Sankhyā: The Indian Journal of Statistics
1992, Special Volume 54, pp. 299–309
Dedicated to the memory of R. C. Bose

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 Γ of the orthogonal group. Later Γ 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 proces, in terms of the Gram matrix of a basis for $\mathrm{Pol}_e(X)$, 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 Γ be a closed subgroup of $O(d)$ and let X be a Γ-invariant subset of $\mathbb{R}^d$, that is, $\gamma(x) \in X$ for all $x \in X$, $\gamma \in \Gamma$.

A *design* ξ on X is a normalized measure on X. If ξ is a design on X, then so is $\xi \circ \gamma$, for $\gamma \in \Gamma$. Any design ξ 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 $\mathrm{Pol}_e(X)$ of polynomials of degree $\leq e$ in d variables, restricted to X. The *volume* $\mathrm{vol}_e(\xi)$ of the ellipsoid

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

is a numerical characteristic for the design ξ. Clearly,

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

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

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

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

(i) *optimal* if $\mathrm{vol}_e(\xi) < \infty$ and $\mathrm{vol}_e(\xi) \leq \mathrm{vol}_e(\xi')$ for all ξ' 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 ξ 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* $\mathrm{Pol}_e(X)$. *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 ξ be a fixed design on X with non-degenerate inner product $\langle \cdot, \cdot \rangle_\xi =: \langle \cdot, \cdot \rangle$ on $\mathrm{Pol}_e(X)$. Let $f_1, \ldots, f_n$ be a $\langle \cdot, \cdot \rangle$-orthonormal basis for $\mathrm{Pol}_e(X)$. Let η 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 η. Then A is a symmetric positive semidefinite matrix and

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

As a consequence we have

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

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

Denote the eigenvalues of A by $\lambda_1, \ldots, \lambda_n$. 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 ξ and η 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 ϕ forces ϕ 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 ξ 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 Γ yields the invariant optimal measure $\overline{\xi}$ in the closed convex hull of the $\xi \circ \gamma$, $\gamma \in \Gamma$. □

Remark 2.3: Continuing the situation in the proof, we observe that optimality of ξ alone implies

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

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

$$\xi \text{ is optimal iff } \mathrm{tr}\, A(\eta) \leq n \text{ for all designs } \eta \text{ on } X. \qquad \ldots(**)$$

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

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

now implies the following:

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

Proof: Choosing an optimal η in the trace formula gives

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

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

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

For an arbitrary basis $g = (g_1, \ldots, g_n)^t$ of $\mathrm{Pol}_e(X)$ with Gram matrix $M(\xi) = [(g_i, g_j)_\xi]$, 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 ξ is rotatable iff $d(x,\xi)$ depends only on the Γ-orbit of ξ. 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

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

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

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

for the components. It is well-known that

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

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

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 ξ on RS has ***strength*** t if any one of the following equivalent conditions holds for all $f \in \mathrm{Pol}_t(RS)$:

(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: $\mathrm{Pol}_i(RS) \cdot \mathrm{Pol}_j(RS) = \mathrm{Pol}_{i+j}(RS)$.

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 $\mathrm{Hom}(\mathbb{R}^d)$, and for $\mathrm{Pol}(\mathbb{R}^d)$.

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

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

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

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

For invariant designs ξ the variables may be separated:

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

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

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

Theorem 3.5 : *Let ξ 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 $|R_0| \le e+1$ such that the even moments of ξ are given by*

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

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 $w : R_0 \to \mathbb{R}^+$ such that, for $i = 0, 1, \ldots, e$,

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

The powers of r are polynomials of degree $\le 2e+1$ 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

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

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 ξ of degree e the conclusion of Theorem 3.5 is that the inner product on $\mathrm{Pol}_e(RS)$ 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

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

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

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

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 $\operatorname{vol}_e(\xi)$ is a finite dimensional problem.

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

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

Here $\operatorname{Harm}_k(\mathbb{R}^d)$ 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

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

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

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

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

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

hence the polynomials $r^{2j} f_{k,i}(y)$ constitute an independent basis for $\operatorname{Pol}_e(RS)$, which we call a *harmonic basis* for $\operatorname{Pol}_e(RS)$. We calculate their inner products $\langle\cdot,\cdot\rangle_\xi$ corresponding to the invariant design ξ 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 μ_{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 ρ 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 ρ. Since R is compact the maximum of det G is attained for an invariant measure ξ^*, 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 μ_{2e}, since μ_{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 ρ.

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

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

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

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

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

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

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

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

The unknown δ 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

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

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

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. α and δ 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 α and δ we refer to [1], and for numerical results to [13].

5. Optimal Experimental Designs

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

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

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*

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

where μ^*_{2i} are the moments of the solution ξ^* 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. □

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

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

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

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

In particular, if ξ is optimal then η is optimal as well. By approximating the weights of η 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 obatin:

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

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

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:

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

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

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 μ^*_{2i}.

We observe that also $r_1X^{\gamma_1}\cup\cdots\cup r_nX^{\gamma_n}$ works, for any $\gamma_i\in O(d)$, since by definition [5] the spherical $2e$-design satisfies

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

Acknowledgement. The authors thank B. Bagchi for several useful remarks, for instance on Definition 3.1, part (i).

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