[15] R. H. Hardin and N. J. A. Sloane, "A new approach to the construction of optimal designs," preprint, 1992.

[16] Y. Hong, "On spherical t-designs in $\mathbb{R}^2$," *Europ. J. Combin.*, **3** (1982), 255–258.

[17] S. Karlin and W. J. Studden, "Optimal experimental designs," *Annals Math. Stat.*, **37** (1966), 783–815.

[18] J. Kiefer, "Optimum experimental designs V, with application to systematic and rotatable designs," in *Proc. 4th Berkeley Sympos. Math. Statist. and Probability*, Univ. Calif. Press, Calif., 1961, **1**, pp. 381–405.

[19] R. Krawczyk and A. Neumaier, "An improved interval Newton operator," *J. Mathematical Analysis and Applications*, **118** (1986), 194–201.

[20] J. H. van Lint, "A survey of perfect codes," *Rocky Mountain J. Math.*, **5** (1975), 199-224.

[21] Mathlab Group, *MACSYMA Reference Manual*, Laboratory for Computer Science, Mass. Inst. Technology, Cambridge, Mass., Version 10, 1983.

[22] A. Neumaier, *Interval Methods for Systems of Equations*, Cambridge University Press, New York, 1991.

[23] A. Neumaier and J. J. Seidel, "Measures of strength $2e$, and optimal designs of degree e," *Sankhyā*, to appear.

[24] P. D. Seymour and T. Zaslavsky, "Averaging sets: a generalization of mean values and spherical designs," *Advances in Math.*, **52** (1984), 213–240.

[25] R. C. St. John and N. R. Draper, "D-optimality for regression designs: a review," *Technometrics*, **17** (1975), 15–23.

References

[1] B. Bajnok, "Construction of spherical 4- and 5-designs," *Graphs and Combinatorics*, **7** (1991), 219–233.

[2] B. Bajnok, "Construction of designs on the 2-sphere," *Europ. J. Combinatorics*, **12** (1991), 377–382.

[3] B. Bajnok, "Construction of spherical t-designs," *Geom. Dedicata*, to appear.

[4] G. E. P. Box and N. R. Draper, *Empirical Model-Building and Response Surfaces*, Wiley, New York, 1987.

[5] J. H. Conway and N. J. A. Sloane, *Sphere-Packings, Lattices and Groups*, Springer-Verlag, New York, 1988.

[6] J. H. Conway and N. J. A. Sloane, "The cell structures of lattices," in *Miscellanea mathematica*, P. Hilton et al., editors, Springer-Verlag, New York, 1991, pp. 71–107.

[7] H. S. M. Coxeter, *Regular Polytopes*, Dover, New York, 3rd ed., 1973.

[8] H. S. M. Coxeter and W. O. J. Moser, *Generators and Relations for Discrete Groups*, Springer-Verlag, New York, 4th Edition, 1984.

[9] P. Delsarte, J.-M. Goethals and J. J. Seidel, "Spherical codes and designs," *Geom. Dedicata*, **6** (1977), 363–388.

[10] V. V. Fedorov, *Theory of Optimal Experiments*, Academic Press, New York, 1972.

[11] Z. Galil and J. Kiefer, "D-optimum weighing designs," *Annals of Statistics*, **8** (1980), 1293–1306.

[12] L. M. Haines, "The application of the annealing algorithm to construction of exact optimal designs for linear regression models," *Technometrics*, **29** (1987), 439–447.

[13] E. Hansen and S. Sengupta, "Bounding solutions of systems of equations using interval analysis," *BIT*, **21** (1981), 203–211.

[14] R. H. Hardin and N. J. A. Sloane, *Operating Manual for Gosset: A General-Purpose Program for Designing Experiments*, Statistical Research Report No. 98, AT&T Bell Laboratories, Murray Hill, New Jersey, Nov. 15, 1991.

Postscript

Conjecture 1 is now a theorem. Sketch of proof: Suppose $\mathcal{E}$ has $I(\mathcal{E})$ given by (1). We will show that the prediction variance at $x \in B^k$ depends only on $r = \|x\|$. It then follows from [23] that the surface points in $\mathcal{E}$ form a spherical 4-design. If the variance at points x with $\|x\| = r$ were not constant, we could find a rotation of $\mathcal{E}$, $\mathcal{F}$ say, with smallest variance at some point x with $\|x\| = r$. By simply averaging the predictions from $\mathcal{E}$ and $\mathcal{F}$ at every point we obtain a design meeting (1). However, we could reduce the variance at x by weighting the prediction from $\mathcal{F}$ at x more heavily. This would reduce the average prediction variance and contradict Theorem 1.

of order 12 (the rotation group of the tetrahedron). The convex hull of these 16 points is a polyhedron with the combinatorial type of a hexakis truncated tetrahedron.

A 22-point design with the same group can be obtained by adjoining the points $(\pm 1, 0, 0)_{\text{cycle}}$, and making x^2, y^2, z^2 roots of

$$\lambda^3 - \lambda^2 + \frac{23}{90}\lambda - \frac{1}{243} \, . \qquad \blacksquare$$

Theorem 5. *There is a 20-point 4-dimensional spherical 4-design with a symmetry group of order 20.*

Proof. We construct the design from the group, which we take to have generators

$$\begin{pmatrix} \cos 2\theta & \sin 2\theta & & \\ -\sin 2\theta & \cos 2\theta & & \\ & & -\cos\theta & -\sin\theta \\ & & \sin\theta & -\cos\theta \end{pmatrix}, \quad \begin{pmatrix} & & - & \\ & & & - \\ - & & & \\ & + & & \end{pmatrix}, \quad \begin{pmatrix} + & & & \\ & - & & \\ & & + & \\ & & & - \end{pmatrix},$$

where $\theta = \pi/5$. Taking the points to be $(a, b, c, d)A$, for A in the group, we obtain from (6) the equations

$$a^2 + b^2 + c^2 + d^2 = 1, \quad (a^2 + b^2)(c^2 + d^2) = 1/6 \, ,$$

$$\begin{aligned} c(a^2 - b^2) - a(c^2 - d^2) &= 2bd(a + c) \, , \\ ac(a^2 + c^2) - bd(b^2 - d^2) &= 3ac(b^2 + d^2) - 3bd(a^2 - c^2) \, . \end{aligned}$$

Therefore $a^2 + b^2 = \frac{1}{2} + \frac{1}{6}\sqrt{3}$, $c^2 + d^2 = \frac{1}{2} - \frac{1}{6}\sqrt{3}$, and after some calculation we find that both b and d are roots of integral polynomials of degree 72. In particular, we find the solution $a = -.737040\ldots$, $b = -.495426\ldots$, $c = -.459434\ldots$, $d = .015674\ldots$. $\blacksquare$

A similar analysis could be made for the 36-point 6-dimensional design mentioned in (8), which appears to have a group of order 36.

Other designs mentioned in (8) can be obtained from the authors (write to the second author at AT&T Bell Laboratories, 600 Mountain Avenue, Murray Hill, NJ 07974, USA; electronic mail address njas@research.att.com).

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taking the solution with $\alpha \doteqdot 22.73°$, $\beta \doteqdot 77.23°$. (It is straightforward to verify using MACSYMA that these points satisfy Eq. (6).) This design has symmetry group $[2,3]^+$ in the notation of [8]. This is the rotation group of a triangular prism, and is abstractly a dihedral group of order 6. Figure 1 shows two views of the convex hull of this design. A label 1, Y, H indicates a point whose first coordinate is respectively 1, $\pm x_+$ or $\pm x_-$.

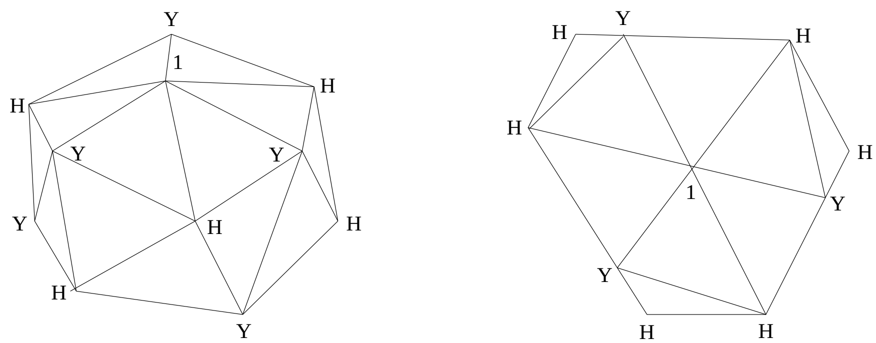

Figure 1: Two views of convex hull of a 14-point spherical 4-design.

The points in the above design are arranged in rings of sizes 1, 3, 3, 3, 3, 1 proceeding from the North to South pole. We indicate this by the formula $1+3^4+1$. The following seven designs are constructed in a precisely similar way. (We omit the details.)

Points	Structure	Group	Order
17	$1+3^5+1$	$[2,3]^+$	6
18	$1+4^4+1$	$[2,4]^+$	8
19	$1+3^6$	$[3]^+$	3
21	3^7	$[2,3]^+$	6
23	$1+3^7+1$	$[2,3]^+$	6
25	5^5	$[2,5]^+$	10
27	$1+5^5+1$	$[2,5]^+$	10

The two remaining designs have a different structure.[1] A 16-point 4-design is given by the points

$$\left(\pm\frac{1}{\sqrt{3}}, \pm\frac{1}{\sqrt{3}}, \pm\frac{1}{\sqrt{3}}\right)^+, \quad (\pm x, \pm y, \pm z)^-_{\text{cycle}},$$

where the superscript + (or −) specifies the product of the signs, the subscript "cycle" indicates that all cyclic shifts are to be used, and x^2, y^2, z^2 are roots of

$$\lambda^3 - \lambda^2 + \frac{7}{45}\lambda - \frac{1}{243}.$$

(In particular, $x \doteqdot .1827$, $y \doteqdot .3888$, $z \doteqdot .9030$.) The symmetry group of this design is $[3,3]^+$

[1] We are grateful to J. H. Conway for assistance in understanding the structure of the last two designs.

Proof. Let the vertices of the icosahedron be $(0,\tau,\pm 1)$, $(\pm 1,0,\tau)$, $(\pm\tau,1,0)$ and their negatives, where $\tau=(1+\sqrt{5})/2$ (we omit the scale factor needed to make these points lie on the unit sphere). The first three pairs are in one hemisphere. Right multiplication of these twelve points by

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix} ,$$

where $\cos\theta = 5^{-1/4}\tau^{-1/2}$, $\sin\theta = 5^{-1/4}\tau^{1/2}$ sends $(0,\tau,1)$ to $(0,0,1)$, and further multiplication of the first three pairs by

$$\begin{bmatrix} u & v & 0 \\ -v & u & 0 \\ 0 & 0 & 1 \end{bmatrix} , \quad (u^2+v^2=1) ,$$

accomplishes the desired rotation. We now use MACSYMA [21] to verify that the resulting points satisfy Eq. (6). ■

A. Blokhuis and J. J. Seidel (personal communication) have found a proof of Theorem 3 that avoids the use of a computer.

Theorem 4. *Three-dimensional spherical 4-designs with n points exist for $n=12$, 14 and all $n\geq 16$.*

Proof. 4-designs with p and q points can be combined to give a 4-design with $p+q$ points. The icosahedron and dodecahedron provide 4-designs with 12 and 20 points (see also Theorem 3). We will construct 4-designs with 14, $16-19$, $21-23$, 25 and 27 points. The remaining numbers above 16 can then be obtained as a sum of two smaller numbers.

The following 14 points form a spherical 4-design:

$$\begin{array}{llll} \pm 1 & 0 & 0 & \text{(2 points)} \\ \pm x_- & y_+\cos\left(\pm\alpha+\dfrac{2\pi m}{3}\right) & y_+\sin\left(\pm\alpha+\dfrac{2\pi m}{3}\right) & \text{(6 points)} \\ \pm x_+ & y_-\cos\left(\pm\beta+\dfrac{2\pi m}{3}\right) & y_-\sin\left(\pm\beta+\dfrac{2\pi m}{3}\right) & \text{(6 points)} \end{array}$$

where $m=0,1,2$, the $\pm$ signs in the second and third rows are linked,

$$\begin{aligned} x_\pm &= \frac{1}{3}\sqrt{2\pm\sqrt{\frac{7}{5}}}, \quad y_\pm = \frac{1}{3}\sqrt{7\pm\sqrt{\frac{7}{5}}} , \\ \sin^2 3\alpha &= \frac{53w}{7}, \ \sin^2 3\beta = \frac{689}{9826w}, \ w = \frac{7+2\sqrt{35}}{53+19\sqrt{35}} , \end{aligned}$$

In fact, our program GOSSET has found what appear to be spherical 4-designs containing n points in k dimensions for the following values of n and k:

$$\begin{array}{ll} k & n \\ 1 & 2,4,6,8,\ldots \\ 2 & \geq 5 \\ 3 & 12,14,\geq 16 \\ 4 & \geq 20 \\ 5 & \geq 29 \\ 6 & 27,36,\geq 39 \\ 7 & \geq 53 \\ 8 & \geq 69 \end{array} \tag{8}$$

These are consistent with the preceding estimates. Furthermore, since the program seems to be very successful at finding I-optimal designs in low dimensions (whether or not they are spherical 4-designs), we are tempted to predict that this list of values is complete.

Conjecture 2. *In dimensions $k \leq 8$, (8) gives a complete list of the parameters of spherical 4-designs.*

Dimensions 1 and 2 are trivial (see also [16]). In dimensions $k \geq 3$ we have numerical coordinates for the putative designs listed in (8), but except for the first few cases we have not formally proved that the designs exist. (However, since Newton's method converges to these designs — see below — we expect that it would be straightforward to formally establish their existence using the interval-Newton methods described in [13], [19], [22].)

Consider for example the putative 29-point 5-dimensional design. GOSSET produces a set of $b = 29$ points which, when supplemented by $c = 3$ copies of the center point, form a quadratic design which has I-value within 10^{-8} of the value given by (1). We then use a separate program to verify that the equations (6) are satisfied with an error of 10^{-6} (or less), and apply Newton's method in $5 \times 29 = 145$ dimensional space to find a nearby set of 29 points which satisfy (6) to within 10^{-20} (or less). We regard this as strong evidence that the claimed design exists.

Except for the 27-point 6-dimensional design (which is almost certainly unique), there appear to be many different designs for each case.

We now discuss some of the smallest cases, where we have proved that the designs exist.

Theorem 3. *Infinitely many distinct spherical 4-designs containing 12 points in 3 dimensions may be obtained by placing an icosahedron so there is a vertex at the North and South poles and rotating the Northern hemisphere about the North-South axis by an arbitrary amount.*

vertices of a 24-cell, was up to now the smallest known example of a 4-dimensional spherical 4-design.

Many similar examples can be obtained from Sobolev's theorem (see for example [5, p. 93]), but these designs usually contain large numbers of points.

Seymour and Zaslavsky [24] show that spherical t-designs exist for all k and t, provided n is sufficiently large. Bajnok [1]–[3] has given explicit constructions for such designs, but his constructions also require large number of points.

3. New spherical 4-designs

It follows immediately from the definition that a set of n points $(x_{i1}, \ldots, x_{ik}) \in B^k$, $1 \le i \le n$, is a spherical 4-design if and only if the following equations are satisfied:

$$\sum_{r=1}^{k} x_{ir}^2 = 1, \quad 1 \le i \le n \; ; \tag{6a}$$

$$\sum_{i=1}^{n} x_{ir}^2 = \frac{n}{k}, \quad 1 \le r \le k \; ; \tag{6b}$$

$$\sum_{i=1}^{n} x_{ir}^4 = \frac{3n}{k(k+2)}, \quad 1 \le r \le k \; ; \tag{6c}$$

$$\sum_{i=1}^{n} x_{ir}^2 x_{is}^2 = \frac{n}{k(k+2)}, \quad 1 \le r < s \le k \; ; \tag{6d}$$

and

$$\sum_{i=1}^{n} x_{ir}^{\alpha} x_{is}^{\beta} x_{it}^{\gamma} x_{iu}^{\delta} = 0 \; , \tag{6e}$$

for $(\alpha, \beta, \gamma, \delta) = (1,0,0,0), (1,1,0,0), (3,0,0,0), (2,1,0,0), (1,1,1,0), (3,1,0,0), (2,1,1,0), (1,1,1,1)$, where r, s, t, u are distinct numbers in the range 1 to k. The final equation in both (6b) and (6c) can be omitted, leaving a set of

$$n + \frac{1}{24}(k^4 + 10k^3 + 35k^2 + 50k - 48) \tag{7}$$

equations in nk unknowns. Therefore, when nk is greater than or equal to this quantity, we might reasonably expect a solution to exist. It follows that we can expect spherical 4-designs to exist in dimensions

2 3 4 5 6 7 8 9 10 11 12

provided the number of points is at least

12 16 23 31 42 55 71 89 111 137 166

Conjecture 1. *If $I(\mathcal{E})$ is equal to (1) then the b surface points form a spherical 4-design.*

It follows from Theorem 1 that, for fixed n, $I(\mathcal{E})$ is bounded below by the minimum of (1) taken over all pairs (c, b) with $c + b = n$.

An analog of Conjecture 1 does hold when we consider D-optimal designs. A D-optimal design is one for which the value of det $M_{\mathcal{E}}$ is maximized. Introducing an appropriate scaling, we define the D-value of a design $\mathcal{E}$ to be

$$D(\mathcal{E}) = \{\det \ M_{\mathcal{E}}\}^{-2/(k+1)(k+2)} \ . \tag{4}$$

D-optimal designs have received a great deal of attention over the past 35 years (see [4], [11], [25]), but for reasons presented in [15] we feel that for most purposes the I-optimality criterion is preferable.

The following result is a consequence of the work of Kiefer [18] and Neumaier and Seidel [23].

Theorem 2.

$$D(\mathcal{E}) \geq \frac{nk}{b}(k+2)^{\frac{k-1}{k+2}} \left\{ \frac{b}{ck2^{k-1}} \right\}^{\frac{2}{(k+1)(k+2)}} \ , \tag{5}$$

with equality if and only if the b surface points form a spherical 4-design.

It seems likely that the techniques used to prove Theorem 2, when combined with the results of Karlin and Studden [17] and Fedorov [10] on L-optimal designs (which include I-optimality as a special case), will also serve to establish Conjecture 1.

2. Previously known examples of 4-designs

Delsarte, Goethals and Seidel [9] show that a spherical 4-design in k dimensions must contain at least $k(k+3)/2$ points, and they call a design *tight* if it contains exactly this many points. Tight spherical 4-designs are known in dimensions 1 (the points ± 1), 2 (the vertices of a regular pentagon), 6 (the 27 vertices of the Schläfli polytope [6], [7], [9]), and 22 (the 275-point arrangement associated with the McLaughlin group [5, p. 292], [9]).

There are also some well-known examples of spherical t-designs with n points in k dimensions for larger t, for example with $(k, n, t) = (3, 12, 5), (4,24,5), (7,56,5), (8,240,7)$ (see [5], [9]). These are automatically 4-designs. The first of these, the set of vertices of an icosahedron, is the smallest known example of a 3-dimensional spherical 4-design, and the second, the set of

However, we soon realized that a straightforward argument shows that the I-value of a design is given by (1) whenever the b surface points form a spherical 4-design.

To our surprise the converse also appears to be true: in all the cases we have examined, whenever the I-value of a design is given by (1), the b surface points form a spherical 4-design. To make this precise we introduce some notation for describing experimental designs for fitting quadratic models.

Let $\mathcal{E} = \{(x_{i1}, \ldots, x_{ik}),\ 1 \le i \le n\}$ be a set of n points in the k-dimensional unit ball B^k, consisting of c copies of the center of the ball and $b = n - c$ points on S^{k-1}. The $n \times \binom{k+2}{2}$ design matrix X corresponding to $\mathcal{E}$ has as rows the vectors

$$1, x_{i1}, \ldots, x_{ik}, x_{i1}^2, \ldots, x_{ik}^2, x_{i1}x_{i2}, x_{i1}x_{i3}, \ldots, x_{i,k-1}x_{ik} \ ,$$

$(1 \le i \le n)$, and $M_{\mathcal{E}} = \frac{1}{n} X'X$ is the moment matrix for the design (the dash indicates transposition). The *average prediction variance* or *I-value* of $\mathcal{E}$ is

$$I(\mathcal{E}) = \text{trace}\ M M_{\mathcal{E}}^{-1} \tag{2}$$

where

$$M \ = \ \begin{bmatrix} 1 & 0 & \alpha u & 0 \\ 0 & \alpha I & 0 & 0 \\ \alpha u' & 0 & \beta(2I + J) & 0 \\ 0 & 0 & 0 & \beta I \end{bmatrix} \tag{3}$$

is the moment matrix for the ball. The blocks in (3) have sizes $1, k, k$ and $k(k-1)/2$, $u = (1, 1, \ldots, 1)$, I is an identity matrix, J is an all-1's matrix, $\alpha = 1/(k+2)$, and $\beta = 1/((k+2)(k+4))$.

Our earlier remarks can be formalized as follows.

Theorem 1. *$I(\mathcal{E})$ is never less than (1), and, in each dimension $k \ge 2$, (1) can be attained provided n is sufficiently large.*

Sketch of proof. It is known (cf. [18]) that the I-optimal design measure on B^k consists of a certain mass at the center point and the remaining mass uniformly distributed over S^{k-1}. $I(\mathcal{E})$ is equal to (1) if the moments of order ≤ 4 of the b surface points are the same as the corresponding moments of S^{k-1}. If, for some n, $I(\mathcal{E})$ were less than (1), by averaging over the orthogonal group we would obtain a rotationally symmetric design measure on B^k that had smaller I-value than the I-optimal measure, which is impossible. The second assertion follows from the theorem of Seymour and Zaslavsky [24] on the existence of spherical t-designs. ■

New Spherical 4-Designs

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1. Introduction

A spherical t-design [9] is a finite subset of the k-dimensional unit sphere S^{k-1} such that, for all polynomials f of degree at most t, the average of f over the subset is equal to the average of f over S^{k-1}. We have recently discovered a number of new spherical 4-designs, as well as numerical evidence for the existence or nonexistence of certain others. The way this came about was as follows.

In 1991 we wrote a general-purpose computer program (GOSSET, see [14],[15]) that searches for optimal experimental designs of various types in various spaces. An I-optimal experimental design consists of n points (which need not be distinct) arranged in the space so as to minimize a quantity called the "average prediction variance" and denoted by I (defined in (2); see [4], [12] for background). When using our program to search for I-optimal designs for fitting a quadratic model in the k-dimensional unit ball B^k, we discovered that the I-values of many of the best designs in low dimensions could be described by a single remarkable formula. It is convenient to restrict such designs to arrangements consisting of a certain number (c say) of copies of the center point of the ball, with the remaining $b = n - c$ points distributed over the boundary (or surface) S^{k-1}. In this situation we observed that the I-values of many of the best designs in low-dimensional balls are given by

$$\frac{n}{(k+2)(k+4)} \left\{ \frac{8}{c} + \frac{k^2(k^2+5k+10)}{2b} \right\} . \tag{1}$$

This formula gave the exact I-values of a very large number of designs, including polygons, the icosahedron, the 24-cell, as well as of infinitely many asymmetric designs.

Furthermore (1) appeared to be a lower bound on the I-value of any quadratic design in the ball, a bound which seemed to be attained in each dimension $k \geq 2$ provided the number of points (n) was sufficiently large.

We therefore provisionally decided to call designs whose I-value was equal to (1) *perfect*, by analogy with perfect codes (see for example van Lint [20]).

New Spherical 4-Designs*

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January 25, 1994

Dedicated to J. H. van Lint on the occasion of his 60th birthday

ABSTRACT

This paper gives a number of new spherical 4-designs, and presents numerical evidence that spherical 4-designs containing n points in k-dimensional space with $k \leq 8$ exist precisely for the following values of n and k: n even and ≥ 2 for $k = 1$; $n \geq 5$ for $k = 2$; $n = 12$, 14, ≥ 16 for $k = 3$; $n \geq 20$ for $k = 4$; $n \geq 29$ for $k = 5$; $n = 27$, 36, ≥ 39 for $k = 6$; $n \geq 53$ for $k = 7$; and $n \geq 69$ for $k = 8$.

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