_2 &= (410 + \sqrt{30})/7200, \\ a_1^2 &= (2 + \sqrt{2})(18 + \sqrt{30})/98, & a_2^2 &= (2 - \sqrt{2})(18 - \sqrt{30})/98, \\ b_1^2 &= (2 - \sqrt{2})(18 + \sqrt{30})/98, & b_2^2 &= (2 + \sqrt{2})(18 - \sqrt{30})/98, \\ c_1^2 &= (13 - 2\sqrt{30})/49, & c_2^2 &= (13 + 2\sqrt{30})/49. \end{aligned}$$

This formula also has symmetry of the group D_{4d} and was first obtained in [2].

The calculation of the parameters of the best cubatures for $n \geq 10$ was carried out with the use of high-precision arithmetic (more than 30 decimal digits in the mantisse) on the computers of the Siberian Supercomputer Center. The systems of nonlinear algebraic equations were solved by a Newton-type numerical method similar to [7].

The cubature $n = 10$, $N = 42$, $M = 5$, $B_0 = C_0 = 0$,

$$
\begin{aligned}
A_0 &= 0.1707368048833795E-1, & & \\
A_1 &= 0.2208270226198964E-1, & a_1 &= 0.9635859193619932E+0, \\
A_2 &= 0.2366264992934368E-1, & a_2 &= 0.4190127133746219E+0, \\
A_3 &= 0.2432888483971895E-1, & a_3 &= 0.7249667564133890E+0, \\
A_4 &= 0.2528591841740224E-1, & a_4 &= 0.1947604331832231E+0, \\
A_5 &= 0.2537142442946100E-1, & a_5 &= 0.4943310656026484E+0, \\
b_1 &= 0.7710698688737620E-1, & c_1 &= 0.2560404041952213E+0, \\
b_2 &= 0.2205903040844950E+0, & c_2 &= 0.8807770795010205E+0, \\
b_3 &= 0.4797191177902702E+0, & c_3 &= 0.4942598204608329E+0, \\
b_4 &= 0.7213078384591524E+0, & c_4 &= 0.6646678688214653E+0, \\
b_5 &= 0.8583324505779122E+0, & c_5 &= 0.1374852787212724E+0.
\end{aligned}
$$

The cuubature $n = 12$, $N = 58$, $M = 7$, $B_0 = C_0 = 0$,

$$
\begin{aligned}
A_0 &= 0.1080668094738448E-1, & & \\
A_1 &= 0.1534631500768976E-1, & a_1 &= 0.9752107546726020E+0, \\
A_2 &= 0.1647228010740910E-1, & a_2 &= 0.2013757821457838E+0, \\
A_3 &= 0.1768832068955872E-1, & a_3 &= 0.8091166365336792E+0, \\
A_4 &= 0.1795325045042185E-1, & a_4 &= 0.4297100226541010E+0, \\
A_5 &= 0.1808174912167061E-1, & a_5 &= 0.1062559919703926E+0, \\
A_6 &= 0.1816125836101417E-1, & a_6 &= 0.5718669807444403E+0, \\
A_7 &= 0.1859515602538967E-1, & a_7 &= 0.6340476258553069E+0, \\
b_1 &= 0.2151032513600321E+0, & c_1 &= 0.5190929806149267E-1, \\
b_2 &= 0.3342269401944399E+0, & c_2 &= 0.9207280525830828E+0, \\
b_3 &= 0.4314221777519450E+0, & c_3 &= 0.3990052293243727E+0, \\
b_4 &= 0.6283022507470571E+0, & c_4 &= 0.6485256958184419E+0, \\
b_5 &= 0.8990890828883328E+0, & c_5 &= 0.4246745638738026E+0, \\
b_6 &= 0.8010558027685969E+0, & c_6 &= 0.1768551870457772E+0, \\
b_7 &= 0.1383990010901307E+0, & c_7 &= 0.7608083363400422E+0.
\end{aligned}
$$

Let us now give a summary table containing the main characteristics of the best cubatures of the group D_4 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	$D_{\infty h}$	[14]	19	134	0.9950	1.1542	O	[17]
3	6	0.8889	2.2913	O_h	[14]	20	150	0.9800	0.5903	O	[18]
4	10	0.8333	1.7550	D_{4d}	[13]	21	162	0.9959	0.9850	D_4	
5	14	0.8571	1.8696	O_h	[15]	22	178	0.9906	0.8271	D_4	
6	18	0.9074	1.8033	D_{4d}	[2]	23	192	1.0000	1.2936	O	[17]
7	22	0.9697	2.1197	D_{4h}	[13]	24	210	0.9921	0.9418	D_4	
8	30	0.9000	1.7299	O	[16]	25	226	0.9971	1.0524	D_4	
9	34	0.9804	2.0546	D_{4h}	[4]	26	246	0.9878	0.6234	O	[10]
10	42	0.9603	1.7392	D_4		27	262	0.9975	0.8524	D_4	
11	48	1.0000	1.6928	O	[17]	28	282	0.9941	0.7105	D_4	
12	58	0.9713	1.7165	D_4		29	302	0.9934	0.7301	D_4	
13	66	0.9899	1.9098	D_{4h}	[4]	30	322	0.9948	0.6672	D_4	
14	78	0.9615	1.6954	O	[18]	31	342	0.9981	0.4297	O	[10]
15	86	0.9922	1.7104	O_h	[19]	32	366	0.9918	0.3121	O	[10]
16	98	0.9830	1.6605	D_4		33	386	0.9983	0.5511	D_4	
17	110	0.9818	1.4290	D_4		34	410	0.9959	0.4788	D_4	
18	122	0.9863	1.2664	D_4		35	432	1.0000	0.7666	O	[10]

Here $\eta = (n+1)^2/(3N)$ is the so called effectivity coefficient (see, for example, [16, 19]), G is the symmetry group of the cubature, L is a reference to the original source.

The table shows that, for all n, the best cubatures of the group D_4 have $\eta \leq 1$ and $\eta = 1$ for $n = 12k - 1$, $k = 1, 2, \dots$. It also demonstrates that, in principle, $\eta \to 1$ as n grows. We can also notice that, in principle, as n grows, the quantity E_{n+1} weakly decreases for the best cubatures while remaining a quantity of order 1. The analogous situation also holds for other symmetry groups (see, for example, [6, 7]).

Note that the cubatures for n = 1, 3, 4, 6, 10, 11, 12, 16, 18, 22, 24, 28, 30, 34 given in this table are the best to date not only for the group D_4 but also for all the symmetry groups.

4. Conclusion

We have presented an algorithm for finding the best cubature formulas for the sphere invariant under the general dihedral group of rotations D_4. Computations by this algorithm are carried out with the aim to find the parameters of all the best cubatures of the given symmetry kind up to the 35th accuracy order n. The parameters of new cubatures for n = 10, 12 are 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 are determined. Therefore, it is not impossible that the results obtained in the article can be improved for some n.

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Anatolii Stepanovich Popov
Institute of Computational Mathematics and Mathematical Geophysics SB RAS,
6, Akad. Lavrent'eva ave.,
Novosibirsk, 630090, Russia
Email address: popov@labchem.sscc.ru