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Optimum Experimental Designs with a Lack of a Priori Information II

Designs for the Estimation of the Whole Response Function

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Experimental designs are studied in the case when the aim of the experimenter is "the interpolation" of the observed response function. The observations are supposed to be uncorrelated. No a priori properties of the response function are supposed, unless that it is continuous.

1. INTRODUCTION

In this part we shall consider the estimation of the whole function $\theta \in \Theta$. The notation and the assumptions on the sets A and Θ are the same as in Part I [3].

In Section 2 we specify first what an estimate for θ under a design ξ is. It is a second order random process $\{Z_\theta(a);\ a \in A\}$. which is continuous in the quadratic mean and such that every random variable $Z_\theta(a);\ a \in A$ is in the span of the set of random variables $\{X_\theta(F)\colon F \in \mathscr{F}\}$ (see (1)) observed in the experiment. The estimate is unbiased if the mean of the process is equal to θ. But, if the set A is uncountable, there is no unbiased estimate for θ. Therefore sequences of asymptotically unbiased and efficient estimates are used. We construct examples of such sequences (Lemma 1). The optimum properties of sequences of asymptotically unbiased and efficient estimates depend on the metric of A and not only on the topology induced by the metric. We must use the concept of a sequence of asymptotically unbiased and efficient estimates for θ which is adapted to the metric of A. In Lemma 2 we show that the sequence constructed in Lemma 1 is asymptotically the best of such sequences under a given design. If there is an isometry τ of A into a Euclidean space E^n such that the interior of $\tau(A)$ is nonvoid and the boundary of $\tau(A)$ is of the Lebesgue measure zero, then the Lebesgue measure in E^n which is normed to one on $\tau(A)$ gives asymptotically the optimum design for estimating $\theta \in \Theta$ (Theorem 3). The criterion for optimality which is used is a generalization of the minimax criterion used in the finitedimensional regression experiments [1, § 2].

Let ξ be a design, and

$$\mathscr{E}_\xi = \{\{X_\theta(F) : F \in \mathscr{F}, \xi(F) > 0\}; \theta \in \Theta\}$$

the variant of the experiment corresponding to the design ξ (see [2]). That means for every $\theta \in \Theta$

$$\{X_\theta(F) : F \in \mathscr{F}, \xi(F) > 0\} \tag{1}$$

is an orthogonal random set function with the properties

a)

$$X_\theta(\bigcup_{i=1}^{n} F_i) = \sum_{i=1}^{n} X_\theta(F_i) ,$$

for disjoint sets $F_1, \ldots, F_n$,

b)

$$\mathrm{E}\, X_\theta(F) = \int_F \theta \,\mathrm{d}\xi ,$$

$$\operatorname{cov}[X_\theta(F), X_\theta(F')] = \xi(F \cap F'); \; F, F' \in \mathscr{F} .$$

We denote by $L_2\{X_\theta(F) : F \in \mathscr{F}, \xi(F) > 0\}$ the span of the set (1) in the Hilbert space of all random variables with finite variances.

Intuitively a (linear) estimate for $\theta \in \Theta$ is a linear mapping from the „sample space" of the orthogonal random set function (1) into the set of all functions defined in A. This mapping and the random set function (1) may induce a random process on A. We shall express more exactly the intuitive feeling by the following definitions:

A (*linear*) *estimate* for $\theta \in \Theta$ (under the design ξ) is a class of second order random processes

$$\{Z_\theta(a);\, a \in A\};\; \theta \in \Theta ,$$

such that

i)

$$Z_\theta(a) \in L_2\{X_\theta(F) : F \in \mathscr{F}, \xi(F) > 0\} \; ; \quad \theta \in \Theta , \quad a \in A ,$$

ii)

$$\mathrm{E}\, Z_\theta(\cdot) \in \Theta \; ; \quad \theta \in \Theta ;$$

iii) the mapping

$$(a, a') \in A \times A \to \operatorname{cov}[Z_\theta(a), Z_\theta(a')]$$

does not depend on $\theta \in \Theta$ and is continuous on $A \times A$.

The *bias* of the estimate is the

$$\sup_{a\in A} |\mathrm{E}\, Z_\theta(a) - \theta(a)| \; ; \quad \theta \in \Theta \, .$$

The estimate is *unbiased* if the bias is zero. It is *efficient* if for every $a \in A$, $\{Z_\theta(a); \theta \in \Theta\}$ is the best linear estimate for $\mathrm{E}\, Z_\theta(a)$ (in the sense of [2]).

From Lemma 2 in Part I [3] it follows immediately that there is no unbiased estimate for $\theta \in \Theta$ if A is uncountable.

A sequence $\{\mathscr{Z}_n\}_{n=1}^{\infty}$ of estimates:

$$\mathscr{Z}_n = \{\{Z_\theta^{(n)}(a) : a \in A\}; \theta \in \Theta\} \; ; \quad n = 1, 2, \ldots,$$

is *asymptotically unbiased* if

$$\lim_{n\to\infty} \sup_{a\in A} |E\, Z_\theta^{(n)}(a) - \theta(a)| = 0 \; ; \quad \theta \in \Theta \, .$$

It is also *asymptotically efficient* if moreover $\{Z_\theta^{(n)}(a); \theta \in \Theta\}$ is the best linear estimate for $\mathrm{E}\, Z_\theta^{(n)}(a)$.

Denote by d the metric in A and by $G(n, a)$ the set $\{a' : a' \in A, d(a', a) < 1/n\}$ $(\overline{G(n, a)} = \{a' : a' \in A, d(a', a) \leqq 1/n\})$.

Lemma 1. Let ξ be a design such that $\xi(U) > 0$ for every open set $U \subset A$ (A is the support of ξ), and that $\xi[\overline{G(n, a)} - G(n, a)] = 0$; $n = 1, 2, \ldots$; $a \in A$. Denote by $\{S_\theta^{(n)}(a); \theta \in \Theta\}$ the best linear estimate for the functional $g_n(\cdot \mid a, \xi)$ under the design ξ, where

$$g_n(\theta|a, \xi) = \frac{\int_{G(n,a)} \theta \, \mathrm{d}\xi}{\xi(G(n, a))} \; ; \quad n = 1, 2, \ldots, a \in A \, , \quad \theta \in \Theta \, . \tag{2}$$

Then $\{\{S_\theta^{(n)}(a) : a \in A\}; \theta \in \Theta\}$; $n = 1, 2, \ldots$, is an asymptotically unbiased and efficient sequence of estimates for $\theta \in \Theta$.

Proof. According to Lemma 2 in Part I [3], the functionals $g_n(\cdot \mid a, \xi)$ are estimable under ξ and the covariance of the best linear estimate for $g_n(\cdot \mid a, \xi)$ and $g_n(\cdot \mid b, \xi)$ is equal to

$$\mathrm{cov}_\xi[g_n(\cdot \mid a, \xi), g_n(\cdot \mid b, \xi)] \equiv \mathrm{cov}\,[S_\theta^{(n)}(a), S_\theta^{(n)}(b)] = \\ = \frac{\xi[G(n, a) \cap G(n, b)]}{\xi[G(n, a)]\, \xi[G(n, b)]} \, . \tag{3}$$

Evidently, for every F_1, F_2. $F \in \mathscr{F}$ we may write: $|\xi(F_1) - \xi(F_2)| \leqq \xi(F_1 \,\Delta\, F_2)$ and $\xi((F_1 \cap F) \,\Delta\, (F_2 \cap F)) \leqq \xi(F_1 \,\Delta\, F_2)$. Hence for a_k, b_k, a, $b \in A$, we have

$$\begin{aligned} &|\xi[G(n, a_k) \cap G(n, b_k)] - \xi[G(n, a) \cap G(n, b)]| \leqq \\ &\leqq |\xi[G(n, a_k) \cap G(n, b_k)] - \xi[G(n, a_k) \cap G(n, b)]| + \\ &+ |\xi[G(n, a_k) \cap G(n, b)] - \xi[G(n, a) \cap G(n, b)]| \leqq \\ &\leqq \xi[G(n, b_k) \,\Delta\, G(n, b)] + \xi[G(n, a_k) \,\Delta\, G(n, a)]\,. \end{aligned}$$

To show the continuity of $\xi[G(n, \cdot) \cap G(n, \cdot)]/\xi[G(n, \cdot)]\, \xi[G(n, \cdot)]$ on $A \times A$ it is sufficient to prove that

$$\lim_{k \to \infty} \xi[G(n, a_k) \,\Delta\, G(n, a)] = 0 \tag{4}$$

if $\lim_{k \to \infty} d(a_k, a) = 0$.

We may write:

$$\begin{aligned} &\bigcap_{m=1}^{\infty} \bigcup_{k \geqq m} G(n, a_k) - \overline{G(n, a)} = \\ &= \{a' : \forall_{m \geqq 1} \exists_{k \geqq m}\, d(a', a_k) < 1/n\} \cap \{a' : d(a', a) > 1/n\} \subset \\ &\subset \{a' : \forall_{m \geqq 1} \exists_{k \geqq m}\, d(a', a) < 1/n + d(a, a_k)\} \cap \{a' : d(a', a) > 1/n\} = \emptyset\,. \end{aligned}$$

Thus $[\bigcup_{k \geqq m} G(n, a_k) - \overline{G(n, a)}] \searrow \emptyset$ with $m \to \infty$. Hence $0 \leqq \xi[G(n, a_m) - \overline{G(n, a)}] \leqq$ $\leqq \xi[\bigcup_{k \geqq m} G(n, a_k) - \overline{G(n, a)}] \to 0$. Analogically: $\bigcap_{m=1}^{\infty} [G(n, a) - \bigcap_{k=m}^{\infty} G(n, a_k)] =$ $= \{a' : d(a', a) < 1/n\} \cap \{a' : \forall_{m \geqq 1} \exists_{k \geqq m}\, d(a', a_k) \geqq 1/n\} = \emptyset$. Therefore $0 \leqq$ $\leqq \xi[G(n, a) - G(n, a_m)] \leqq \xi[G(n, a) - \bigcap_{k=m}^{\infty} G(n, a_k)] \to 0$ with $m \to \infty$ and (4) is proved.

Since

$$\begin{aligned} &\left| \int_{G(n,a)} \theta \,\mathrm{d}\xi - \int_{G(n,b)} \theta \,\mathrm{d}\xi \right| \leqq \\ &\leqq \sup_{a' \in A} |\theta(a')|\, \xi[G(n. a) \,\Delta\, G(n, b)]\,, \end{aligned}$$

the limit (4) implies also the continuity of $g_n(\theta \mid \cdot, \xi)$ in A.

Finally

$$\begin{aligned} &\sup_{a \in A} |g_n(\theta \mid a, \xi) - \theta(a)| \leqq \\ &\leqq \sup_{a \in A} \sup_{a' \in G(n,a)} |\theta(a') - \theta(a)| \to 0 \end{aligned}$$

with $n \to \infty$. □

In the sequel we shall assume that any design ξ satisfies the conditions stated in Lemma 1. Let $\{\mathscr{Z}_n\}_{n=1}^{\infty}$ be an asymptotically unbiased and efficient sequence of estimates for $\theta \in \Theta$ under the design ξ. We shall denote by $h_n(\cdot \mid a)$ the functional on Θ defined by

$$(5) \qquad h_n(\theta \mid a) = \mathrm{E}\, Z_\theta^{(n)}(a)\,; \quad \theta \in \Theta$$

That means that $Z_\theta^{(n)}(a)$ is the best linear estimate for $h_n(\cdot \mid a)$ and, analogically as in Part I, we denote by $\mathrm{var}_\xi\, h_n(\cdot \mid a)$ the variance of $Z_\theta^{(n)}(a)$. Since $h_n(\cdot \mid a)$ is estimable under ξ, there is a $\varphi_a^{(n)} \in L_2(A, \mathscr{F}, \xi)$ such that

$$(6) \qquad h_n(\theta \mid a) = \int \varphi_a^{(n)} \theta \, \mathrm{d}\xi\,; \quad \theta \in \Theta\,,$$

and

$$(7) \qquad \mathrm{var}_\xi\, h_n(\cdot \mid a) = \int [\varphi_a^{(n)}]^2 \, \mathrm{d}\xi$$

(see [2], theorem 4). We shall say that $\{\mathscr{Z}_n\}_{n=1}^{\infty}$ is *adapted to the metric of* A if for every $a \in A$, $n = 1, 2, \ldots$, the function $\varphi_a^{(n)}$ is zero outside of $G(n, a)$.

Lemma 2. If $\{\mathscr{Z}_n\}_{n=1}^{\infty}$ is an asymptotically unbiased and efficient sequence of estimates for $\theta \in \Theta$ under the design ξ, which is adapted to the metric of A, then

$$(8) \qquad \liminf_{n \to \infty} \frac{\mathrm{var}_\xi\, h_n(\cdot \mid a)}{\mathrm{var}_\xi\, g_n(\cdot \mid a, \xi)} \geqq 1\,; \quad a \in A\,.$$

Proof. We may write

$$(9) \qquad \left[\int \varphi_a^{(n)} \, \mathrm{d}\xi\right]^2 \leqq \xi[G(n, a)] \int [\varphi_a^{(n)}]^2 \, \mathrm{d}\xi\,.$$

The sequence $\{\mathscr{Z}_n\}_{n=1}^{\infty}$ is asymptotically unbiased and the function on A which is identically equal to 1, is an element of Θ. Hence

$$(10) \qquad \lim_{n \to \infty} \int \varphi_a^{(n)} \, \mathrm{d}\xi = 1\,.$$

The inequality (8) follows directly from (9) and (10). Moreover the convergence in (10) is uniform in A. Thus

$$(11) \qquad \forall_{\varepsilon > 0}\ \exists_{n_\varepsilon}\ \forall_{n \geqq n_\varepsilon}\ \forall_{a \in A}\ \mathrm{var}_\xi\, h_n(\cdot \mid a) \geqq (1 - \varepsilon)\, \mathrm{var}_\xi\, g_n(\cdot \mid a, \xi)\,. \qquad \square$$

If we omit the assumption that $\varphi_a^{(n)}$ is zero outside of $G(n, a)$, we may obtain contradictory results as the following example shows. Take $A = \langle 0, 1 \rangle$, ξ the Lebesgue measure on $\langle 0, 1 \rangle$. $\varphi_a^{(n)} = \chi_{G(n,a)} / \xi[G(2n, a)]$. Then

$$\lim_{n \to \infty} \frac{\mathrm{var}_\xi\, h_n(\cdot \mid a)}{\mathrm{var}_\xi\, g_n(\cdot \mid a, \xi)} = \lim_{n \to \infty} \frac{\xi[G(n, a)]}{\xi[G(2n, a)]} = 2;\ a \in (0, 1)\,;$$

thus "$g_n(\cdot \mid a, \xi)$ is better than $h_n(\cdot \mid a)$". On the other hand $\{h_n(\cdot \mid a)\}_{n=1}^{\infty}$ is a subsequence of $\{g_n(\cdot \mid a, \xi)\}_{n=1}^{\infty}$ and both sequences must be considered as asymtotically equivalent.

Denote by E^m the m-dimensional Euclidean space and by λ the Lebesgue measure on E^m. Let us suppose that there is an isometry τ of A into E^m such that the interior of $\tau(A)$ is nonvoid and the boundary of $\tau(A)$ has a zero measure λ. There is a sequence of compact sets $C_1 \subset C_2 \subset \ldots \subset A$ such that the sequence $\tau(C_1), \tau(C_2), \ldots$ converges to the interior of $\tau(A)$. (Since every open set in E^m is a F^σ – set.)

Theorem 3. Let $\{\mathscr{X}_n\}_{n=1}^{\infty}$ be an asymptotically unbiased sequence of estimates for $\theta \in \Theta$ under the design ξ, which is adapted to the metric of A. Then

$$\lim_{k\to\infty} \liminf_{n\to\infty} \frac{\sup\limits_{a\in C_k} \operatorname{var}_\xi h_n(\cdot \mid a)}{\sup\limits_{a\in C_k} \operatorname{var}_\mu g_n(\cdot \mid a, \mu)} \geqq 1$$

where $\mu(\cdot) = \lambda\tau(\cdot)/\lambda[\tau(A)]$.

Proof. Without restriction on generality we may suppose that $A \equiv \tau(A)$. From (3) it follows

$$(12)\quad \frac{\operatorname{var}_\xi h_n(\cdot \mid a)}{\operatorname{var}_\mu g_n(\cdot \mid a', \mu)} = \frac{\operatorname{var}_\xi h_n(\cdot \mid a)}{\operatorname{var}_\xi g_n(\cdot \mid a, \xi)} \cdot \frac{\mu[G(n, a')]}{\xi[G(n, a)]}\,; \quad a', a \in A\,, \quad n = 1, 2, \ldots$$

Take a compact set $C \subset A^0$ (A^0 is the interior of A), take $\varepsilon > 0$ and take n_ε according to (11). There is an $n_c \geqq n_\varepsilon$ such that for every $a \in C$ and every $n \geqq n_c$, $\{x : : x \in E^m, \|x - a\| < 1/n\} \subset A$. Denote $\delta_n = \mu\{x : x \in E^m, \|x\| < 1/n\}$. Using (11) and (12) we may write

$$\frac{\operatorname{var}_\xi h_n(\cdot \mid a)}{\sup\limits_{a'\in C} \operatorname{var}_\mu g_n(\cdot \mid a', \mu)} \geqq (1 - \varepsilon)\frac{\delta_n}{\xi[G(n, a)]}\,; \quad a \in C\,, \quad n \geqq n_c\,.$$

Hence for every $\varepsilon > 0$

$$\frac{\sup\limits_{a\in C} \operatorname{var}_\xi h_n(\cdot \mid a)}{\sup\limits_{a\in C} \operatorname{var}_\mu g_n(\cdot \mid a, \mu)} \geqq$$

$$\geqq (1 - \varepsilon)\frac{\delta_n}{\inf\limits_{a\in C} \xi[G(n, a)]}\,;$$

$$C \subset A^0\,, \quad n \geqq n_c\,.$$

Thus

$$\liminf_{n\to\infty} \frac{\sup_{a\in C} \operatorname{var}_\xi h_n(\cdot \mid a)}{\sup_{a\in C} \operatorname{var}_\mu g_n(\cdot \mid a, \mu)} \geqq$$

(13) $$\geqq \liminf_{n\to\infty} \frac{\delta_n}{\inf_{a\in C} \xi[G(n, a)]}\,; \quad C \subset A^0\,.$$

Suppose that for some $\varepsilon > 0$, $j_0 \geqq 1$

(14) $$\liminf_{n\to\infty} \frac{\delta_n}{\inf_{a\in C_j} \xi[G(n, a)]} < 1 - \varepsilon\,; \quad j = j_0, j_0 + 1, \ldots$$

Then for a given C_j there is a sequence $\{n_k\}_{k=1}^{\infty}$ such that

(15) $$(1 - \varepsilon)\, \xi[G(n_k, a)] > \mu[G(n_k, a)]\,; \quad a \in C_j\,, \quad k = 1, 2, \ldots$$

There is a decreasing sequence of open sets $U_1, U_2, \ldots$ such that $C_j = \bigcap_{m=1}^{\infty} U_m$. But to every m there is an n_k such that $U_m \supset \bigcup_{a\in C_j} G(n_k, a) \supset C_j$. Since C_j is compact we may directly suppose that to every m there is an n_k such that U_m is a finite union of open spheres $G(n_k, a)$; $a \in C_j$. Then (15) implies:

$$(1 - \varepsilon)\, \xi(U_m) > \mu(U_m)\,; \quad m = 1, 2, \ldots, \quad \text{hence}$$

$$\mu(C_j) = \lim_{m\to\infty} \mu(U_m) \leqq (1 - \varepsilon) \lim_{m\to\infty} \xi(U_m) = (1 - \varepsilon)\, \xi(C_j)\,.$$

Finally, since A^0 is a union of C_{j0}, C_{j0+1}, we have $1 = \mu(A^0) = (1 - \varepsilon)\, \xi(A^0) \leqq \leqq 1 - \varepsilon$. The supposition (14) is not possible; thus to every $\varepsilon > 0$, $j_0 \geqq 1$, there is a $j \geqq j_0$ such that

(16) $$\liminf_{n\to\infty} \frac{\delta_n}{\inf_{a\in C_i} \xi[G(n, a)]} \geqq 1 - \varepsilon\,; \quad i = 1, 2, \ldots, j\,.$$

Putting (16) into (13) and taking the limit $\varepsilon \to 0$ we obtain the statement of Theorem 3. □

Theorem 3 shows that the normalized Lebesgue measure can be considered as the design which minimalizes the maximal variance of the approximate estimate for $\theta(a)$; $a \in A$. This optimal design depends on the metric in A, that means on the way of approximating the function θ by estimable functionals. This can be shown in the following example. Take $A = \langle 0, 1\rangle$, $d_1(a, b) = |b - a|$, $d_2(a, b) = |b^2 - a^2|$; $a, b \in \langle 0, 1\rangle$ and $\tau_1 : a \in \langle 0, 1\rangle \to x = a \in E^1$, $\tau_2 : a \in \langle 0, 1\rangle \to x = a^2 \in E^1$. τ_1, τ_2 are isometries of (A, d_1) or (A, d_2) onto $\langle 0, 1\rangle \in E^1$, but $\lambda\tau_1(\cdot) \neq \lambda\tau_2(\cdot)$.

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[1] J. Kiefer, J. Wolfowitz: Optimum Design in Regression Problems. Ann. Math. Statist. *30* (1959), 271—294.

[2] A. Pázman: The Ordering of Experimental Designs. A Hilbert Space Approach. Kybernetika *10* (1974), 5, 373—388.

[3] A. Pázman: Optimum Experimental Designs with a Lack of a priori Information I — Designs for the Estimation of a Finite-Dimensional Set of Functionals. Kybernetika *11* (1975), 5, 355—367.

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