JOURNAL OF COMPUTATIONAL PHYSICS **59**, 167–175 (1985)

Note

Efficient Integration on the Hypersphere

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Received October 25, 1983; revised April 10, 1984

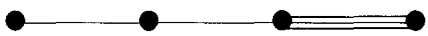
1. INTRODUCTION

Various applications require the integration of functions on spherical surfaces in Euclidean 4-space. The concept of spherical t-designs confers an advantage for the solution of that class of numerical problems. By definition, all points of a t-design are equally weighted. Furthermore, suitably chosen spherical designs possess an automorphism group acting transitively on the points. The most interesting group in this context is I_4, the hypericosahedral group of order 14,400. It allows the construction of a unique 19-design containing 3600 integration points furnishing the exact integration of hyperspherical harmonics up to 19th order, while 20th order harmonics are integrated with minimized errors.

2. THE 600-CELL AND ITS AUTOMORPHISM GROUP

Cubature formulas invariant under finite rotation groups have been considered by Sobolev [9], while the special case of the hypericosahedral group was discussed by Salihov [8]. In connection with the theory of spherical designs invented by Delsarte *et al.* [4], powerful integration formulas can be found. Examples are the 9-designs in $\mathbb{R}^3$ and 19-designs in $\mathbb{R}^4$ given by Goethals *et al.* [5]. The unique optimal 9-orbit for any 3-dimensional orthogonal group was constructed by Neutsch [7].

The largest finite orthogonal group in 4-dimensional Euclidean space is the hypericosahedral group I_4, which can be defined as the automorphism group of the regular 600-cell (cf. Coxeter [2]). To this end we consider the root system of Coxeter type H_4:

 (1)

It has 120 members. In a suitable coordinate frame (x, y, z, t) these are

$$(0, 0, 0, 1), \qquad \tfrac{1}{2}(1, 1, 1, 1), \qquad \tfrac{1}{2}(1, \lambda, \lambda', 0) \tag{2}$$

0021-9991/85 $3.00

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and all even coordinate permutations and sign reversals, where

$$\lambda = \tfrac{1}{2}(-1+\sqrt{5}) \tag{3}$$

and

$$\lambda' = \tfrac{1}{2}(-1-\sqrt{5}). \tag{4}$$

They are the 120 vertices of a regular 600-cell.

3. Invariant Polynomials under the Hypericosahedral Group

The degrees of the I_4-invariant polynomials can be calculated with the help of the Molien series

$$M(I_4, \varepsilon) = |I_4|^{-1} \sum_{\mu \in I_4} |\det(1-\varepsilon\mu)|^{-1} \tag{5}$$

which reduces to

$$M(I_4, \varepsilon) = [(1-\varepsilon^2)(1-\varepsilon^{12})(1-\varepsilon^{20})(1-\varepsilon^{30})]^{-1} \tag{6}$$

(Coxeter and Moser [3]). Hence there is a set of four basic invariant polynomials $P_2, P_{12}, P_{20}, P_{30}$ of degrees 2, 12, 20, and 30. The natural choice for P_2 is

$$P_2 = x^2 + y^2 + z^2 + t^2 = \tfrac{1}{3}\langle 2, 0, 0, 0\rangle. \tag{7}$$

Here the symbol $\langle a, b, c, d\rangle$ denotes

$$\langle a, b, c, d\rangle = x^a y^b z^c t^d + \text{all even permutations of the exponents.} \tag{8}$$

The invariant P_{12} is unique up to a constant factor and the addition of multiples of P_2^6. For convenience we choose P_{12} such that the coefficient of $\langle 12, 0, 0, 0\rangle$ vanishes:

$$\begin{aligned} P_{12} = {} & 2\langle 10, 2, 0, 0\rangle - 6\langle 8, 4, 0, 0\rangle - 12\langle 8, 2, 2, 0\rangle \\ & + 7\langle 6, 6, 0, 0\rangle + (9 - 33\sqrt{5})\langle 6, 4, 2, 0\rangle + (9 + 33\sqrt{5})\langle 6, 4, 0, 2\rangle \\ & + 10\langle 4, 4, 4, 0\rangle + 116\langle 6, 2, 2, 2\rangle - 135\langle 4, 4, 2, 2\rangle \end{aligned} \tag{9}$$

and

$$P_{20} = \Delta\Delta(P_{12}^2), \tag{10}$$

$$P_{30} = \Delta(P_{12}P_{20}), \tag{11}$$

where Δ is the Laplacian in Euclidean 4-space

$$\Delta = \partial_x^2 + \partial_y^2 + \partial_z^2 + \partial_t^2. \tag{12}$$

As usual, the average of a function P over the hypersphere

$$\Omega_4 = \{(x, y, z, t) \in \mathbb{R}^4 \mid x^2 + y^2 + z^2 + t^2 = 1\} \tag{13}$$

is defined by

$$M_4(P) = \frac{1}{\operatorname{Vol} \Omega_4} \int_{\Omega_4} P \, d\Omega_4. \tag{14}$$

Hence

$$M_4(\langle a, b, c, d\rangle) = 12 \cdot 2^{-2(a+b+c+d)} \cdot \frac{(2a)!\,(2b)!\,(2c)!\,(2d)!}{a!\,b!\,c!\,d!(a+b+c+d+1)!} \tag{15}$$

and thus

$$M_4(P_2) = 1, \tag{16}$$

$$M_4(P_{12}) = 1/14, \tag{17}$$

$$M_4(P_{20}) = 12672/7, \tag{18}$$

$$M_4(P_{30}) = 13542912/91. \tag{19}$$

These results were obtained through the use of the REDUCE 3 algebraic manipulation system (Hearn [6]).

We recall the following definitions: A finite set N of unit vectors in Euclidean 4-space is called a spherical t-design if for all polynomials P of degree $\leqslant t$ the N-average of P equals $M_4(P)$ (Delsarte, Goethals, and Seidel [4]). Furthermore, if N is transitively permuted by a finite orthogonal group G, we say that N is a t-orbit of G (Neutsch [7]).

We are now able to formulate the following

THEOREM. *Every orbit of the hypericosahedral group I_4 which is contained in the surface of the unit hypersphere is an* 11*-design. There are infinitely many* 19*-orbits of I_4, but no* 20*-orbits. Exactly one of these* 19*-orbits is optimal with respect to integration of polynomials of degree* 20.

The 3600 integration points are of the form $C_1 E_1 + C_2 E_2$, where E_1 and E_2 are vertices of the 600-cell which are mutually orthogonal, while the coefficients C_1 and C_2 are approximately:

$$C_1 = 0.97129\ 92948\ 30434\ 51205\ 35832,$$

$$C_2 = 0.23786\ 06311\ 72753\ 45523\ 39919.$$

Proof. In analogy to the 3-dimensional case (Neutsch [7]), the first two assertions are obvious because P_{12} and P_{20} are the smallest degree nonconstant I_4-invariant polynomials. The point (x, y, z, t) generates a 19-orbit of the group if

$$P_2(x, y, z, t) = M_4(P_2) = 1 \tag{20}$$

and

$$P_{12}(x, y, z, t) = M_4(P_{12}) = \tfrac{1}{14}. \tag{21}$$

The point (x, y, z, t) compatible with (20, 21) yields an extremum of P_{20} if for all vectors $\mathbf{v}$ tangent to the intersection of (20) and (21)

$$\mathbf{v}\nabla P_{20} = 0 \tag{22}$$

holds, where ∇ denotes the gradient. This means that ∇P_2, ∇P_{12}, ∇P_{20} are linearly dependent. Hence ∇P_2, ∇P_{12}, ∇P_{20}, ∇P_{30} are also linearly dependent:

$$\det(\nabla P_2, \nabla P_{12}, \nabla P_{20}, \nabla P_{30}) = 0. \tag{23}$$

The reflection $t \to -t$ is an element of I_4; thus all invariants of I_4 are even functions of t. If we set $t = 0$, the fourth line of the determinant (23) vanishes. The hyperplane $t = 0$ is therefore a solution of (23), and similarly, all its images under I_4. The union of these 60 hyperplanes forms the complete solution of (23) as the determinant is a homogeneous polynomial of degree 60. Without loss of generality, we may set $t = 0$ and use

$$P^*(x, y, z) = P(x, y, z, 0). \tag{24}$$

Equations (20)–(22) reduce to

$$P_2^*(x, y, z) = 1, \tag{25}$$

$$P_{12}^*(x, y, z) = \tfrac{1}{14}, \tag{26}$$

$$\det(\nabla P_2^*, \nabla P_{12}^*, \nabla P_{20}^*) = 0. \tag{27}$$

The subgroup of I_4 fixing $(0, 0, 0, 1)$ is isomorphic to the icosahedral group I_3. We use as the basic invariants of I_3:

$$Q_2 = x^2 + y^2 + z^2, \tag{28}$$

$$Q_6 = 4x^2y^2z^2 + \lambda(x^4y^2 + y^4z^2 + z^4x^2) + \lambda'(x^2y^4 + y^2z^4 + z^2x^4), \tag{29}$$

$$\begin{aligned} Q_{10} = \sqrt{5}(x^4 + y^4 + z^4 - 2x^2y^2 - 2y^2z^2 - 2z^2x^2((\lambda'^6 - \lambda^6)\, x^2y^2z^2 \\ + \lambda^2(x^2y^4 + y^2z^4 + z^2x^4) - \lambda'^2(x^4y^2 + y^4z^2 + z^4x^2)), \end{aligned} \tag{30}$$

as defined in Neutsch [7, Eqs. (13)–(15)]. P_2^*, P_{12}^*, and P_{20}^* are invariant under I_3 and can be expressed in terms of Q_2, Q_6, Q_{10}:

$$P_2^* = Q_2, \tag{31}$$

$$P_{12}^* = -\tfrac{3}{2}Q_2^3 Q_6 - 6Q_6^2 - \tfrac{1}{2}Q_2 Q_{10}, \tag{32}$$

$$P_{20}^* = 480Q_2^{10} - 26880Q_2^7 Q_6 - 90096Q_2^4 Q_6^2 - 92928Q_2 Q_6^3 - 8960Q_2^5 Q_{10} + 11616Q_2^2 Q_6 Q_{10} + 1936Q_{10}^2. \tag{33}$$

Hence (27) can be rewritten as

$$\det(\nabla Q_2, \nabla Q_6, \nabla Q_{10}) \det \frac{\partial(P_2^*, P_{12}^*, P_{20}^*)}{\partial(Q_2, Q_6, Q_{10})} = -46464 Q_6 Q_{10} \det(\nabla Q_2, \nabla Q_6, \nabla Q_{10}) = 0. \tag{34}$$

There are three cases to be distinguished:

$$\text{case 1:} \quad \det(\nabla Q_2, \nabla Q_6, \nabla Q_{10}) = 0, \tag{35}$$

$$\text{case 2:} \quad Q_{10}(x, y, z) = 0, \tag{36}$$

$$\text{case 3:} \quad Q_6(x, y, z) = 0. \tag{37}$$

The icosahedral group I_3 transitively permutes the 12 vertices, 20 faces, and 30 edges of a regular icosahedron inscribed into the unit sphere.

Case 1. We use the same procedure as with I_4 above (Eq. (23)), and find the complete solution to be the union of the 15 planes normal to the icosahedron's 15 pairs of edge-centres. For reasons of transitivity we may restrict ourselves to one of these planes, e.g., $z = 0$. Condition (25) reduces to

$$P_2^*(x, y, 0) = Q_2(x, y, 0) = x^2 + y^2 = 1. \tag{38}$$

We substitute

$$2x^2 = 1 + \mu 5^{-1/2}; \; 2y^2 = 1 - \mu 5^{-1/2} \tag{39}$$

and obtain

$$Q_6(x, y, 0) = -\tfrac{1}{40}(\mu - 1)(\mu^2 - 5), \tag{40}$$

$$Q_{10}(x, y, 0) = \tfrac{1}{200}(3\mu + 5)\,\mu^2(\mu^2 - 5). \tag{41}$$

Using (32) we derive

$$21\mu^6 - 119\mu^4 + 175\mu^2 - 125 = 0. \tag{42}$$

The only real solution for μ^2 is

$$\mu^2 = \frac{1}{9}\left(17 + \frac{2}{\sqrt[3]{7}}\left[\sqrt[3]{1177 + 135\sqrt{65}} + \sqrt[3]{1177 - 135\sqrt{65}}\right]\right) \tag{43}$$

or

$$\mu = \pm 1.9830449011 \tag{44}$$

and

$$x = \pm 0.9712992948; \qquad y = \pm 0.2378606312 \tag{45}$$

for positive μ. The values of x and y are interchanged for the negative solution. Hence

$$P_{20}^*(x, y, 0) = \frac{44}{39{,}375}(2123\mu^4 - 3875\mu^2 + 1{,}598{,}375), \tag{46}$$

$$P_{20}^*(x, y, 0) = 1805.889296 < M_4(P_{20}). \tag{47}$$

Case 2. Case 2 has no real solutions.

Case 3. Using

$$Q_6(x, y, z) = 0 \tag{48}$$

and (26) and (32) we find

$$Q_{10}(x, y, z) = -\tfrac{1}{7}. \tag{49}$$

Thus

$$P_{20}^*(x, y, z) = \frac{88{,}176}{49} = 1799.510204 < M_4(P_{20}) \tag{50}$$

by virtue of (33). Both cases (1 and 3) yield values of P_{20} smaller than $M_4(P_{20})$; hence there is no 20-orbit of I_4. The optimal 19-orbit is given by case 1. The length of that orbit is 3600. Points are generated by application of I_4 to any one of them, e.g.,

$$(x, y, z, t) = (\sqrt{(1+\delta)/2}, \sqrt{(1-\delta)/2}, 0, 0), \tag{51}$$

with

$$\delta^2 = \frac{1}{45}\left[17 + \frac{2}{\sqrt[3]{7}}\left(\sqrt[3]{1177 + 135\sqrt{65}} + \sqrt[3]{1177 - 135\sqrt{65}}\right)\right]. \tag{52}$$

Numerical values with an accuracy of 25 digits are

$$x = 0.9712992948304345120535832, \tag{53}$$

$$y = 0.2378606311727534552339919. \tag{54}$$

This completes the proof of the theorem.

4. Conclusions

We have demonstrated the existence of a unique optimal 19-orbit of the group I_4 containing 3600 points. These equally weighted points are generated by simple operations like reflections in the roots of the Coxeter system H_4. They are all the vectors of the form $C_1 E_1 + C_2 E_2$, where (E_1, E_2) represent the 120×30 ordered pairs of vertices of the 600-cell (given by Eq. (2)) which are orthogonal to each other. Obviously, simply generated and equally weighted points confer an advantage in integration procedures.

Appendix

We list the vertices and centres of the edges, faces, and cells of the 600-cell. For each vector given there are additional ones (not listed here) that are formed by even permutations of the coordinates and/or sign reversals. Their number is given in each case. The definition of the following quantities is helpful:

$$\lambda = (-1 + 5^{1/2})/2, \tag{A1}$$

$$\lambda' = (-1 - 5^{1/2})/2, \tag{A2}$$

$$s = ((5 + 5^{1/2})/2)^{1/2}, \tag{A3}$$

$$s' = ((5 - 5^{1/2})/2)^{1/2}. \tag{A4}$$

The 120 vertices are

$$(0, 0, 0, 1) \qquad \# = 8, \tag{A5}$$

$$\tfrac{1}{2}(1, 1, 1, 1) \qquad \# = 16, \tag{A6}$$

$$\tfrac{1}{2}(1, \lambda, \lambda', 0) \qquad \# = 96. \tag{A7}$$

The 720 edge centres are

$$5^{-1/2}(0, 0, s, s') \qquad \# = 48, \tag{A8}$$

$$20^{-1/2}(s+s', s+s', s-s', s-s') \qquad \# = 96, \tag{A9}$$

$$20^{-1/2}(0, s, s+s', 2s-s') \qquad \# = 96, \tag{A10}$$

$$20^{-1/2}(0, s', s+2s', s-s') \qquad \# = 96, \tag{A11}$$

$$20^{-1/2}(s, 2s, s', s-s') \qquad \# = 192, \tag{A12}$$

$$20^{-1/2}(s, 2s', s', s+s') \qquad \# = 192. \tag{A13}$$

The 1200 face centres are

$$3^{-1/2}(0, 1, 1, 1) \qquad \# = 32, \tag{A14}$$

$$3^{-1/2}(0, 0, \lambda, \lambda') \qquad \# = 48, \tag{A15}$$

$$12^{-1/2}(1, 1, 1, 3) \qquad \# = 64, \tag{A16}$$

$$12^{-1/2}(0, \lambda, 3, \lambda') \qquad \# = 96, \tag{A17}$$

$$12^{-1/2}(0, \lambda^2, \lambda^2, \lambda-\lambda') \qquad \# = 96, \tag{A18}$$

$$12^{-1/2}(1, 1, \lambda-\lambda', \lambda-\lambda') \qquad \# = 96, \tag{A19}$$

$$12^{-1/2}(1, 2\lambda', \lambda, \lambda^2) \qquad \# = 192, \tag{A20}$$

$$12^{-1/2}(1, \lambda'^2, \lambda', 2\lambda) \qquad \# = 192, \tag{A21}$$

$$12^{-1/2}(1, 2, \lambda'^2, \lambda^2) \qquad \# = 192, \tag{A22}$$

$$12^{-1/2}(\lambda, 2, \lambda', \lambda-\lambda') \qquad \# = 192. \tag{A23}$$

The 600 cell centres are

$$2^{-1/2}(0, 0, 1, 1) \qquad \# = 24, \tag{A24}$$

$$8^{-1/2}(1, 1, 1, \lambda-\lambda') \qquad \# = 64, \tag{A25}$$

$$8^{-1/2}(\lambda, \lambda, \lambda, \lambda'^2) \qquad \# = 64, \tag{A26}$$

$$8^{-1/2}(\lambda', \lambda', \lambda', \lambda^2) \qquad \# = 64, \tag{A27}$$

$$8^{-1/2}(0, 1, \lambda^2, \lambda'^2) \qquad \# = 96, \tag{A28}$$

$$8^{-1/2}(0, \lambda', \lambda, \lambda-\lambda') \qquad \# = 96, \tag{A29}$$

$$8^{-1/2}(1, 2, \lambda, \lambda') \qquad \# = 192. \tag{A30}$$

Acknowledgments

W. Neutsch is grateful for the support from the Deutsche Forschungsgemeinschaft through a research stipend. The authors thank the Regionales Hochschulrechenzentrum der Universität Bonn for the use of their computing facilities.

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