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CUBATURE FORMULAS ON THE SPHERE THAT ARE INVARIANT UNDER THE CYCLIC ROTATION GROUPS $\mathbf{C_{kh}}$

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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 cyclic rotation groups C_{kh} is described. This algorithm is applied for finding the parameters of the best cubature formulas of 19th and 31st orders of accuracy.

Keywords: numerical integration, invariant cubature formulas, invariant polynomials, cyclic rotation group.

1 Introduction

Cubature formulas on the sphere that are invariant under various cyclic and dihedral groups of symmetry were considered in [1] – [9]. In particular, in [9], we described the general algorithm for constructing the best cubature formulas (in a sense) on the sphere that are invariant under the dihedral groups of rotations with inversion. All cubature formulas invariant under these groups possess central symmetry and hence are accurate for all odd functions.

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In the present article, we describe an analogous general algorithm for constructing the best cubature formulas invariant under the cyclic rotation groups C_{kh}. We apply this algorithm for finding parameters of the best cubature formulas of 19th and 31st orders of accuracy. The parameters of these cubature formulas are given with 16 significant digits.

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 [10])

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

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 the best cubature formulas on the sphere that are invariant under the transformations of the cyclic rotation groups C_{kh}. 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 [10]):

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 of the group C_{kh} are of the form

$$V(f) = A_0 \sum_{j=1}^{2} f(a_{0j}) + \sum_{i=1}^{L} A_i \sum_{j=1}^{k} f(a_{ij}) + \sum_{i=1}^{M} B_i \sum_{j=1}^{2k} f(b_{ij}), \qquad (3)$$

where 2 points a_{0j} lie at the poles of the rotation axis z and have coordinates $(0, 0, \pm 1)$; k points a_{ij} lie in the equator plane $z = 0$ and are generated by the point $(a_i, b_i, 0)$ of the group C_k; $2k$ points b_{ij} are the points of general position of the group C_{kh} and are generated by the points $(c_i, d_i, \pm e_i)$ 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 $u = \cos(2\pi/k)$, $v = \sin(2\pi/k)$, $l = 1, 2, \ldots, k-1$.

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

Theorem 1. *For cubature formula (3) 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 C_{kh}.*

It is well known (see, for instance, [8]) that every polynomial invariant under the cyclic group C_{kh} is representable on the unit sphere as a polynomial of basis invariant forms

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

where θ and φ are the angular coordinates of the spherical coordinate system. The form u has degree 2, the forms v and w have degree k. Since $u^k = v^2 + w^2$, the polynomial w occur in the basis at most in degree 1. For the group C_{kh}, the basis polynomials are of the form $u^i v^j w^l$ where $i, j = 0, 1, \ldots;\ l = 0, 1;$ $2i + kj + kl \le n$. Note that $u = v = w = 0$ at the nodes a_{0j}; $u = 1$ at the nodes a_{ij}.

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 cyclic groups C_{kh}, we keep the following rules.

The parameters of cubature formula (3) are the weights A_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} have one free parameter (the weight A_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}, $k/2$ nodes a_{ij}, $2k/3$ nodes b_{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 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, as a rule, to use first the nodes a_{0j} and a_{ij}, and only in the last place, the nodes b_{ij}.

However, two essential restrictions are available here. The first restriction is quite analogous to corresponding restrictions for the groups D_{kh} and D_{kd} (see [9]). The matter is in the fact that the basis polynomials of degree $n \geq 2$ contain the polynomials of the form $(1-u)^i v^j w^l$ with $i \geq 1$. These polynomials are equal to zero at the nodes a_{ij}, but the integral $U((1-u)^i) > 0$. Therefore, correct integration of these polynomials is possible only in the case when the nodes a_{0j} and b_{ij} are used. For a cubature formula of order n, the number of basis functions that require to use the nodes a_{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 $n-2$. Thus, for value M in (3), the condition $3M \geq m_0$ must perform when $A_0 = 0$, and the condition $3M + 1 \geq m_0$ must perform when $A_0 > 0$.

The second restriction is specific for cyclic groups C_k. The matter is in the fact that we should fix the net of nodes relatively to the rotations around the axis z. Thus, we have in cubature formula (3) $2L + 3M - 1$ free parameters when $A_0 = 0$ and $2L + 3M$ free parameters when $A_0 > 0$. As a result, the condition $3M - 1 \geq m_0$ must perform when $A_0 = 0$, and the condition $3M \geq m_0$ must perform when $A_0 > 0$.

Then, we take the value L in (3) by 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 $A_0 = 0$.

After this, we substitute m basis functions for f in formula (3) 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 above, 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.

3 Construction of the concrete best cubature formulas

Cubature formulas of the form (3) are of special interest in the case when the value k is even. In this case, the formula is invariant to operation of inversion when the point (x, y, z) is changed to point $(-x, -y, -z)$. Hence, such formula is accurate for all odd functions. Let us construct two specific formulas invariant under the group C_{4h}.

The cubature formula $n = 19$, $N = 130$. Here $k = 4$, $m = 50$, $m_0 = 41$. Thus, we put in (3) $A_0 > 0$, $L = 4$, $M = 14$. Solving the system of nonlinear equations numerically, we get $A_0 = 0.7660304343888119E-2$,

Таблица 1. Parameters of cubature formula for $n = 19$.

i	w_i	x_i
1	$0.6645295553789985E-2$	$0.1000000000000000E+1$
2	$0.7940547602282251E-2$	$0.7904189241617745E+0$
3	$0.7972378890136528E-2$	$0.9448501758339844E+0$
4	$0.8573377575291844E-2$	$0.5355707815845251E+0$
5	$0.6510520973163796E-2$	$0.4569317630202860E+0$
6	$0.7136235937493791E-2$	$0.6768475178116094E+0$
7	$0.7255717442273412E-2$	$0.2550834114536487E-1$
8	$0.7281549870918769E-2$	$0.3801363982928767E+0$
9	$0.7584573244599878E-2$	$0.2316546737838826E+0$
10	$0.7604391975980193E-2$	$0.9565112919395244E+0$
11	$0.7710938137623127E-2$	$0.2550707877707171E+0$
12	$0.7815627698858543E-2$	$0.3406958784534529E+0$
13	$0.7816964422838738E-2$	$0.1265273973753093E+0$
14	$0.7978327624980708E-2$	$0.6587478998720094E-1$
15	$0.8003983653837969E-2$	$0.8545200203022775E+0$
16	$0.8082139286016494E-2$	$0.5560935780500953E+0$
17	$0.8234836915868764E-2$	$0.8008040968867047E+0$
18	$0.8503316918823482E-2$	$0.6372961542422668E+0$
i	y_i	z_i
1	$0.0000000000000000E+0$	$0.0000000000000000E+0$
2	$0.6125666692915498E+0$	$0.0000000000000000E+0$
3	$0.3275028934627734E+0$	$0.0000000000000000E+0$
4	$0.8444903421075583E+0$	$0.0000000000000000E+0$
5	$0.8205661456207424E+0$	$0.3433432169190062E+0$
6	$0.6780381392043270E+0$	$0.2866037672756531E+0$
7	$0.4221549660163514E+0$	$0.9061647252016296E+0$
8	$0.7091057139942805E+0$	$0.5938563842155619E+0$
9	$0.2001058495398148E+0$	$0.9519946224081478E+0$
10	$0.1057784060118048E+0$	$0.2718401685067600E+0$
11	$0.9516217161691417E+0$	$0.1713330164951382E+0$
12	$0.4854220420066139E+0$	$0.8051656721066536E+0$
13	$0.8755565979006869E+0$	$0.4662525727392884E+0$
14	$0.6833847676185643E+0$	$0.7270803060398921E+0$
15	$0.4187154839704564E+0$	$0.3073644065046921E+0$
16	$0.2551482270805925E+0$	$0.7909862923395531E+0$
17	$0.2057535931812009E+0$	$0.5624751170518516E+0$
18	$0.5134609294410294E+0$	$0.5746403098683307E+0$

other parameters are given in the table 1. The value $E_{n+1} = E_{20} = 1.836$ here.

Note that we apply in our tables the successive numeration of the nodes a_{ij} and b_{ij}, that is, in the first place, parameters of L nodes a_{ij} are given, and then, parameters of M nodes b_{ij} are given. For instance, in the table 1, we have $A_1 = w_1$, $a_1 = x_1$, $b_1 = y_1$, $B_1 = w_5$, $c_1 = x_5$, $d_1 = y_5$, $e_1 = z_5$, and so on.

The cubature formula $n = 31$, $N = 334$. Here $k = 4$, $m = 128$, $m_0 = 113$. Thus, we put in (3) $A_0 > 0$, $L = 7$, $M = 38$. Solving the system of nonlinear

Таблица 2. Parameters of cubature formula for $n = 31$.

i	w_i	x_i
1	$0.2857339278630283E-2$	$0.1000000000000000E+1$
2	$0.2873537417366394E-2$	$0.8793751898836127E+0$
3	$0.2925017946201064E-2$	$0.9636862144257188E+0$
4	$0.3063663254389160E-2$	$0.2293385666097021E+0$
5	$0.3230945413086455E-2$	$0.7663501491578905E+0$
6	$0.3240268313587605E-2$	$0.4337949015455863E+0$
7	$0.3295024947194438E-2$	$0.6150137924079744E+0$
8	$0.2481078352389441E-2$	$0.9287280945604399E+0$
9	$0.2544339109601428E-2$	$0.8020041742158256E+0$
10	$0.2680646437944871E-2$	$0.9145470748022536E+0$
11	$0.2695623016780501E-2$	$0.5109491471577080E+0$
12	$0.2707778655827009E-2$	$0.8897630855513612E+0$
13	$0.2739392220982742E-2$	$0.1033741140760991E+0$
14	$0.2875113563849260E-2$	$0.1146664694579942E+0$
15	$0.2881836718777421E-2$	$0.8006152334270228E+0$
16	$0.2898792068067391E-2$	$0.9820285897118167E+0$
17	$0.2912246071018620E-2$	$0.2438037712016351E+0$
18	$0.2922320956053537E-2$	$0.6942640490970199E+0$
19	$0.2927474138016341E-2$	$0.9540215911252631E+0$
20	$0.2937885924814594E-2$	$0.6710616805188693E+0$
21	$0.2937909913742207E-2$	$0.7026195834450003E+0$
22	$0.2947113171411905E-2$	$0.2703390775138423E+0$
23	$0.2961140394583733E-2$	$0.3787816208007406E+0$
24	$0.2980612397123625E-2$	$0.5506779631254267E+0$
25	$0.2985412263204448E-2$	$0.1077936400960356E+0$
26	$0.3005224475267694E-2$	$0.8249966809803215E-1$
27	$0.3006877310250035E-2$	$0.1326327383084290E+0$
28	$0.3013188531135578E-2$	$0.2696713895149357E+0$
29	$0.3022434440257125E-2$	$0.2668525422272480E+0$
30	$0.3022477703759273E-2$	$0.2707950862015674E-1$
31	$0.3080688499240702E-2$	$0.2302716240599156E+0$
32	$0.3090732982201134E-2$	$0.4135492675046034E+0$
33	$0.3095559039029059E-2$	$0.4166298304027775E+0$
34	$0.3098263332925083E-2$	$0.5731412043011793E+0$
35	$0.3099021810902918E-2$	$0.1858722590884954E+0$
36	$0.3122989485055384E-2$	$0.4266121527846227E+0$
37	$0.3125974147960563E-2$	$0.5683596527046579E+0$
38	$0.3136102663525452E-2$	$0.8149439620595171E+0$
39	$0.3143631563871559E-2$	$0.8364230149298469E+0$
40	$0.3170648697498085E-2$	$0.3222479827541115E+0$
41	$0.3207344069418187E-2$	$0.3872788409458259E+0$
42	$0.3224542526230039E-2$	$0.7140627661750236E+0$
43	$0.3261588091925836E-2$	$0.5655316727341512E+0$
44	$0.3273197293190835E-2$	$0.6819330515989615E+0$
45	$0.3274582129587377E-2$	$0.5153286715336740E+0$

equations, we get $A_0 = 0.3061270189405236E{-}2$, other parameters are given in the table 2. The value $E_{n+1} = E_{32} = 1.388$ here.

i	y_i	z_i
1	$0.0000000000000000E+0$	$0.0000000000000000E+0$
2	$0.4761294733758457E+0$	$0.0000000000000000E+0$
3	$0.2670372261049524E+0$	$0.0000000000000000E+0$
4	$0.9733467120535248E+0$	$0.0000000000000000E+0$
5	$0.6424231073721422E+0$	$0.0000000000000000E+0$
6	$0.9010116444270046E+0$	$0.0000000000000000E+0$
7	$0.7885163505901200E+0$	$0.0000000000000000E+0$
8	$0.2524388893035526E+0$	$0.2715487682559495E+0$
9	$0.3089789787357818E+0$	$0.5111959460322284E+0$
10	$0.3730640570039191E+0$	$0.1562909381327583E+0$
11	$0.3672637170039674E-1$	$0.8588260258285930E+0$
12	$0.1805783724560172E+0$	$0.4191814678528347E+0$
13	$0.4121951192800001E+0$	$0.9052121166780348E+0$
14	$0.6100073968834808E+0$	$0.7840552126792337E+0$
15	$0.1161314865069427E+0$	$0.5878169152434128E+0$
16	$0.1323010537879169E+0$	$0.1345967315919189E+0$
17	$0.2953903954441597E+0$	$0.9237446808654455E+0$
18	$0.2719386529720772E+0$	$0.6663683659592064E+0$
19	$0.3032796901739156E-1$	$0.2981996277028217E+0$
20	$0.7477446138978959E-1$	$0.7376211770706274E+0$
21	$0.4609008916506171E+0$	$0.5421218396589832E+0$
22	$0.1051450093988163E-1$	$0.9627077585845821E+0$
23	$0.1640330898865588E+0$	$0.9108334804813842E+0$
24	$0.2288260302019346E+0$	$0.8027405738033020E+0$
25	$0.9810609694786695E+0$	$0.1609344752388981E+0$
26	$0.7630327821974979E+0$	$0.6410731456360189E+0$
27	$0.1428626447935778E+0$	$0.9808153860188939E+0$
28	$0.6816402489012675E+0$	$0.6801793239689824E+0$
29	$0.4992458501266768E+0$	$0.8243441646776828E+0$
30	$0.8807090467283320E+0$	$0.4728829402968177E+0$
31	$0.8244043743811370E+0$	$0.5170419776517715E+0$
32	$0.7299735423231610E+0$	$0.5441650768421126E+0$
33	$0.3704449059040935E+0$	$0.8301747744350343E+0$
34	$0.4270814928179717E+0$	$0.6993643960229650E+0$
35	$0.9214461315996310E+0$	$0.3411576319847099E+0$
36	$0.5635730017497922E+0$	$0.7073807622456229E+0$
37	$0.6057391472681832E+0$	$0.5568189927115049E+0$
38	$0.5466231217372238E+0$	$0.1925344163649413E+0$
39	$0.4159332637279392E+0$	$0.3569258469490403E+0$
40	$0.9289682155940478E+0$	$0.1821381125050895E+0$
41	$0.8451916845516509E+0$	$0.3683288146756921E+0$
42	$0.5872369596127509E+0$	$0.3811392386349718E+0$
43	$0.7318359583055115E+0$	$0.3802499931171156E+0$
44	$0.7051391216796678E+0$	$0.1942836385642256E+0$
45	$0.8352707436040760E+0$	$0.1917267461113150E+0$

The calculation of parameters of all cubature formulas 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 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 cyclic rotation groups C_{kh}. Computations by this algorithm were carried out with the aim to find the parameters of the best cubature formulas of 19th and 31st orders of accuracy n. The parameters of these cubature formulas were given with 16 significant digits. We note that both new formulas contain lesser number of nodes in comparison with any other known today formulas for respective n.

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 possible that the results obtained in the article can be improved by the value E_{n+1} for some n.

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