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Optimum Experimental Designs with a Lack of a Priori Information I

Designs for the Estimation of a Finite-dimensional Set of Functionals

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Designs of regression experiments with uncorrelated observations are considered. The continuity of the observed "response function" is the only a priori information known by the experimenter. Optimum designs for estimating several linear functionals (parameters of the response function) are studied and an algorithm is proposed for computing such designs. An example is given.

1. INTRODUCTION AND RESULTS

The aim of this paper is to continue in the investigation of designs of infinite-dimensional regression experiments with uncorrelated observations, which was begun in [3]. The set-up in the present paper is a special case of the one in [3]; namely we shall suppose that

i) the "set of regulating points" A is a compact metric space,*

ii) the experimenter has a lack of a priori information about the form of the "response function" and he knows only that the response function is a continuous function in A.

Let us denote by $\mathscr{F}$ the Borel σ-algebra on A and by Θ the set of possible response functions, Θ will be the set of all continuous real functions defined in A.* As described in [3], the experimenter observes the values of uncorrelated random variables $X_\theta(a)$; $a \in A$ with the means

$$\mathrm{E}X_\theta(a) = \theta(a)\,,$$

* In Section 5 it is shown that we may suppose that A is a locally compact Hausdorff space, Θ is the set of all functions defined in A which are zero outside a countable union of compact subsets of A and $\mathscr{F}$ is the Baire σ-algebra.

and the variances

$$\mathrm{D}X_\theta(a) = 1\ ; \quad a \in A\ .$$

(If $\mathrm{D}X_\theta(\cdot)$ is a continuous function in A, then the estimation and design problem may be transformed into an equivalent one with $\mathrm{D}X_\theta(\cdot) = 1$, [3].)

A *design* of the experiment is a probability measure ξ on $\mathscr{F}$. For every $F \in \mathscr{F}$, $\xi(F)$ is proportional to the number of observations performed on the set F. Therefore we may say in a generalized set-up that the experimenter observes random variables $X_\theta(F)$; $F \in \mathscr{F}$, with the means and the covariances

$$\mathrm{E}X_\theta(F) = \int_F \theta\, \mathrm{d}\xi\ , \quad \operatorname{cov}\left[X_\theta(F),\, X_\theta(F')\right] = \xi(F \cap F')\ .$$

The aim of the experimenter is to estimate real functionals defined on the set Θ by linear unbiased estimates with minimal variances. A (*linear*) *estimate* is here a set of random variable $\{Y_\theta : \theta \in \Theta\}$ with Y_θ in the span of the set $\{X_\theta(F) : F \in \mathscr{F}\}$ in the Hilbert space of random variables with finite variances. The estimate is an *unbiased estimate* for a functional g if $g(\theta) = \mathrm{E}Y_\theta$ for every $\theta \in \Theta$. (For details see [3]). We shall say briefly that g *is estimable* if there is an unbiased linear estimate for g and we speak about the variance of g instead of the variance of the best linear estimate for g.

In Part I optimal designs for the estimation of a finite-dimensional set of functionals are studied. In Part II optimal designs for the estimation of the whole response function will be specified. In both parts it is a problem of an infinite-dimensional regression experiment since the dimension of Θ is infinite.

It is proved in Section 2 that any functional which is estimable at least with respect to one design has the form

$$g(\theta) = \int \theta\, \mathrm{d}\upsilon\ ; \quad \theta \in \Theta\ ,$$

where υ is a finite generalized measure on $(A, \mathscr{F})$. There is a unique optimal design for estimating g and it is equal to $(\upsilon^+ + \upsilon^-)/[\upsilon^+(A) + \upsilon^-(A)]$, where $\upsilon = \upsilon^+ - \upsilon^-$ is the Jordan decomposition of υ (Lemma 3).

If $g_1, \ldots, g_n$ are linearly independent functionals: $g_i(\cdot) = \int .\, \mathrm{d}\upsilon_i$; $i = 1, 2, \ldots, n$, then they always may be estimated simultaneously (under a suitably chosen design). We shall specify a complete class of decisions in the following decision problem (Theorem 4): The strategy space of the chance is the linear span $\mathscr{L}$ of $\{g_1, \ldots, g_n\}$. The decision space of the experimenter is the set Ξ of all designs which allow the simultaneous estimation of $g_1, \ldots, g_n$. The loss of the experimenter is the variance of $g \in \mathscr{L}$ under a design $\xi \in \Xi$.

In Theorem 5 there is a proof of the existence and uniqueness of a design which minimalizes the determinant of the covariance matrix D of $g_1, \ldots, g_n$ under some restrinctions on $g_1, \ldots, g_n$. In Theorem 6 the convergence of an iterative procedure for computing this optimum design is proved. The obtained algorithm allows the computation of optimum designs for an arbitrary finite-dimensional set of functionals G. It is sufficient to take a maximal linearly independent subset of G, $g_1, \ldots, g_n$ and to compute the design which minimalizes the determinant of the covariance matrix of $g_1, \ldots, g_n$: $\det D$. The ordering of designs according to the $\det D$ does not depend on the choice of the maximal linearly independent set in G (Lemma 7). The optimum design is computed in an illustrative example at the end of the paper (the estimation of four trigonometric coefficients of a continuous function defined in $\langle 0, 2\pi \rangle$).

2. THE COMPARISON OF DESIGNS AND THE COMPLETE CLASS THEOREM

We shall use the following statements discused in [3]:

1. A functional $g(\cdot)$ on Θ is estimable under a design ξ iff there is an $l \in L_2(A, \mathscr{F}, \xi)$ such that

$$g(\theta) = \int \theta l \, \mathrm{d}\xi \, ; \quad \theta \in \Theta \, . \tag{1}$$

2. The covariance of two functionals $g_1(\cdot)$, $g_2(\cdot)$ which are estimated under ξ is equal to

$$\operatorname{cov}_\xi (g_1, g_2) = \int (P_\Theta l_1) (P_\Theta l_2) \, \mathrm{d}\xi \, , \tag{2}$$

where P_Θ is the projection of $L_2(A, \mathscr{F}, \xi)$ onto the closure of Θ in $L_2(A, \mathscr{F}, \xi)$.

If υ is a finite generalized measure on $(A, \mathscr{F})$, we denote by υ^+, υ^- the components of the Jordan decomposition of υ and by $\bar{\upsilon}$ the measure $\bar{\upsilon} = (\upsilon^+ + \upsilon^-)/[\upsilon^+(A) + \upsilon^-(A)]$.

Lemma 1. A functional g defined on Θ is estimable under at least one design ξ iff there is a finite generalized measure υ defined on $(A, \mathscr{F})$ and such that

$$g(\theta) = \int \theta \, \mathrm{d}\upsilon \, ; \quad \theta \in \Theta \, . \tag{3}$$

Proof. If (1) is true for some ξ, we take $\upsilon(F) = \int_F l \, \mathrm{d}\xi$; $F \in \mathscr{F}$. We have $[\upsilon^+(A) + \upsilon^-(A)]^2 \leqq \int l^2 \, \mathrm{d}\xi < \infty$. If (3) is true for some finite generalized measure υ, consider the design $\bar{\upsilon}$. Evidently

$$g(\theta) = \int \theta \frac{d\upsilon}{d\bar{\upsilon}} d\bar{\upsilon} ; \quad \theta \in \Theta$$

and $d\upsilon/d\bar{\upsilon}$ is bounded on A; $d\upsilon/d\bar{\upsilon} \in L_2(A, \mathscr{F}, \bar{\upsilon})$.

Using a known result from the measure theory [1, § 56], we remark here that g is estimable under at least one design iff it can be expressed as a difference of two positive linear functionals on Θ.

Lemma 2. The covariance of two functionals g_1, g_2 which are estimated under the design ξ is equal to

$$\text{(4)} \qquad \operatorname{cov}_\xi (g_1, g_2) = \int \frac{d\upsilon_1}{d\xi} \frac{d\upsilon_2}{d\xi} d\xi ,$$

where υ_1, υ_2 are the generalized measures associated with g_1, g_2 according to Lemma 1.

Proof. From (2) it follows that it is sufficient to prove that Θ is dense in $L_2(A, \mathscr{F}, \xi)$. Any Borel probability measure on a metric space is regular [2, II, 1]. That means, to $F \in \mathscr{F}$ and to $\varepsilon > 0$ we may find an open (closed) set $U \supset F$ $(C \subset F)$ such that $\xi(U - C) < \varepsilon$. Further we may find a continuous function θ_ε which is zero on U^c and is equal to one on C and such that $0 \leqq \theta_\varepsilon(a) \leqq 1$; $a \in A$.
Therefore

$$\|\chi_F - \theta_\varepsilon\|^2 = \int_{U-C} |\chi_F - \theta_\varepsilon|^2 d\xi < \varepsilon .$$

Hence Θ is dense in the set $\{\chi_F : F \in \mathscr{F}\}$ and therefore also in $L_2(A, \mathscr{F}, \xi)$. □

Lemma 3. Let g be an estimable functional. Then

$$\text{(5)} \qquad \min_\xi \operatorname{var}_\xi g = \operatorname{var}_{\bar{\upsilon}} g = [\upsilon^+(A) + \upsilon^-(A)]^2 ,$$

where υ is the generalized measure associated with g. $\bar{\upsilon}$ is the unique design which minimalizes $\operatorname{var}_\xi g$.

Proof. For any design ξ we may write

$$\operatorname{var}_\xi g = \int \left(\frac{d\upsilon}{d\xi}\right)^2 d\xi = [\upsilon^+(A) + \upsilon^-(A)]^2 \int \left(\frac{d\bar{\upsilon}}{d\xi}\right)^2 d\xi \geqq$$

$$\geqq [\upsilon^+(A) + \upsilon^-(A)]^2 \left[\int \frac{d\bar{\upsilon}}{d\xi} d\xi\right]^2 = [\upsilon^+(A) + \upsilon^-(A)]^2 ,$$

where the equality occurs iff $d\bar{\upsilon}/d\xi = 1$ a.e. $[\xi]$. □

Consider a set $g_1, \ldots, g_n$ of functionals

$$g_i(\theta) = \int \theta \, \mathrm{d}\upsilon_i \, ; \quad \theta \in \Theta \, , \quad i = 1, 2, \ldots, n \, .$$

They are simultaneously estimable under the design

$$\varkappa = \frac{1}{n} \sum_{i=1}^{n} \bar{\upsilon}_i \, ,$$

as follows from (1). If ξ is a design and $g_1, \ldots, g_n$ are estimable under ξ, we denote by $D(\xi)$ the covariance matrix of $g_1, \ldots, g_n$. According to (4) we may write

$$D_{ij}(\xi) = \int f_i f_j \frac{\mathrm{d}\zeta}{\mathrm{d}\xi} \, \mathrm{d}\zeta \, ; \quad i, j = 1, \ldots, n \, , \tag{6}$$

where

$$f_i = \frac{\mathrm{d}\upsilon_i}{\mathrm{d}\zeta} \, ; \quad i = 1, \ldots, n \, ,$$

and where ζ is a design such that $\zeta \sim \varkappa$.

Evidently $\det D \neq 0$ iff $g_1, \ldots, g_n$ are linearly independent. We take a fixed ζ such that $\mathrm{d}\zeta/\mathrm{d}\varkappa$ is bounded and we denote by $\mathscr{A}$ the minimal σ-algebra which ensures the measurability of $f_1, \ldots, f_n$.

Theorem 4. Let ξ be a design such that $g_1, \ldots, g_n$ are estimable under ξ. Then there is a design μ such that

a) $\upsilon_i(F) = 0$; $i = 1, 2, \ldots, n$ iff $\mu(F) = 0$,

b) $\mathrm{d}\mu/\mathrm{d}\zeta$ is an $\mathscr{A}$-measurable function,

c) $g_1, \ldots, g_n$ are estimable under the design μ,

d) the matrix $D(\xi) - D(\mu)$ is nonnegative definite.

Proof. We have $\zeta \ll \xi$ since $\upsilon_i \ll \xi$; $i = 1, \ldots, n$. Further $\mathrm{d}\zeta/\mathrm{d}\xi$ is integrable with respect to ζ since $(\mathrm{d}\upsilon_i/\mathrm{d}\xi)^2$ and therefore also $(\mathrm{d}\zeta/\mathrm{d}\xi)^2$ are integrable with respect to ξ.

Denote

$$\psi_1 = \mathrm{E}_\zeta \left[\frac{\mathrm{d}\zeta}{\mathrm{d}\xi} \middle| \mathscr{A} \right] ,$$

the conditional mean of $\mathrm{d}\zeta/\mathrm{d}\xi$ with respect to ζ under the condition that the algebra $\mathscr{A}$ is given. We may decompose $\xi : \xi = \xi_0 + \xi_1$, where $\xi_0 \sim \zeta$ and $\xi_1 \perp \zeta$ (the Lebesgue theorem of measure theory [1]).

Denote

$$\psi_2 = \mathrm{E}_\zeta\left[\frac{\mathrm{d}\xi_0}{\mathrm{d}\zeta}\middle| \mathscr{A}\right]$$

and define the design μ by

$$\mu(F) = \int_F \psi_2 \,\mathrm{d}\zeta/\xi_0(A)\,; \quad F \in \mathscr{F}\,. \tag{7}$$

Evidently

$$\psi_1\psi_2 \geqq \mathrm{E}_\zeta^2\left[\left(\frac{\mathrm{d}\zeta}{\mathrm{d}\xi}\right)^{1/2}\left(\frac{\mathrm{d}\xi_0}{\mathrm{d}\zeta}\right)^{1/2}\middle| \mathscr{A}\right] = 1$$

Thus using (6) we obtain for any numbers $a_1, \ldots, a_n$:

$$\sum_{i,j=1}^{n} a_i D_{ij}(\xi)\, a_j = \mathrm{E}_\zeta\left\{\left(\sum_{i=1}^{n} a_i f_i\right)^2 \mathrm{E}_\zeta\left[\frac{\mathrm{d}\zeta}{\mathrm{d}\xi}\middle| \mathscr{A}\right]\right\} \geqq$$

$$\geqq \mathrm{E}_\zeta\left\{\left(\sum_{i=1}^{n} a_i f_i\right)^2 \frac{\mathrm{d}\zeta}{\mathrm{d}\mu}\right\}\Big/\xi_0(A) \geqq \sum_{i,j=1}^{n} a_i D_{ij}(\mu)\, a_j\,.$$

Evidently $\mathrm{d}\upsilon_i/\mathrm{d}\mu = (\mathrm{d}\upsilon_i/\mathrm{d}\zeta)(\mathrm{d}\zeta/\mathrm{d}\mu)$; $i = 1, \ldots, n$, are $\mathscr{A}$-measurable functions. If $\upsilon_i(F) = 0$; $i = 1, \ldots, n$, then $\zeta(F) = 0$ and, according to (7) also $\mu(F) = 0$. □

Theorem 4 implies that the set of designs which have the properties a, b, is a complete class in the decision problem mentioned in the introduction. Indeed it is sufficient to realize that $\sum_{i,j=1}^{n} a_i D_{ij}(\xi)\, a_j$ is the variance of $g(\cdot) = \sum_{i=1}^{n} a_i g_i(\cdot)$ under the design ξ.

3. DESIGNS MINIMALIZING THE DETERMINANT OF THE COVARIANCE MATRIX

The ordering of designs according to the determinant of $D(\xi)$ is a criterion of optimality in the discussed decision problem. The importance of this criterion has been discussed many times; also in [3].

Theorem 5. Let $g_1, \ldots, g_n$ be linearly independent estimable functionals on Θ. Let us suppose that the σ-algebra $\mathscr{A}$ is a finite algebra.

There is a unique design μ such that

$$\min_\xi \det D(\xi) = \det D(\mu)\,,$$

where the minimum is taken over the set of all designs under which the functionals $g_1, \ldots, g_n$ are estimable. μ is the unique design which has the properties a, b, of Theorem 4 and which is the solution of the equation

$$\mu^2(B) = \frac{1}{n} \sum_{i,j=1}^{n} v_i(B)\, v_j(B) \{D^{-1}(\mu)\}_{ij} \tag{8}$$

for every atom B of the algebra $\mathscr{A}$.

Proof. We shall suppose in the proof, without restrictions on generality that $\zeta = \varkappa$. We shall use the following notation. $\mathscr{B}$ is the set of all atoms of $\mathscr{A}$ which have a positive measure $\varkappa$. Ξ is the set of all designs ξ such that $\xi \sim \varkappa$ and that $\mathrm{d}\xi/\mathrm{d}\varkappa$ is an $\mathscr{A}$-measurable function.

Designs from Ξ are uniquely determined by their values on $\mathscr{B}$. Ξ_0 is the set of all designs which minimalize det $D(\cdot)$. Ξ_1 is the set of all designs from Ξ which are the solution of (8). According to Theorem 4, $\Xi_0 \subset \Xi$.

1) We shall prove first that $\Xi_0 \neq \emptyset$. Denote

$$K = \{\{\alpha(B)\}_{B\in\mathscr{B}} : \alpha(B) \in R, \alpha(B) \geqq 0, \sum_{B\in\mathscr{B}} \alpha(B) = 1\} .$$

K is a compact set in a Euclidean space and it is the closure of Ξ. The function det $D(\cdot)$ is continuous on Ξ as it is evident from the expression

$$D_{ij}(\xi) = \sum_{B\in\mathscr{B}} \frac{v_i(B)\, v_j(B)}{\xi(B)} ; \quad i, j = 1, \ldots, n , \quad \xi \in \Xi \tag{9}$$

which follows from (6). We may extend det $D(\cdot)$ on K taking det $D(\cdot) = \infty$ on the boundary of K. The extension is continuous, since $\lim_{n\to\infty} \sum_{B\in\mathscr{B}} \xi_n^{-1}(B) = \infty$ implies $\lim_{n\to\infty} \det D(\xi) = \infty$. Therefore the infinum of det $D(\cdot)$ is attained on K and trivially it is finite. Hence it is attained on Ξ.

2) We shall prove that $\Xi_0 \subset \Xi_1$. Take $\mu \in \Xi_0$, $\xi \in \Xi$ and consider the design

$$\xi^\alpha = \alpha\xi + (1 - \alpha)\, \mu .$$

Evidently $\xi^\alpha \in \Xi$ for $\alpha \in (0 - \varepsilon, 1\rangle$, where ε is the min $\{\mu(B) : B \in \mathscr{B}\}$. Using a known formula of the matrix theory we obtain

$$\frac{\mathrm{d} \ln \det D(\xi^\alpha)}{\mathrm{d}\alpha} = \operatorname{Tr} D^{-1}(\xi^\alpha) \frac{\mathrm{d}D(\xi^\alpha)}{\mathrm{d}\alpha} ,$$

where the derivative exists and is continuous for $\alpha \in (0 - \varepsilon, 1\rangle$. Since μ maximalizes the function $\ln \det D(\cdot)$, we obtain by a simple computation

$$0 = \frac{\mathrm{d} \ln \det D(\xi^\alpha)}{\mathrm{d}\alpha}\bigg|_{\alpha=0} = \sum_{B \in \mathscr{B}} \left\{ \sum_{i,j=1}^{n} \frac{v_i(B)\, v_j(B)}{\mu^2(B)} D_{ij}^{-1}(\mu) - n \right\} \xi(B),$$

for every $\xi \in \Xi$. Therefore μ is the solution of (8).

3) We shall use the notation

$$(10) \qquad \varphi(a, \xi) = \sum_{i,j=1}^{n} \frac{\mathrm{d}v_i}{\mathrm{d}\varkappa}(a) \frac{\mathrm{d}v_j}{\mathrm{d}\varkappa}(a) \left[\frac{\mathrm{d}\varkappa}{\mathrm{d}\xi}(a)\right]^2 D_{ij}^{-1}(\xi); \quad a \in A, \xi \in \Xi.$$

For every $\varepsilon > 0$ we may consider a two-person game $\Gamma_\varepsilon = (\Xi_\varepsilon, \Xi_\varepsilon, H)$. Here the strategy space is $\Xi_\varepsilon = \{\xi : \xi \in \Xi, \xi(B) \geqq \varepsilon, B \in \mathscr{B}\}$; it is a compact convex set in a Euclidean space. The pay-off function H is

$$(11) \qquad H(\xi, \eta) = \operatorname{Tr} D^{-1}(\xi)\, D(\eta); \quad \xi, \eta \in \Xi.$$

It is continuous on $\Xi_\varepsilon \times \Xi_\varepsilon$, concave in ξ and convex in η, as it follows from (9). Therefore if $\Xi_\varepsilon \neq \emptyset$, the game Γ_ε has a value ϑ_ε and the players have optimal strategies $\xi_\varepsilon, \eta_\varepsilon$.

Take $\mu \in \Xi_0$ and take $\varepsilon > 0$ such that $\mu \in \Xi_\varepsilon$. Then $\mu \in \Xi_\delta$ for every $\delta : 0 < \delta < \varepsilon$. $\operatorname{Tr} D^{-1}(\mu)\, D(\eta)$ is the sum and $\det D^{-1}(\mu)\, D(\eta)$ is the product of the eigenvalues of the matrix $D^{-1}(\mu)\, D(\eta)$. Therefore using the inequality between the arithmetic and the geometric means we obtain

$$(12) \qquad n \leqq n \left[\frac{\det D(\eta)}{\det D(\mu)}\right]^{1/n} \leqq \operatorname{Tr} D^{-1}(\mu)\, D(\eta); \quad \eta \in \Xi.$$

Therefore $\vartheta_\delta \geqq \inf_{\eta = \Xi} \operatorname{Tr} D^{-1}(\mu)\, D(\eta) \geqq n = \operatorname{Tr} D^{-1}(\xi_\delta)\, D(\xi_\delta) \geqq \vartheta_\delta$. Thus n is the value of Γ_δ, μ is an optimal strategy of Player I, and according to (12) every optimal strategy of Player II is in Ξ_0; this is true for $\delta \leqq \min \{\mu(B) : B \in \mathscr{B}\}$.

4) We shall prove that Ξ_1 is a one-point subset of Ξ_0. Tak $\lambda \in \Xi_1$, $\mu \in \Xi_0$ and find $\varepsilon > 0$ so that $\lambda, \mu \in \Xi_\varepsilon$. Then for every $\delta < \varepsilon$ we may write $\vartheta_\delta \geqq \operatorname{Tr} D^{-1}(\lambda)\,.$ $.\, D(\eta_\delta) = \int \varphi(\cdot, \lambda)\, (\mathrm{d}\lambda/\mathrm{d}\eta_\delta)^2\, \mathrm{d}\eta_\delta = n \int [\mathrm{d}\lambda/\mathrm{d}\eta_\delta]^2\, \mathrm{d}\eta_\delta \geqq n[\int (\mathrm{d}\lambda/\mathrm{d}\eta_\delta)\, \mathrm{d}\eta_\delta]^2 = n = \vartheta_\delta$. The equality $\int (\mathrm{d}\lambda/\mathrm{d}\eta_\delta)^2\, \mathrm{d}\eta_\delta = [\int (\mathrm{d}\lambda/\mathrm{d}\eta_\delta)\, \mathrm{d}\eta_\delta]^2$ implies $\mathrm{d}\lambda/\mathrm{d}\eta_\delta = 1$ a.e. $[\eta_\delta]$. Thus λ is the unique strategy of Player II in the game Γ_δ. Therefore Ξ_1 is a one-point set. According to part 3 of the proof we have $\lambda \in \Xi_0$. □

Theorem 5 allows to construct an algorithm for an iterative computation of the desing μ minimalizing det $D(\cdot)$. Let us denote by U the mapping

$$(U\eta)(F) = \int_F \sqrt{[\varphi(\cdot, \eta)/n]}\, d\eta \,; \quad F \in \mathscr{F} \tag{13}$$

which will be defined for every finite measure η on $(A, \mathscr{F})$ and $\varphi(a, \eta)$ is given by the expression (10). If the algebra $\mathscr{A}$ is finite we obtain the following formula, equivalent to (13):

$$(U\eta)(B) = \left[\frac{1}{n} \sum_{i,j=1}^{n} v_i(B)\, D_{ij}^{-1}(\eta)\, v_j(B)\right]^{1/2} ; \quad B \in \mathscr{B} \tag{14}$$

where $D(\eta)$ is given by (9).

We shall denote by W the set of finite measures: $W \equiv \{\eta : \eta/\eta(A) \in \Xi\}$.

Theorem 6. Let us suppose that the algebra $\mathscr{A}$ is finite and let ξ be a design: $\xi \in \Xi$. Then

a) U mapps W into W and μ is the unique fixed point of U in W. Moreover $(U^n\xi)(A) \leqq 1$ for every $n = 1, 2, \ldots$ with equality iff $\xi = \mu$.

b)

$$\sum_{B \in \mathscr{B}} \frac{[(U^n\xi)(B) - \mu(B)]^2}{\mu(B)} \leqq 2[1 - (U^n\xi)(A)] ; \quad n = 1, 2, \ldots \tag{15}$$

c) The sequence $\{U^n\xi\}_{n=1}^{\infty}$ has a subsequence which converges to μ.

Proof. a) Take $\eta \in W$ and denote $\bar{\eta} = \eta/\eta(A)$. We have

$$(U\eta)(A) = \eta^{1/2}(A) \int [\varphi(\cdot, \bar{\eta})/n]^{1/2}\, d\bar{\eta} \leqq \tag{16}$$

$$\leqq \eta^{1/2}(A) \left[\int (\varphi(\cdot, \bar{\eta})/n)\, d\bar{\eta}\right]^{1/2} = \eta^{1/2}(A)$$

with equality iff $\bar{\eta} = \mu$. Denote

$c = \min_{B \in \mathscr{B}} \left[\frac{1}{n} \sum_{i,j=1}^{n} v_i(B)\, Q_{ij}\, v_j(B)\right]^{1/2}$, where $Q_{ij} = \sum_{B \in \mathscr{B}} v_i(B)\, v_j(B)$. From (14) we obtain

$$(U\eta)(B) \geqq [\min_{B \in \mathscr{B}} \eta(B)]^{1/2}\, c \tag{17}$$

Therefore $\min_{B\in\mathscr{B}} \eta(B) < c^2$ implies $\min_{B\in\mathscr{B}} (U\eta)(B) > \min_{B\in\mathscr{B}} \eta(B)$, and $\min_{B\in\mathscr{B}} \eta(B) \geqq c^2$ implies $\min_{B\in\mathscr{B}} (U\eta)(B) > c^2 > 0$. It follows that U mapps W into W.

From the inequality (16) it follows

$$(18) \qquad (U^n\xi)(A) \leqq [(U^{n-1}\xi)(A)]^{1/2} \leqq \ldots \leqq [\xi(A)]^{1/2n} = 1$$

with equality iff $\xi = \mu$. Theorem 5 implies that μ is the fixed point of U. On the other hand if $\lambda \in W$, and $U\lambda = \lambda$ then

$$\lambda(A) = \sum_{B\in\mathscr{B}} \frac{1}{n} \sum_{i,j=1}^{n} \frac{v_i(B)\, D_{ij}^{-1}(\lambda)\, v_j(B)}{\lambda(B)} = \frac{1}{n} \operatorname{Tr} D^{-1}(\lambda)\, D(\lambda) = 1\,,$$

i.e. $\lambda \in \Xi$. But, according to Theorem 5, μ is the unique fixed point of U in Ξ.

b) From the proof of Theorem 5 it follows

$$\int\left(\frac{\mathrm{d}U\eta}{\mathrm{d}\mu}\right)^2 \mathrm{d}\mu = \int\frac{\varphi(\cdot,\eta)}{n}\left(\frac{\mathrm{d}\eta}{\mathrm{d}\mu}\right)^2 \mathrm{d}\mu = \frac{\eta(A)}{n} \operatorname{Tr} D^{-1}(\eta)\, D(\mu) \leqq \eta(A)\,.$$

Therefore

$$\sum_{B\in\mathscr{B}} \frac{[(U^n\xi)(B) - \mu(B)]^2}{\mu(B)} = \sum_{B\in\mathscr{B}} \frac{\{U[U^{n-1}\xi](B)\}^2}{\mu(B)} - 2(U^n\xi)(A) + 1 \leqq$$

$$\leqq 2[1 - (U^n\xi)(A)]\,.$$

c) Denote $\delta = \min\{c, \min_{B\in\mathscr{B}} \xi(B)\} > 0$, and $C = \{\eta : \eta \in W, \min_{B\in\mathscr{B}} \eta(B) \geqq \delta\}$. According to (17) $U^n\xi \in C$; $n = 0, 1, 2, \ldots$. The set of all limit points of $\{U^n\xi\}_{n=1}^{\infty}$ is nonvoid and compact, since C is compact. Denote by S the minimal convex set containing all limit points of $\{U^n\xi\}_{n=1}^{\infty}$. It is also compact and, according to the Brawer fixed point theorem, S contains a fixed point of the mapping U. Part a) of Theorem 6 implies that $\mu \in S$. Therefore $\mu = \sum_{i=1}^{N} \alpha_i\xi_i$, where $\alpha_i > 0$, $\sum_{i=1}^{N} \alpha_i = 1$ and $\xi_1, \ldots, \xi_N$ are limit points of $\{U^n\xi\}_{n=1}^{\infty}$. It follows that $\xi_1(A) = \ldots = \xi_N(A) = 1$. Hence (17) and (18) imply $\xi_1 = \ldots = \xi_N = \mu$. □

The design μ is computed if we start by an arbitrary $\xi \in \Xi$ and compute subsequently $U\xi$, $U^2\xi$, etc. At each step we compute $(U^n\xi)(A) = \sum_{B\in\mathscr{B}} (U^n\xi)(B)$, which is always less than one. If $(U^n\xi)(A)$ is near to one, then, according (15), $U^n\xi$ is "almost" the optimum design μ. Part c) of Theorem 6 ensures that this is always attained by a finite number of steps.

4. OPTIMUM DESIGNS FOR ARBITRARY FINITE-DIMENSIONAL SETS OF FUNCTIONALS

Let G be a set of linear functionals and $\mathscr{L}(G)$ the linear span of G; we consider the case of $\mathscr{L}(G)$ being finite-dimensional. Denote by $g_1, \ldots, g_n$; $h_1, \ldots, h_n$ two maximal linearly independent subsets of $\mathscr{L}(G)$.

Lemma 7. $g_1, \ldots, g_n$ are estimable under ξ iff every $g \in G$ is estimable under ξ. For any two designs ξ, η allowing the simultaneous estimability of $\mathscr{L}(G)$ we have

$$\frac{\det D^g(\xi)}{\det D^g(\mu)} = \frac{\det D^h(\xi)}{\det D^h(\mu)},$$

where D^g; D^h are the covariance matrices of $g_1, \ldots, g_n$; $h_1, \ldots, h_n$.

Proof. Take $g = \sum_i \alpha_i g_i \in G$. If $\upsilon_1, \ldots, \upsilon_n$ are the generalized measures associated with $g_1, \ldots, g_n$ then $\mathrm{d}\upsilon_i/\mathrm{d}\xi \in L_2(A, \mathscr{F}, \xi)$; $i = 1, \ldots, n$ imply $\sum_i \alpha_i(\mathrm{d}\upsilon_i/\mathrm{d}\xi) \in L_2(A, \mathscr{F}, \xi)$ and the first statement follows from (1).

There is a non-singular $n \times n$ matrix J such that

$$g_i(\theta) = \sum_{j=1}^{n} J_{ij} h_j(\theta)\,; \quad \theta \in \Theta\,, \quad i = 1, \ldots, n\,.$$

Using (6) we obtain

$$D^g(\xi) = J\, D^h(\xi)\, J\,.$$

Therefore $\det D^g(\xi) = (\det J)^2 \det D^h(\xi)$. □

5. REMARKS ABOUT DESIGNS ON LOCALLY COMPACT HAUSDORFF SPACES

In most applications it is sufficient to suppose that A is a compact metric space. However, we may repeat all the statements of Sections 2–4 if:

i) A is a locally compact Hausdorff space,

ii) if Θ is the set of all functions continuous in A each of which is zero ouside a compact subset of A (the same is obtained if Θ is the set of all functions which are continuous and each of which is zero outside a countable union of compact subsets of A), and

iii) if a design is a probability (Baire) measure on the minimal σ-algebra which ensures the measurability of every $\theta \in \Theta$ (the Baire σ-algebra).

To prove this the following statements, taken from [1, chapt. 10], have to be used:

A) If $C \subset A$ is compact, $F \subset A$ is closed and $C \cap F = \emptyset$, then there is a continuous function $f : f(a) \in \langle 0, 1 \rangle$; $a \in A$, $f(a) = 1$ for $a \in C$, $f(a) = 0$ for $a \in F$.

B) If C is a compact Baire set, then there is a decreasing sequence of open sets $\{U_n\}_{n=1}^{\infty}$ such that

a) $C = \bigcap_{n=1}^{\infty} U_n$.

b) There is a compact set C_0 such that $U_1 \subset C_0$.

C) Every Baire measure ξ is regular, that means to every $\varepsilon > 0$ and every Baire set F we may find a compact Baire set $C \subset F$ and an open set $U \supset F$ such that $\xi(U - F) < \varepsilon$.

The statements A, B, C imply that Θ is dense in $L_2(A, \mathscr{F}, \xi)$ (as in Lemma 2), where $\mathscr{F}$ is now the Baire σ-algebra. Any other statement depends on the topology of A, on the set Θ and on the σ-algebra $\mathscr{F}$ only through Lemma 2.

Example. Take $A = \langle 0, 2\pi \rangle$. Any $\theta \in \Theta$ may be expressed by a trigonometric series

$$\theta(a) = \sum_{i=1}^{\infty} \alpha_i \cos ia + \sum_{i=1}^{\infty} \beta_i \sin ia .$$

Suppose that the experimenter will estimate the truncated series

$$\tilde{\theta}(a) = \alpha_0 + \alpha_1 \cos a + \beta_1 \sin a + \beta_2 \sin 2a .$$

An optimum design is thus the design which gives a minimum for the determinant of the covariance matrix of the functionals

$$g_0(\theta) = \int_0^{2\pi} \theta(x) \, dx ,$$

$$g_1(\theta) = \int_0^{2\pi} \sin x \, . \, \theta(x) \, dx ,$$

$$g_2(\theta) = \int_0^{2\pi} \cos x \, . \, \theta(x) \, dx ,$$

$$g_3(\theta) = \int_0^{2\pi} \sin 2x \, . \, \theta(x) \, dx .$$

For computational reasons we have divided $\langle 0, 2\pi \rangle$ into 50 intervals $I_1, \ldots, I_{50}$ of equal length, and we have computed in fact the optimum designs for the functionals

$$\tilde{g}_i(\theta) = \int h_i(x)\, \theta(\cdot)\, \mathrm{d}x\,; \quad i = 0, 1, 2, 3,$$

where

$$h_0(\cdot) = \sum_{i=1}^{50} \chi_{I_i}(\cdot)\,, \quad h_1(\cdot) = \sum_{i=1}^{50} \int_{I_i} \sin x\, \mathrm{d}x \,.\, \chi_{I_i}(\cdot)\,,$$

$$h_2(\cdot) = \sum_{i=1}^{50} \int_{I_i} \cos x\, \mathrm{d}x \,.\, \chi_{I_i}(\cdot)\,, \quad h_3(\cdot) = \sum_{i=1}^{50} \int_{I_i} \sin 2x\, \mathrm{d}x \,.\, \chi_{I_i}(\cdot)\,.$$

We started with the design $\xi : \xi(I_i) = i/1275$; $i = 1, 2, \ldots, 50$. The sequence $(U\xi)(A), \ldots, (U^{20}\xi)(A)$ was increasing and the sequence det $D(\xi), \ldots,$ det $D(U^{20}\xi)$ was decreasing. The computed optimum design is

$$\mu(I_1) = 0{\cdot}0173, \quad \mu(I_2) = 0{,}0181, \quad \mu(I_3) = 0{,}0195,$$
$$\mu(I_4) = 0{,}0206, \quad \mu(I_5) = 0{,}0217, \quad \mu(I_6) = 0{,}0224,$$
$$\mu(I_7) = 0{,}0226, \quad \mu(I_8) = 0{,}0221, \quad \mu(I_9) = 0{,}0212,$$
$$\mu(I_{10}) = 0{,}0199, \quad \mu(I_{11}) = 0{,}0186, \quad \mu(I_{12}) = 0{,}0176,$$
$$\mu(I_{13}) = 0{,}0173,$$

and it is periodic: $\mu(B) = \mu(B + \pi/2)$.

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