

## MEASURES OF STRENGTH $2e$ AND OPTIMAL DESIGNS OF DEGREE $e$

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**SUMMARY.** Kiefer's theory of optimal rotatable designs is reproved and discussed in the context of Euclidean  $t$ -designs. Existence of nearly optimal experimental designs is shown for arbitrary degree and strength, and an explicit construction is given yielding many optimal designs from spherical  $2e$ -designs.

### 1. INTRODUCTION

The word design covers various notions. Companions to the ordinary  $t$ -designs in set theory are the spherical  $t$ -designs [5] on the unit sphere  $S$  in Euclidean  $\mathbb{R}^d$ . Recently [14] this last notion was generalized to a measure (both finite and infinite) of strength  $t$  in  $\mathbb{R}^d$ . On the other hand, optimal designs have been developed since the late fifties by Kiefer [11] and others, both experimental (finite) and abstract (as a measure). We restrict to  $D$ -optimality in terms of the determinant of the information matrix. The present paper relates these notions in the setting of the space of polynomials of degree  $\leq \frac{1}{2}t$  in  $\mathbb{R}^d$  and their inner products.

In Section 2 we introduce the relevant notions, and give simple proofs of Kiefer's theorem and the Equivalence theorem for a subset  $X$  of  $\mathbb{R}^d$  admitting a subgroup  $\Gamma$  of the orthogonal group. Later  $\Gamma$  will be the full orthogonal group, and  $X = RS$  a union of concentric spheres with radii from  $R$ , a possibly infinite symmetric subset of  $\mathbb{R}$ . In Section 3 we recall various definitions for measures of strength  $2e$ , a.o. in terms of moments. We recognize rotatable designs of degree  $e$  as measures of strength  $2e$ . For invariant measures the moments reduce to integrals over  $R$ , which are approximated by finite sums following Gauss-Christoffel. Section 4 gives a setting for the optimization process, in terms of the Gram matrix of a basis for  $\text{Pol}_e(X)$ , by use of spherical harmonics. Finally, Section 5 discusses the relevance of measures of strength  $2e$  for [almost] optimal experimental designs of degree  $e$ .

### 2. KIEFER'S THEOREM

Let  $\mathbb{R}^d$  denote a vector space of dimension  $d$  over the reals, with positive definite inner product  $(\cdot, \cdot)$  and orthogonal group  $O(d)$ . Let  $\Gamma$  be a closed subgroup of  $O(d)$  and let  $X$  be a  $\Gamma$ -invariant subset of  $\mathbb{R}^d$ , that is,  $\gamma(x) \in X$  for all  $x \in X$ ,  $\gamma \in \Gamma$ .

A design  $\xi$  on  $X$  is a normalized measure on  $X$ . If  $\xi$  is a design on  $X$ , then so is  $\xi \circ \gamma$ , for  $\gamma \in \Gamma$ . Any design  $\xi$  on  $X$  defines a positive semi-definite inner product

$$\langle f, g \rangle_\xi := \int_X f(x)g(x) d\xi(x)$$

on the linear space  $\text{Pol}_e(X)$  of polynomials of degree  $\leq e$  in  $d$  variables, restricted to  $X$ . The volume  $\text{vol}_e(\xi)$  of the ellipsoid

$$\{f \in \text{Pol}_e(X) : \langle f, f \rangle_\xi \leq 1\}$$

is a numerical characteristic for the design  $\xi$ . Clearly,

$$\text{vol}_e(\xi) < \infty \text{ iff } \langle \cdot, \cdot \rangle_\xi \text{ nondegenerate.}$$

Moreover, since  $O(d)$  acts in  $\text{Pol}_e(X)$  with  $|\det| = 1$ , we have

$$\text{vol}_e(\xi \circ \gamma) = \text{vol}_e(\xi) \text{ for } \gamma \in \Gamma.$$

*Definition 2.1:* A design  $\xi$  on the  $\Gamma$ -invariant set  $X$  in  $\mathbb{R}^d$  is called:

- (i) *optimal* if  $\text{vol}_e(\xi) < \infty$  and  $\text{vol}_e(\xi) \leq \text{vol}_e(\xi')$  for all  $\xi'$  on  $X$ ,
- (ii) *rotatable* if  $\langle \cdot, \cdot \rangle_\xi = \langle \cdot, \cdot \rangle_{\xi \circ \gamma}$  for all  $\gamma \in \Gamma$ ,
- (iii) *invariant* if  $\xi \circ \gamma = \xi$  for all  $\gamma \in \Gamma$ .

The notions *optimal* and *rotatable* depend on the degree  $e$  of the polynomials involved. We will mention this dependence only if necessary.

For any design  $\xi$  on  $X$ , there is an invariant design

$$\bar{\xi} := \int_\Gamma \xi \circ \gamma d\gamma$$

on  $X$ . Clearly, invariant designs are rotatable. It is a consequence of the following theorem that optimal designs are also rotatable. The theorem goes back to Kiefer [11], cf. Kiefer-Wolfowitz [12] and generalizations in Karlin-Studden [10] (Theorem X.7.4).

*Theorem 2.2:* Let  $\Gamma \leq O(d)$  act on  $X \subset \mathbb{R}^d$ , and let there exist an optimal design of degree  $e$  on  $X$ . Then all optimal designs of degree  $e$  on  $X$  define the same inner product on  $\text{Pol}_e(X)$ . Moreover, the set of all optimal designs of degree  $e$  on  $X$  is a closed convex set consisting of rotatable designs, and containing an invariant design.

*Proof:* Let  $\xi$  be a fixed design on  $X$  with non-degenerate inner product  $\langle \cdot, \cdot \rangle_\xi =: \langle \cdot, \cdot \rangle$  on  $\text{Pol}_e(X)$ . Let  $f_1, \dots, f_n$  be a  $\langle \cdot, \cdot \rangle$ -orthonormal basis for  $\text{Pol}_e(X)$ . Let  $\eta$  denote another design on  $X$ , and let

$$A = A(\eta) := [\langle f_i, f_j \rangle_\eta]$$

be the Gram matrix of our basis in the inner product corresponding to  $\eta$ . Then  $A$  is a symmetric positive semidefinite matrix and

$$\text{vol}_e(\eta) \cdot (\det A)^{1/2} = \text{vol}_e(\xi).$$

As a consequence we have

$$\xi \text{ is optimal iff } \det A(\eta) \leq 1 \text{ for all designs } \eta \text{ on } X. \quad \dots (*)$$

Moreover,  $\det A(\eta) = 1$  iff  $\eta$  is also optimal.

Denote the eigenvalues of  $A$  by  $\lambda_1, \dots, \lambda_n$ . Then the function

$$\phi(s) := -\log \det((1-s)I + sA) = -\sum_{i=1}^n \log(1-s + s\lambda_i)$$

is convex for  $0 \leq s \leq 1$ , since

$$\phi''(s) = \sum_{i=1}^n \left( \frac{\lambda_i - 1}{1-s + s\lambda_i} \right)^2 \geq 0$$

Now suppose that both  $\xi$  and  $\eta$  are optimal, so that, in particular,  $\det A = 1$ . Then also

$$\eta_s := (1-s)\xi + s\eta, \text{ with } A(\eta_s) = (1-s)I + sA(\eta)$$

is a design on  $X$ . Hence (\*) implies  $\phi(0) = \phi(1) = 0 \leq \phi(s)$  for  $0 \leq s \leq 1$ , and the convexity of  $\phi$  forces  $\phi$  to be constant and  $\phi''(s) = 0$ . Hence  $\lambda_i = 1$  for all  $i$ , and  $A = I$ . We conclude that  $\langle \cdot, \cdot \rangle_\eta = \langle \cdot, \cdot \rangle$ , proving the first claim and the convexity of the set of the optimal designs. Clearly, this set is closed. Since  $\xi \circ \gamma$  is optimal whenever  $\xi$  is, we infer  $\langle \cdot, \cdot \rangle_{\xi \circ \gamma} = \langle \cdot, \cdot \rangle = \langle \cdot, \cdot \rangle_\xi$  which proves rotatability. Finally, integration over  $\Gamma$  yields the invariant optimal measure  $\bar{\xi}$  in the closed convex hull of the  $\xi \circ \gamma$ ,  $\gamma \in \Gamma$ .  $\square$

*Remark 2.3:* Continuing the situation in the proof, we observe that optimality of  $\xi$  alone implies

$$0 \leq \phi'(0) = -\sum_{i=1}^n (\lambda_i - 1) = n - \text{tr } A,$$

hence  $\text{tr } A \leq n$ . On the other hand,  $\text{tr } A \leq n$  implies  $\sqrt[n]{\det A} \leq \text{tr } A/n \leq 1$  by the arithmetic-geometric mean inequality, hence  $\det A \leq 1$ . Therefore we can reformulate (\*) as

$$\xi \text{ is optimal iff } \text{tr } A(\eta) \leq n \text{ for all designs } \eta \text{ on } X. \quad \dots (**)$$

Moreover,  $\text{tr } A(\eta) = n$  iff  $\eta$  is also optimal. The trace formula

$$\text{tr } A(\eta) = \int_X d(x, \xi) d\eta(x) \quad \text{for } d(x, \xi) := f_1^2(x) + \dots + f_n^2(x)$$

now implies the following:

**Theorem 2.4:**  $\max_{x \in X} d(x, \xi) \geq n = \dim \text{Pol}_e(X)$ , with equality iff  $\xi$  is optimal. In this case,  $d(x, \xi) = n$  for all  $x \in X$  except on a set of zero measure with respect to  $\xi$ .

*Proof:* Choosing an optimal  $\eta$  in the trace formula gives

$$n = \text{tr } A(\eta) \leq \max d(x, \xi).$$

If equality holds, then  $d(x, \xi) \leq n$  for all  $x \in X$ , and the trace formula gives  $\text{tr } A(\eta) \leq n$  for all  $\eta$ . Thus  $\xi$  is optimal by (\*\*).

Conversely, if  $\xi$  is optimal then the trace formula applied to all unit measures  $\eta$  with one-point support gives  $\max d(x, \xi) \leq n$ ; and since  $\text{tr } A(\eta) = n$ , the trace formula for  $\eta = \xi$  shows that  $d(x, \xi) = n$  almost everywhere.  $\square$

For an arbitrary basis  $g = (g_1, \dots, g_n)^t$  of  $\text{Pol}_e(X)$  with Gram matrix  $M(\xi) = \langle (g_i, g_j) \rangle_\xi$ , the information matrix in statistics, we have

$$d(x, \xi) = g^t(x) M(\xi)^{-1} g(x) = \langle M(\xi)^{-1} g(x), M(\xi)^{-1} g(x) \rangle_\xi.$$

We see that Theorem 2.4 is just another form of the equivalence theorem of Kiefer and Wolfowitz [12].

We also see that  $\xi$  is rotatable iff  $d(x, \xi)$  depends only on the  $\Gamma$ -orbit of  $\xi$ . In particular, in the case  $\Gamma = O(d)$  a rotatable design is the same notion as the one introduced by Box and Hunter [2], cf. [16].

### 3. MEASURES OF STRENGTH $t = 2e$

From now on we specialize to the case  $\Gamma = O(d)$ . The  $O(d)$ -invariant set  $X$  is a union of spheres, possibly infinitely many. We use the notation

$$RS := \bigcup_{r \in R} rS, \quad rS := \{x \in \mathbb{R}^d : (x, x) = r^2\}, \quad r \in R \subset \mathbb{R}$$

where  $R = -R$  is symmetric about 0. Thus the whole space  $\mathbb{R}^d$ , the unit sphere  $S$ , a union of  $p$  concentric spheres, the unit ball, the case  $R = \{r \in \mathbb{R} : r^2 \in 2\mathbb{Z}\}$  for lattices, they all are covered by the notation  $RS$ . The unit sphere  $S$  has the standard Borel measure  $d\sigma$ .

The space  $\text{Pol}_e(RS)$  of the polynomials of degree  $\leq e$  is the sum, for  $k = 0, 1, \dots, e$ , of the subspaces  $\text{Hom}_k(R, S)$  of the homogeneous polynomials of degree  $k$ , all restricted to  $RS$ . We shall write

$$f = \sum_{k=0}^e f_k, \quad f \in \text{Pol}_e(RS), \quad f_k \in \text{Hom}_k(RS),$$

for the components. It is well-known that

$$\dim \text{Hom}_e(RS) = \dim \text{Hom}_e(\mathbb{R}^d) = \binom{d-1+e}{d-1};$$

$$\dim \text{Pol}_e(RS) = \sum_{i=0}^{2p-1} \binom{d-1+e-i}{d-1},$$

$$\dim \text{Pol}_e(\mathbb{R}^d) = \binom{d+e}{d},$$

which are equal if  $2p \geq e+1$ , where  $p$  is the number of spheres, the one-point sphere  $O$  being counted as half a sphere.

We refer to [14], [6] for the following definitions, and their equivalence.

*Definition 3.1:* A measure  $\xi$  on  $RS$  has *strength*  $t$  if any one of the following equivalent conditions holds for all  $f \in \text{Pol}_t(RS)$ :

- (i)  $\int_{RS} f d\xi = \int_{RS} f d(\xi \circ \gamma), \forall \gamma \in \Gamma$ ;
- (ii)  $\int_{RS} f d\xi = \int_{RS} f d\bar{\xi}$ ;
- (iii)  $\int_{RS} f(y) d\xi(y) = \sum_{k=0}^t \mu_k \int_S f_k(x) d\sigma(x), \mu_k = \int_{RS} \|y\|^k d\xi(y)$ .

A *Euclidean  $t$ -design* is a measure of strength  $t$  having finite support.

In (ii), the measure  $\bar{\xi}$  is the invariant measure introduced in Section 2. The equivalence with (iii) is proved as follows:

$$\begin{aligned} \int_{RS} f d\xi &= \int_{\Gamma} d\gamma \int_{RS} f d\xi \circ \gamma = \int_{RS} d\xi(y) \int_{\Gamma} f(\gamma^{-1}y) d\gamma \\ &= \sum_{k=0}^t \int_{RS} \|y\|^k d\xi(y) \int_{\Gamma} f_k\left(\frac{\gamma^{-1}y}{\|y\|}\right) d\gamma = \sum_{k=0}^t \mu_k \int_S f_k(x) d\sigma(x) \end{aligned}$$

The notion of strength is related to the designs introduced in Section 2.

*Theorem 3.2:* A design is rotatable of degree  $e$  iff it has strength  $2e$ .

The proof is a direct consequence of the following lemma, cf. [6].

*Lemma 3.3:*  $\text{Pol}_i(RS) \cdot \text{Pol}_j(RS) = \text{Pol}_{i+j}(RS)$ .

Here the product  $F \cdot G$  is the linear space spanned by the products  $fg$  of  $f \in F$  and  $g \in G$ . The lemma follows from the analogous formulae for  $\text{Hom}(\mathbb{R}^d)$ , and for  $\text{Pol}(\mathbb{R}^d)$ .

*Theorem 3.4:* If a design  $\xi$  is rotatable of degree  $e$ , then the inner product  $\langle \cdot, \cdot \rangle_{\xi}$  is uniquely determined by the first  $e+1$  even moments

$$\mu_{2i} = \int_{RS} (y, y)^i d\xi(y), \quad i = 0, 1, \dots, e$$

*Proof:* We apply Theorem 3.2 and Definition 3.1, (iii). The polynomials  $f, g \in \text{Pol}_e(RS)$  are written in terms of their homogeneous components.  $\text{Hom}_k$  and  $\text{Hom}_l$  are  $\langle \cdot, \cdot \rangle_{\sigma}$  orthogonal if  $k$  and  $l$  have opposite parity. Hence

$$\begin{aligned} \langle f, g \rangle_{\xi} &= \sum_{k,l=0}^e \langle f_k, g_l \rangle_{\xi} = \sum_{k,l=0}^e \mu_{k+l} \int_S f_k(x) g_l(x) d\sigma(x) \\ &= \sum_{i=0}^e \mu_{2i} \sum_{k=0}^{2i} \langle f_k, g_{2i-k} \rangle_{\sigma}. \quad \square \end{aligned}$$

For invariant designs  $\xi$  the variables may be separated:

$$y = rx \in RS, \quad r \in R, \quad x \in S; \quad d\xi(y) = d\rho(r) d\sigma(x);$$

$$\mu_{2i} = \int_{RS} r^{2i} d\rho d\sigma = \int_R r^{2i} d\rho(r),$$

where  $\rho(r)$  is a normalized symmetric measure on  $R$ .

**Theorem 3.5:** *Let  $\xi$  be an invariant design of degree  $e$  with nondegenerate inner product  $\langle \cdot, \cdot \rangle_\xi$ . Then there is a unique symmetric weighted finite set  $(R_0, w)$  of size  $|R_0| \leq e + 1$  such that the even moments of  $\xi$  are given by*

$$\mu_{2i} = \sum_{r \in R_0} w_r r^{2i}, \quad i = 0, 1, \dots, e.$$

$R_0$  is in the closed convex hull of  $R$ ,  $-R_0 = R_0$ ,  $w_{-r} = w_r$ , and  $R_0 = R$  if  $|R| < e + 1$ ,  $|R_0| = e + 1$  otherwise.

*Proof:* The problem is to find finite symmetric  $R_0$  and  $w : R_0 \rightarrow \mathbb{R}^+$  such that, for  $i = 0, 1, \dots, e$ ,

$$\int_R r^{2i} d\rho(r) = \sum_{r \in R_0} w_r r^{2i}, \quad \int_R r^{2i+1} d\rho(r) = 0.$$

The powers of  $r$  are polynomials of degree  $\leq 2e + 1$  which are independent with respect to the radical of  $\langle \cdot, \cdot \rangle_\rho$ . Hence for given measure  $d\rho(r)$  we need symmetric  $R_0$  and  $w$  such that

$$\int_R f(r) d\rho(r) = \sum_{r \in R_0} w_r f(r), \quad \forall f \in \text{Pol}_{2e+1}(R).$$

This is solved by the  $(e + 1)$ -point Gauss-Christoffel quadrature formula, cf. [4], p. 35 and [7], p. 80. Then  $R_0$  is the set of the  $e + 1$  zeros of the orthogonal polynomial of degree  $e + 1$  associated with  $d\rho$ , and  $w_r$ ,  $r \in R$ , are the corresponding Christoffel numbers.

**Remark 3.6:** For the invariant design  $\xi$  of degree  $e$  the conclusion of Theorem 3.5 is that the inner product on  $\text{Pol}_e(RS)$  may be taken as restricted to at most  $(e + 1)/2$  concentric spheres, the origin being counted as half a sphere. The radii of these spheres are determined uniquely.

If the finite support of a Euclidean design is contained in the unit sphere  $S$ , then a cubature formula (arbitrary positive weights) or a spherical design (equal weights) are obtained. We repeat their definitions from [8] and [5] for future reference.

**Definition 3.7:** A finite set  $Y \subset S$  is a *spherical  $t$ -design* if

$$|Y|^{-1} \sum_{y \in Y} f(y) = \int_S f(x) d\sigma(x), \quad \text{for all } f \in \text{Pol}_t(S).$$

A finite weighted set  $(Y, w)$ ,  $Y \subset S$ , is a cubature formula for  $S$  of strength  $t$  if

$$\sum_{y \in Y} w_y f(y) = \left( \sum_{y \in Y} w_y \right) \int_S f(x) d\sigma(x) \quad \text{for all } f \in \text{Pol}_t(S).$$

4. THE OPTIMIZATION PROBLEM

We are now in a position to determine the even moments of an invariant optimal design of degree  $e$  on  $RS$ , and to show their existence if  $R$  is compact and  $|R| \geq e+1$ . From Theorem 3.5 we know that for an invariant optimal design of degree  $e$  there are only a finite number of moments to determine. Therefore, the optimization problem to minimize  $\text{vol}_e(\xi)$  is a finite dimensional problem.

We shall use spherical harmonics, and first recall the simple but basic formula

$$\text{Hom}_k(\mathbb{R}^d) = \text{Harm}_k(\mathbb{R}^d) \oplus r^2 \text{Hom}_{k-2}(\mathbb{R}^d).$$

Here  $\text{Harm}_k(\mathbb{R}^d)$  is the space of the homogeneous polynomials of degree  $k$  which are harmonic, that is, which are annulled by the Laplace operator. It follows that

$$h_k := \dim \text{Harm}_k(\mathbb{R}^d) = \binom{d+k-1}{d-1} - \binom{d+k-3}{d-1}.$$

We let  $f_{k,1}, \dots, f_{k,h_k}$  denote any  $\langle \cdot, \cdot \rangle_\sigma$ -orthonormal basis for  $\text{Harm}_k(\mathbb{R}^d)$ , and notice that  $\text{Harm}_k(RS) \cong \text{Harm}_k(\mathbb{R}^d)$ . By iteration of the basic formula, and substitution of  $l = k + 2j$ , this implies

$$\text{Pol}_e(\mathbb{R}^d) = \sum_{l=0}^e \text{Hom}_l(\mathbb{R}^d) = \sum_{k=0}^e \sum_{k+2j \leq e} r^{2j} \text{Harm}_k(\mathbb{R}^d).$$

Assuming  $|R| \geq e + 1$ , we have as in Section 3,

$$\text{Pol}_e(RS) \cong \text{Pol}_e(\mathbb{R}^d),$$

hence the polynomials  $r^{2j} f_{k,i}(y)$  constitute an independent basis for  $\text{Pol}_e(RS)$ , which we call a *harmonic basis* for  $\text{Pol}_e(RS)$ . We calculate their inner products  $\langle \cdot, \cdot \rangle_\xi$  corresponding to the invariant design  $\xi$  that we wish to establish:

$$\begin{aligned} \langle r^{2j} f_{k,i}(y), r^{2j'} f_{k',i'}(y) \rangle_\xi &= \int_R r^{2(j+j'+k)} d\rho(r) \int_S f_{k,i}(x) f_{k',i'}(x) d\sigma(x) \\ &= \mu_{2(j+j'+k)} \delta_{k,k'} \delta_{i,i'}. \end{aligned}$$

As a consequence, the Gram matrix  $G$  of the harmonic basis reads

$$G = \sum_{k=0}^e \oplus h_k M_k, \quad M_k := \begin{bmatrix} \mu_{2k} & \cdots & \mu_{2k+2j} \\ \vdots & \ddots & \vdots \\ \mu_{2k+2j} & \cdots & \mu_{2k+4j} \end{bmatrix}$$

with  $j = \lceil \frac{1}{2}(e - k) \rceil$ . For example, for  $e = 3$ ,

$$G = \begin{bmatrix} \mu_0 & \mu_2 \\ \mu_2 & \mu_4 \end{bmatrix} \oplus h_1 \begin{bmatrix} \mu_2 & \mu_4 \\ \mu_4 & \mu_6 \end{bmatrix} \oplus h_2 \mu_4 \oplus h_3 \mu_6.$$

Theorem 4.1: Let  $-R = R \subset \mathbb{R}$  be compact and  $|R| \geq e + 1$ . Then optimal designs of degree  $e$  on  $RS$  exist. Their even moments  $\mu_{2i}^*$  follow from the unique solution of the optimization problem to maximize

$$\det G = \prod_{k=0}^e (\det M_k)^{h_k},$$

the determinant of the Gram matrix  $G$  of a harmonic basis, over the normalized measures  $\rho$  on  $R$ .

*Proof:* By Theorem 2.2, the class of the optimal designs of degree  $e$  on  $RS$ , if not empty, contains an invariant design  $\xi = \rho\sigma$ . The optimization problem is to maximize over  $R$  the determinant  $\det G$ , which is positive by  $|R| \geq e + 1$ , and whose moments depend only on the radial measure  $\rho$ . Since  $R$  is compact the maximum of  $\det G$  is attained for an invariant measure  $\xi^*$ , say, which is optimal as well by Theorem 2.2, and unique by Theorem 3.4.

Corollary 4.2: For an invariant optimal design of degree  $e$  with compact  $R$  and  $e \leq |R| - 1$ , some non-zero points of the finite set  $R_0$  must lie on the boundary of  $R$ .

*Proof:*  $\det G$  is a strictly increasing function of  $\mu_{2e}$ , since  $\mu_{2e}$  occurs in  $M_{2e}$  linearly with a positive coefficient. Hence the unique maximum of  $\det G$  is attained on the boundary of the admissible domain for  $\rho$ .

Example 4.3: We illustrate Theorem 4.1 and Theorem 3.5 in the case of the unit ball  $B = [-1, 1]S$ , for  $e = 1, 2, 3$ . We are in particular interested in the discrete solutions. The dimensions of the spaces of harmonic polynomials are

$$h_0 = 1, \quad h_1 = d, \quad h_2 = \frac{1}{2}(d+2)(d-1), \quad h_3 = \frac{1}{6}(d+4)d(d-1),$$

corresponding to the bases for  $\text{Harm}_{\leq e}$  consisting of the polynomials

$$1, x_i, x_i x_j \text{ and } x_i^2 - x_1, \quad x_i x_j x_k \text{ and } x_i(3x_j^2 - x_i^2),$$

in number 1,  $d$ ,  $\binom{d}{2}$  and  $d-1$ ,  $\binom{d}{3}$  and  $d(d-1)$ .

For  $e = 1$ , the discrete measure and the moments are

$$\xi(-1) = \xi(1) = \frac{1}{2}; \quad \mu_0 = \mu_2 = 1.$$

For  $e = 2$  the discrete measure and the moments are

$$\xi(0) = \delta, \quad \xi(-1) = \xi(1) = \frac{1}{2}(1 - \delta); \quad \mu_0 = 1, \quad \mu_2 = \mu_4 = 1 - \delta.$$

The unknown  $\delta$  is determined by the optimization of

$$\det G = (\mu_0 \mu_4 - \mu_2^2) \mu_2^{h_1} \mu_4^{h_2} = \delta(1 - \delta)^{\frac{1}{2}d(d+3)},$$

which yields  $\delta = 2/(d+1)(d+2)$ .

For  $e = 3$  the measure and the moments are

$$\xi(-1) = \xi(1) = \frac{1}{2}(1 - \delta), \quad \xi(-\sqrt{\alpha}) = \xi(\sqrt{\alpha}) = \frac{1}{2}\delta;$$

$$\mu_0 = 1, \quad \mu_2 = 1 - \delta + \delta\alpha, \quad \mu_4 = 1 - \delta + \delta\alpha^2, \quad \mu_6 = 1 - \delta + \delta\alpha^3.$$

The unknown  $0 < \delta < 1$  and  $0 < \alpha < 1$  follow from the optimization of

$$\begin{aligned} \det G &= (\mu_0\mu_4 - \mu_2^2)(\mu_2\mu_6 - \mu_4^2)^{h_1} \mu_4^{h_2} \mu_6^{h_3} \\ &= \alpha^d (\delta(1 - \delta)(1 - \alpha)^2)^{d+1} (1 - \delta + \delta\alpha^2)^{h_2} (1 - \delta + \delta\alpha^3)^{h_3}. \end{aligned}$$

Logarithmic differentiation of  $\det G$  w.r.t.  $\alpha$  and  $\delta$  yields:

$$\frac{d}{\alpha} - \frac{2(d+1)}{1-\alpha} + \frac{2h_2\delta\alpha}{1-\delta+\delta\alpha^2} + \frac{3h_3\delta\alpha^2}{1-\delta+\delta\alpha^3} = 0,$$

$$\frac{(d+1)(1-2\delta)}{\delta(1-\delta)} - \frac{h_2(1-\alpha^2)}{1-\delta+\delta\alpha^2} - \frac{h_3(1-\alpha^3)}{1-\delta+\delta\alpha^3} = 0.$$

For a further discussion of these equations in  $\alpha$  and  $\delta$  we refer to [1], and for numerical results to [13].

### 5. OPTIMAL EXPERIMENTAL DESIGNS

For the actual application in statistical experiments the continuous designs  $\xi$  must be approximated by discrete designs having rational weights. An *experimental design* on  $RS$  is a finite collection  $Y$  of points of  $RS$ , with repetitions allowed. In statistical terms,  $n_i$  uncorrelated observations are taken at distinct points  $y_i \in Y$ ,  $i = 1, \dots, r$ , so we have  $\sum_{i=1}^r n_i$  points. The normalized measure  $\xi$  corresponding to the experimental design  $(Y, n)$  is given by

$$\int_Y f(y) d\xi(y) = \frac{\sum_{i=1}^r n_i f(y_i)}{\sum_{i=1}^r n_i}.$$

The first case to consider is that of an experimental design on a single sphere, say on the unit sphere  $S$ , with  $R = \{-1, 1\}$ . The second case deals with an experimental design on the unit ball  $B = [-1, 1]S$ .

**Theorem 5.1:** *An experimental design on the unit sphere is optimal of degree  $e$  iff it is a spherical  $2e$ -design (with repeated points allowed).*

*Proof:* By Theorem 2.2 the optimal designs of degree  $e$  on  $S$  are rotatable on  $S$ , hence by Theorem 3.2 are measures of strength  $2e$  on  $S$ . An optimal experimental design on  $S$  has finite support  $Y \subset S$ , which may be taken to have equal weights. Therefore, it satisfies Definition 3.7 for a spherical  $2e$ -design.

**Theorem 5.2:** *An experimental design  $(Y, n)$  on the unit ball  $B = [-1, 1]S$  is optimal of degree  $e$  iff  $(Y, n)$  is a Euclidean design of strength  $2e$  whose even moments are*

$$\sum_{y \in Y} n_y (y, y)^i = \left( \sum_{y \in Y} n_y \right) \mu_{2i}^*$$

where  $\mu_{2i}^*$  are the moments of the solution  $\xi^*$  of the optimization problem for  $\det G$  in Theorem 4.1.

*Proof:* Theorem 4.1 exhibits an optimal design and its moments. Theorem 2.2 asserts that all rotatable designs of degree  $e$  with the same inner product are optimal, and no others. Theorem 3.4 says that this condition is equivalent to having the same moments.  $\square$

We continue to show the existence of experimental almost optimal designs with small support. The basic ingredient in the following theorem is due to Caratheodory [3].

**Theorem 5.3:** *Let  $X$  be a compact subset of  $\mathbb{R}^n$ , and let  $C$  be the closed convex hull of  $X$ . Then every boundary [interior] point of  $C$  is a convex combination of at most  $n$  [resp.  $n + 1$ ] points from  $X$ .*

**Theorem 5.4:** *Let  $\xi$  be a design on  $X$ , with information matrix  $M(\xi)$  on  $\text{Pol}_e(X)$ . Then there exists a design  $\eta$  on  $X$  with  $M(\eta) = M(\xi)$ , and finite support  $X_0$  of size at most  $\dim \text{Pol}_{2e}(X)$ .*

*Proof:* Let  $g_1, \dots, g_n$  be a basis of  $\text{Pol}_e(X)$ . The set  $\Sigma$  of the  $n \times n$  matrices  $[g_i(x)g_j(x)]$ ,  $x \in X$ , spans a space of dimension  $N \leq \dim \text{Pol}_{2e}(X)$ . The  $n \times n$  information matrix

$$M(\xi) = [(g_i, g_j)_\xi] = \left[ \int_X g_i(x)g_j(x) d\xi(x) \right]$$

is an element of the boundary of the closed convex hull of  $\Sigma$ . Hence  $M(\xi)$  can be written as a convex combination of at most  $N$  matrices from  $\Sigma$ , for  $x \in X_0$ , say, with  $|X_0| \leq N$ . This defines a design  $\eta$  with support  $X_0$  having the desired properties.  $\square$

In particular, if  $\xi$  is optimal then  $\eta$  is optimal as well. By approximating the weights of  $\eta$  by rational numbers we can obtain experimental designs which are arbitrarily close to being optimal. In particular, combining the present results with Theorem 5.1 we obtain:

**Corollary 5.5:** *For every  $e \geq 0$  there exist cubature formulae of strength  $2e$  on the unit sphere in  $\mathbb{R}^d$ , which have at most  $\binom{d+2e-2}{d-1}$  points.*

**Example 5.6:** Finally we mention the construction of a class of optimal designs on  $RS$  with finite support, on the basis of a spherical  $2e$ -design  $X$ , cf. [9] Theorem 5.1 and [15] Corollary 5. We wish to find a finite weighted set  $(Y, w)$  with

$$Y = r_1 X \cup \dots \cup r_n X; \quad R_0 := \{r_1, r_2, \dots, r_n\} \subset R,$$

where  $X$  is a spherical  $2e$ -design on  $S \subset \mathbb{R}^d$ , and the weights  $w_r$  are homogeneous on the various spheres. For  $(Y, w)$  we have:

$$\int_{RS} \mathbf{y}^k d\rho d\sigma = \int_R r^k d\rho(r) \cdot \int_S \mathbf{x}^k d\sigma(x),$$

$$\sum_{y \in Y} w_y y^k = \sum_{r \in R_0} w_r r^k \cdot \sum_{x \in X} x^k,$$

$$\sum_{y \in Y} w_y = \sum_{r \in R_0} w_r \cdot |X|.$$

Since  $X$  is a spherical  $2e$ -design, the weighted set  $(Y, w)$  has strength  $2e$  iff  $(R_0, w)$  has strength  $2e$ . In order to obtain optimal designs  $(Y, w)$  of degree  $e$  it suffices to choose  $\rho(r)$  so that it matches the optimal moments  $\mu_{2i}^*$ .

We observe that also  $r_1 X^{\gamma_1} \cup \dots \cup r_n X^{\gamma_n}$  works, for any  $\gamma_i \in O(d)$ , since by definition [5] the spherical  $2e$ -design satisfies

$$\sum_{x \in X} x^k = \sum_{x \in X^\gamma} x^k, \quad \gamma \in O(d), \quad k = 1, \dots, 2e.$$

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