

## Optimum Designs of Experiments for Uncorrelated Observations on Fields

ANDREJ PÁZMAN

The properties of experimental designs in a generalized regression experiment with uncorrelated observations which was described in [8] are studied. It is supposed that the space of all possible "response functions" is a reproducing kernel Hilbert space generated by a given kernel. The stress is upon the principles of the construction of iterative procedures for computing optimum designs for a large class of optimality criteria.

### 1. THE CONSIDERED MODEL OF THE EXPERIMENT

The standard formulation of the design problem of a (finite dimensional) regression experiment is the following (cf. [5]). On a compact set  $A$ ,  $k$  continuous and linearly independent functions  $(f_1, \dots, f_k) = f'$  are given. The expected value of an observation in a point  $a \in A$  is  $\sum_{i=1}^k \alpha_i f_i(a)$ , the vector of the parameters  $\alpha' = (\alpha_1, \dots, \alpha_k)$  being unknown. Observations are uncorrelated and they have positive variances depending continuously on  $A$ . It may be supposed without loss of generality that the variances are identically equal to 1 (more exactly: if  $\sigma^2(a)$  is the variance of the observation in  $a \in A$ , we obtain unit variances by the substitution  $f_i(\cdot) \rightarrow f_i(\cdot) \sigma^{-1}(\cdot)$ ). Usually an approximated (asymptotic) design theory is considered, wherein the designs are a class  $\mathcal{E}$  of Borel probability measures on  $A$  and the information matrix of a design  $\xi$  is  $M(\xi) = \int_A f(a) f'(a) d\xi(a)$ . This has the usual meaning that  $M^{-1}(\xi)$  is proportional to the covariance matrix of the best linear estimates for  $\alpha_1, \dots, \alpha_k$ . A real function  $\Psi$  is given on the class  $\{M(\xi) : \xi \in \mathcal{E}\}$ . It expresses the aim of the experimenter. The problem of the optimum design theory is the characterization and the computation of designs which are optimal, that is for which the extreme (usually minimal) value of  $\Psi[M(\xi)]$  is attained.

Several aspects may be pointed out in the described (finite-dimensional) model:

- 1) The mapping  $f : a \in A \rightarrow (f_1(a), \dots, f_k(a))' \in E^k$  maps continuously the compact

set  $A$  onto a compact metric space  $f(A)$  (in  $E^k$ ). Instead of  $A$  we may consider  $f(A)$  and instead of  $\xi$ , the induced measure  $\xi f^{-1}$ . Hence without loss of generality it may be supposed that  $A$  is a compact metric space.

2) The function  $K$  defined on  $A \times A$  by

$$(1.1) \quad K(a, a') = \sum_{i=1}^k f_i(a) f_i(a'); \quad a, a' \in A$$

is the kernel of a reproducing kernel Hilbert space  $H(K)$  with the kernel  $K$  (for the definition see [1] or Paragraph 3.1). The space  $H(K)$  is here the set of all functions  $\theta$  expressed as  $\theta(a) = \sum_{i=1}^k \alpha_i f_i(a)$  with arbitrary reals  $\alpha_1, \dots, \alpha_k$ . In other words,  $H(K)$  is the set of possible "response levels" in the regression experiment.

3) Consider a linear function  $h$  of  $\alpha$ . We define a functional  $g$  on  $H(K)$  by  $g(\sum_{i=1}^k \alpha_i f_i) = h(\alpha)$ . Obviously the correspondence between  $h$  and  $g$  is one-to-one.

That means the experimenter estimating some parameters or functions of parameters, estimates some linear functionals defined on  $H(K)$ . Moreover, the variance of the best linear estimate for  $g$  may be expressed as the norm of an element of  $H(K)$ .

4) A discrete design  $\xi$  ( $\xi$  is supported by a finite subset of  $A$ ) may be interpreted so that for any Borel set  $F \subset A$ , the value  $\xi(F)$  is proportional to the number of observations which are performed in points from  $F$ . With such a set we may associate a random variable  $X_\theta^\xi(F)$ , which is the sum of all observations performed in the points from  $F$ , divided by the total number of observations in  $A$ . We have  $E X_\theta^\xi(F) = \int_F \theta d\xi$  and  $\text{var} X_\theta^\xi(F) = \xi(F)$ .

5) The experimenter, who wants to estimate functionals from a given set  $G$ , has to solve the following decision problem: The strategy space of the chance is  $G$ , the strategy space of the experimenter is  $\Xi$  and the loss of the experimenter is the variance of the best linear estimate for  $g$  under the design  $\xi$ . As a consequence, an optimality criterion in the design problem must be a decision criterion in this decision problem.

Points 1–5 stimulate a certain generalization of the standard model (see [8]). We shall describe it:

Consider a compact metric space  $A$ , a symmetric, nonnegative definite and continuous real function  $K$  on  $A \times A$  (a kernel), and the reproducing kernel Hilbert space  $H(K)$  with the kernel  $K$ . Denote by  $\mathcal{F}$  the Borel  $\sigma$ -algebra of subsets of  $A$ . A design is an arbitrary probability measure defined on  $\mathcal{F}$ . A possible "response function" will be any function  $\theta \in H(K)$ . Given the true "response function"  $\theta$  and a design  $\xi$ , the experimenter observes on  $F \in \mathcal{F}$  a random variable  $X_\theta^\xi(F)$ , with a finite mean and a finite variance. It is supposed that there is a probability space  $(\Omega, \mathcal{S}, P)$  such that

$$X_\theta^\xi(F) \in L_2(\Omega, \mathcal{S}, P); \quad F \in \mathcal{F}$$

$$(1.2) \quad E X_{\theta}^{\xi}(F) = \int_F \theta d\xi; \quad F \in \mathcal{F}$$

$$\text{cov} [X_{\theta}^{\xi}(F), X_{\theta}^{\xi}(F')] = \xi(F \cap F'); \quad F, F' \in \mathcal{F}$$

and

$$(1.3) \quad X_{\theta}^{\xi}\left(\sum_{i=1}^n F_i\right) = \sum_{i=1}^n X_{\theta}^{\xi}(F_i)$$

for every finite class of disjoint sets  $F_1, \dots, F_n$ . The last equality is an equality of elements in  $L_2(\Omega, \mathcal{S}, P)$ .\* The aim of the experimenter is to estimate real functionals defined on  $H(K)$ , which are elements of a given set  $G$ . The experimenter deals again with the decision problem  $(G, \Xi, \text{var}_{\xi} g)$ , where  $\Xi$  is the set of all designs on  $A$  and  $\text{var}_{\xi} g$  is the variance of the best linear estimate for  $g$  under the design  $\xi$ .

In a certain sense the space  $H(K)$  may correspond to a field. For instance, let us suppose that  $A$  is a cube  $\langle 0,1 \rangle \times \langle 0,1 \rangle \times \langle 0,1 \rangle$  in  $E^3$  and  $\theta$  is the potential function of an electrostatic field in  $A$  which is constant along two axes (say  $y, z$ ; that means  $\partial\theta/\partial y = \partial\theta/\partial z = 0$ ). The derivative  $|\partial\theta/\partial x|$  is the magnitude of the intensity of the field and  $\int_0^1 [\partial\theta/\partial x]^2 dx$  is the energy of the field. The set of possible potential functions is  $\{\theta : \int_0^1 [\partial\theta/\partial x]^2 dx < \infty\}$  and this is equal to  $H(K)$  with  $K(x_1, y_1, z_1; x_2, y_2, z_2) = \min(x_1, x_2) \min(y_1, y_2) \min(z_1, z_2)$ ,

$$K(x_1, y_1, z_1; x_2, y_2, z_2) = \min(x_1, x_2) \min(y_1, y_2) \min(z_1, z_2),$$

$$H(K) = \left\{ \theta : \iiint_A [\partial^2 \theta / \partial x \partial y \partial z]^2 dx dy dz < \infty \right\}.$$

We give now some remarks on the structure of the paper. The paper is divided into 4 sections. In the first two the main results, their interpretation and their correspondence to the finite-dimensional case are stated. In the last two sections we complement the paper by auxiliary results and by the proofs of all the results (also of the ones from Section 2). These sections are divided into paragraphs labelled as **i.1**, **i.2**, etc. (in the  $i$ -th section). Theorems and propositions (the less important statements) have the same numbers as the paragraphs in which they occur (hence "Theorem **4.1**" or "the theorem in **4.1**" or "the theorem in Paragraph **4.1**" means the same).

\* The mapping

$$\chi_F \in L_2(A, \mathcal{F}, \xi) \rightarrow \left[ X_{\theta}^{\xi}(F) - \int_F \theta d\xi \right] \in L_2(\Omega, \mathcal{S}, P)$$

is an inner product preserving linear mapping which may be extended uniquely to an isometry of  $L_2(A, \mathcal{F}, \xi)$  onto a subspace of  $L_2(\Omega, \mathcal{S}, P)$ . The existence of  $(\Omega, \mathcal{S}, P)$  and of such an isometry for every probability space  $(A, \mathcal{F}, \xi)$  is proved in [6].

Now some notations for inner products and closures in the Hilbert spaces:  $H(K)$  is a real reproducing kernel Hilbert space with the kernel  $K$ ,  $\| \cdot \|_K$  and  $(\cdot, \cdot)_K$  are the norm and the inner product in  $H(K)$ .  $\Xi$  is the set of all designs on  $A$ ; for every  $\xi \in \Xi$ ,  $L_2(\xi)$  (or  $L_2(A, \mathcal{F}, \xi)$ ) is the Hilbert space of  $\xi$ -square integrable functions on  $A$  and  $\| \cdot \|_{\xi}$ ,  $(\cdot, \cdot)_{\xi}$  is the norm and the inner product in  $L_2(\xi)$ . Analogical notations are used in  $L_2(\mathbb{P}) = L_2(\Omega, \mathcal{S}, \mathbb{P})$ . If  $Q \subset L_2(\xi)$  or  $Q \subset H(K)$ , we denote by  $\mathcal{L}\{Q\}$  the set of all finite linear combinations of elements from  $Q$  and we denote by  $[Q]^{\xi}$  (resp. by  $[Q]^K$ ) the closure of  $Q$  in  $L_2(\xi)$  (resp. in  $H(K)$ ). Other notations will be given in what follows.

## 2. THE PROPERTIES AND THE CONSTRUCTION OF OPTIMUM DESIGNS FOR ESTIMATING FUNCTIONALS (RESULTS)

In the whole section  $A$  is a compact metric space,  $K$  is a symmetric nonnegative definite and continuous function defined on  $A \times A$  and  $H(K)$  is the reproducing kernel Hilbert space (of real functions on  $A$ ) with the kernel  $K$  ([1] or 3.1). As explained in Section 1 the experimenter wants to estimate one or several (linear) functionals defined on  $H(K)$ . If observations are performed according to a design  $\xi$ , the estimate of a functional  $g$  is based on the observed random variables  $X_{ij}^{\xi}(F)$ ;  $F \in \mathcal{F}$ . A (linear) estimate is a set of random variables  $\{Y_{\theta} : \theta \in H(K)\}$ , which are elements of  $L_2(\Omega, \mathcal{S}, \mathbb{P})$ , and which have the property: There are real numbers  $c_{ij}$  and sets  $F_{ij}$ ;  $i = 1, 2, \dots, j, j = 1, 2, \dots$  not depending on  $\theta$ , such that for every  $\theta \in H(K)$

$$\lim_{j \rightarrow \infty} \left\| \sum_{i=1}^j c_{ij} X_{ij}^{\xi}(F_{ij}) - Y_{\theta} \right\|_{\mathbb{P}} = 0.$$

It follows that there is an  $l \in L_2(A, \mathcal{F}, \xi)$  such that

$$\lim_{j \rightarrow \infty} \left\| \sum_{i=1}^j c_{ij} \chi_{F_{ij}} - l \right\|_{\xi} = 0$$

(see the footnote 1 and [8]).

By arguments, using the isometry mentioned in the footnote 1, it is proved in [8] that

$$E Y_{\theta} = \int_{\Omega} Y_{\theta} d\mathbb{P} = \int_A \theta d\xi; \quad \theta \in H(K)$$

and

$$(2.1) \quad \text{var } Y_{\theta} = \int_{\Omega} (Y_{\theta} - E Y_{\theta})^2 d\mathbb{P} = \int_A l^2 d\xi; \quad \theta \in H(K).$$

The last value is the variance of the estimate. The estimate is called an unbiased estimate for a functional  $g$  if

$$E Y_{\theta} = g(\theta); \quad \theta \in H(K).$$

It is the *best (linear) estimate* for  $g$  if it has a minimal variance in the set of all unbiased estimates for  $g$ . This minimal variance will be denoted by  $\text{var}_\xi g$  ("the variance of  $g$  under the design  $\xi$ "). We define the covariance  $\text{cov}_\xi(g, g')$  of the best (linear) estimates for two functionals  $g, g'$  analogously.

We denote:

by  $K_\xi$  the kernel on  $A \times A$ , defined by

$$(2.2) \quad K_\xi(a, a') = \int_A K(\cdot, a) K(\cdot, a') d\xi,$$

by  $M_\xi$  the kernel on  $H(K) \times H(K)$ , defined by

$$M_\xi(\theta, \theta') = \int_A \theta, \theta' d\xi,$$

by  $\mathbf{K}$  the operator from  $L_2(\xi)$  into  $L_2(\xi)$ , defined by

$$(\mathbf{K}h)(a) = \int_A K(\cdot, a) h d\xi; \quad a \in A.$$

$H(K_\xi)$  and  $H(M_\xi)$  are the reproducing kernel Hilbert spaces with the kernels  $K_\xi$  and  $M_\xi$ , respectively. By  $P_\xi$  we denote the projection of  $L_2(\xi)$  onto  $[H(K)]^\xi$ . By  $g[K]$  we denote the real function on  $A$  equal to  $g[K(\cdot, a)]$  in  $a \in A$ . We shall write from now on throughout the paper  $\int$  instead of  $\int_A$  to denote integrals over the set  $A$ . The image on the estimability of  $g$  is complemented by

**Theorem 4.1.** A functional  $g$  on  $H(K)$  is estimable (i.e. has a linear unbiased estimate) under the design  $\xi$  iff one of the following four equivalent statements is true:

1) There is an  $l \in L_2(\xi)$  such that

$$g(\theta) = \int l\theta d\xi; \quad \theta \in H(K)$$

2)  $g[K]$  is in the range of the operator  $\mathbf{K}$

3)  $g[K] \in H(K_\xi)$

4)  $g \in H(M_\xi)$

$g[K]$  is the unique element of  $H(K)$  with the property  $g(\theta) = (g[K], \theta)_K; \theta \in H(K)$ . The variance of the best (linear) estimate is

$$(2.3) \quad \text{var}_\xi g = \|g[K]\|_{K_\xi}^2 = \|g\|_{M_\xi}^2 = \|P_\xi l\|_\xi^2.$$

We may write (see 4.1):

$$(\theta, (K_\xi, \theta')_K)_K = (\theta, \mathbf{K}\theta')_K = M_\xi(\theta, \theta'); \quad \theta, \theta' \in H(K).$$

This, together with Theorem 4.1 shows that the operator  $\mathbf{K}$  and the kernels  $K_\xi$  and  $M_\xi$  are different representations of one "object", namely, they are generalizations of the information matrix which is so important in the finite-dimensional case.

Indeed, in the latter case, from  $\theta = \sum_{i=1}^k \alpha_i f_i$ ,  $\theta' = \sum_{i=1}^k \alpha'_i f_i$ , we obtain

$$M_\xi(\theta, \theta') = \sum_{i,j=1}^k \alpha_i M_{ij}(\xi) \alpha_j.$$

The statement 2 (or the statements 3 and 4) in Theorem 4.1 may be read: " $g$  is in the range" of the "information operator".  $\mathbf{K}$  ("information kernels"  $K_\xi$  or  $M_\xi$ ). The equality (2.3) shows that  $\mathbf{K}$ ,  $K_\xi$  and  $M_\xi$  determine the variance of the best estimate for  $g$ , as well as does the information matrix in the finite-dimensional case.

Let us denote  $G$  an  $r$ -dimensional linear space of functionals which are defined on  $H(K)$  (the space of "useful functionals"). According to the statement 1 in Theorem 4.1, every  $g \in G$  is estimable under the design  $\xi$  iff  $r$  linearly independent functionals  $g_1, \dots, g_r \in G$  (a linear basis of  $G$ ) are estimable under  $\xi$ . On the other hand, if  $g_1, \dots, g_r$  are estimable, each with respect to another design  $\xi_i$ , then every  $g \in G$  is estimable with respect to the design  $\xi = r^{-1} \sum_{i=1}^r \xi_i$ .

We denote by  $\Xi$  the set of all designs and by  $\Xi_G$  the set of designs allowing the estimation of every  $g \in G$ . By  $D(\xi)$  we shall denote the covariance matrix

$$(2.4) \quad D_{ij}(\xi) = \text{cov}_\xi(g_i, g_j); \quad i, j = 1, \dots, r, \quad \xi \in \Xi_G$$

An *optimality criterion* for estimating functionals from  $G$  will be a finite real function  $\Phi$  defined on the set  $\{D(\xi) : \xi \in \Xi_G\}$  having the properties

a) The ordering of designs according to  $\Phi[D(\xi)]$  does not depend on the choice of the linear basis  $g_1, \dots, g_r \in G$

b)  $\Phi$  is continuous on  $\{D(\xi) : \xi \in \Xi_G\}$

c) If  $\xi, \eta \in \Xi_G$  and  $\text{var}_\xi g \leq \text{var}_\eta g$  for every  $g \in G$ , then  $\Phi[D(\xi)] \leq \Phi[D(\eta)]$ .

We define a real function  $\Phi^*$  on  $\Xi$  by  $\Phi^*(\xi) = \Phi[D(\xi)]$  for  $\xi \in \Xi_G$  and by  $\Phi^*(\xi) = \infty$  for  $\xi \in \Xi - \Xi_G$ . The aim of the experimenter is to find a design  $\xi^*$  (if it exists) which minimalizes  $\Phi^*(\cdot)$  over  $\Xi$ .  $\xi^*$  is called the  $\Phi$ -optimum design.

A sequence of designs  $\{\xi_n\}_{n=1}^\infty$  is said to converge weakly to a design  $\xi$  if for every function  $f$  which is continuous on  $A$

$$\lim_{n \rightarrow \infty} \int f d\xi_n = \int f d\xi.$$

The set  $\Xi$  with the weak topology is compact and metrizable, since  $A$  is a compact metric space [7]. However, unlike the finite-dimensional case,  $\Phi^*$  may not be a continuous function on  $\Xi$  as the following example shows: Take  $A = \langle 0, 1 \rangle$ ,  $K(a, a') =$

$= \min(a, a')$ . Denote by  $\xi_n$  the design concentrated in the point  $1/n$  and by  $\xi_\infty$  the design concentrated in the point 0. Evidently the sequence  $\{\xi_n\}_{n=1}^\infty$  converges weakly to  $\xi_\infty$ . From (2.2) we obtain  $K_{\xi_n}(a, a') = K(a, 1/n)K(a', 1/n)$ , hence  $H(K_{\xi_n})$  is the span of  $K(\cdot, 1/n)$ . Take  $\Phi^*(\xi) = \|K(\cdot, 0)\|_{K_\xi}^2$ . We have  $\Phi^*(\xi_n) = \infty$  but  $\Phi^*(\xi_\infty) = 1$ .

We shall call an *iterative procedure* a sequence  $\{\xi_i\}_{i=0}^\infty$  of designs which is such that there is a sequence of designs  $\{\varkappa_i\}_{i=0}^\infty$  and a sequence of numbers  $\{\alpha_i\}_{i=0}^\infty$ ,  $\alpha_i \in (0, 1)$ ,  $\sum_{n=0}^\infty \alpha_i < \infty$  so that

$$(2.5) \quad \xi_{n+1} = (1 - \alpha_n) \xi_n + \alpha_n \varkappa_n$$

or

$$(2.6) \quad \xi_n = (1 - \alpha_n) \xi_{n+1} + \alpha_n \varkappa_n$$

for  $n = 0, 1, 2, \dots$

The iterative procedure is *increasing* if (2.5) is true for  $n = 0, 1, 2, \dots$ . It is *decreasing* if (2.6) is true for  $n = 0, 1, 2, \dots$ . The design  $\xi_0$  is the starting design of the iterative procedure. The designs  $\varkappa_0, \varkappa_1, \dots$  are correction designs.

**Theorem 4.3.** Every sequence of designs  $\{\xi_n\}_{n=0}^\infty$ , which is an increasing or a decreasing iterative procedure, is weakly convergent, and

$$\Phi^*[\lim_{n \rightarrow \infty} \xi_n] = \lim_{n \rightarrow \infty} \Phi^*(\xi_n)$$

for every optimality criterion  $\Phi$ .

**Theorem 4.4.** If  $\Phi$  is an optimality criterion such that  $\Phi^*$  is convex on  $\Xi$ , then there is a decreasing iterative procedure weakly converging to a  $\Phi$ -optimum design.

For every design  $\xi \in \Xi$  we denote

$$A_\xi = \{a : a \in A, K(\cdot, a) \in H(K_\xi)\}$$

and

$$T_\xi = \{a : a \in A, K(\cdot, a) \in [H(K_\xi)]^K\}.$$

In the case of a finite-dimensional  $H(K)$  we have  $A_\xi = T_\xi$ , which may not be true in the infinite-dimensional case.

Let  $\xi, \mu$  be two designs each of which allows the simultaneous estimation of every  $g \in G$ . Let  $\varkappa$  be the design (the restriction of  $\mu$  to  $T_\xi$ ) defined as

$$\mu(T_\xi) \varkappa(\cdot) = \mu(\cdot \cap T_\xi).$$

**Proposition 4.5.** If  $\varkappa$  is the restriction of  $\mu$  to  $T_\xi$ , then

$$\text{var}_\varkappa g \leq \text{var}_\mu g ; \quad g \in G .$$

As a consequence,  $\Phi^*(\varkappa) \leq \Phi^*(\mu)$  for every optimality criterion  $\Phi$ .

The proposition 4.5 may not be true if  $\varkappa$  is the restriction of  $\mu$  to  $A_\xi$ .

The construction of an iterative procedure converging to a  $\Phi$ -optimum design which will follow, is based on the assumption that we know increasing iterative procedures for constructing  $\Phi$ -optimum designs for finite-dimensional regression experiments. The actual situation in the experimental design [2, 3] justifies such an assumption.

Take an increasing sequence of finite-dimensional subspaces of  $H(K) : \Theta_1 \subset \Theta_2 \subset \dots \subset H(K)$  such that

$$\left[ \bigcup_{i=1}^{\infty} \Theta_i \right]^K = H(K) .$$

Denote by  $g^{(k)}$  the restriction from  $H(K)$  to  $\Theta_k$  of a functional  $g \in G$ . Take a linear basis  $\{g_1, \dots, g_r\} \subset G$  and denote by  $D^{(k)}(\xi)$  the covariance matrix of the best linear estimates for  $g_1^{(k)}, \dots, g_r^{(k)}$  under a design  $\xi \in \Xi_G$ . We define

$$\Phi_k^*(\xi) = \begin{cases} \Phi[D^{(k)}(\xi)] ; & \xi \in \Xi_G \\ \infty ; & \xi \in \Xi - \Xi_G . \end{cases}$$

Take a sequence  $\{\varepsilon_n\}_{n=1}^{\infty}$  of positive numbers converging to  $\varepsilon \geq 0$  and consider an increasing iterative procedure  $\{\xi_n\}_{n=0}^{\infty}$  which is such that

a)  $\xi_0$  is a design allowing the estimation of every  $g \in G$

$$(2.7) \quad \text{b) } \Phi_n^*(\xi_n) \leq \inf_{\xi \in \Xi} \Phi_n^*(\xi) + \varepsilon_n ; \quad n = 1, 2, \dots$$

We note that design  $\xi_{n+1}$  may be obtained from the design  $\xi_n$  by a finite iterative procedure  $\zeta_0 = \xi_n, \zeta_1, \zeta_2, \dots, \zeta_{m(n)} = \xi_{n+1}$ . The finite sequence  $\{\zeta_i\}_{i=0}^{m(n)}$  is the first  $m(n)$  terms of an iterative procedure converging to a  $\Phi$ -optimum design in the finite-dimensional regression experiment with the set of possible "response functions"  $\Theta_k$ .

**Theorem 4.6.** The described iterative procedure  $\{\xi_n\}_{n=0}^{\infty}$  converges weakly to a design  $\xi^{**}$  and

$$\Phi^*(\xi^{**}) \leq \inf_{\xi \in \Xi} \Phi^*(\xi) + \varepsilon .$$

We end this Section by considering the  $D$ -optimality criterion:

$$(2.8) \quad \Phi[D(\xi)] = \det D(\xi) .$$



It may be proved without difficulty that it has the properties a, b, c of an optimality criterion. The proof of a) is based on the following: If  $g_1, \dots, g_r$  and  $h_1, \dots, h_r$  are two linear bases of  $G$ , then there is a nonsingular  $r \times r$  matrix  $J$  such that  $g_i = \sum_j J_{ij} h_j$ . Hence  $\text{cov}_\xi(g_i, g_j) = (g_i[K], g_j[K])_{K_\xi} = \sum_{k,l} J_{ik} J_{jl} (h_k[K], h_l[K])_{K_\xi} = \sum_{k,l} J_{il} J_{jl} \text{cov}_\xi(h_k, h_l)$ .

This allows also to prove that the expression

$$(2.9) \quad \sum_{i,j=1}^r (g_i[K], K(\cdot, b))_{K_\xi} \{D^{-1}(\xi)\}_{ij} (g_j[K], K(\cdot, b))_{K_\xi}$$

which is defined for every  $b \in A_\xi$ , does not depend on the choice of the linear basis in  $G$ . We shall denote this expression by  $d_G(b, \xi)$ .

Moreover if

$$g_i[K] = \int \mathbf{K} l_i d\xi; \quad i = 1, \dots, r$$

for some  $l_1, \dots, l_r \in H(K)$ , then, from the arguments which are given in 3.10, it follows that the functionals  $(g_i[K], \cdot)_{K_\xi}$  may be uniquely extended from  $H(K_\xi)$  to  $[H(K_\xi)]^K$ . Thus in this special case,  $d_G(b, \xi)$  is defined for every  $b \in T_\xi$  (and it is continuous on  $T_\xi$ ).

The function  $d_G(\cdot, \xi)$  may be useful to express the changes of  $\det D(\xi)$  in increasing iterative procedures with one-point corrections or to stop the iterative procedures at some design  $\xi_n$ , as Proposition 4.8b and Theorems 4.9 and 4.10 show. We say that an increasing iterative procedure  $\{\xi_n\}_{n=0}^\infty$  has one-point corrections if there is a sequence  $\{a_n\}_{n=0}^\infty$  of points from  $A$ , such that

$$\xi_{n+1}(\cdot) = (1 - \alpha_n) \xi_n(\cdot) + \alpha_n \mathcal{Z}_{(\cdot)}(a_n); \quad n = 0, 1, 2, \dots$$

In such a case we have the following:

**Proposition 4.8b.**

$$\frac{\det D(\xi_{n+1})}{\det D(\xi_n)} = \left(\frac{1}{1 - \alpha_n}\right)^r; \quad a_n \notin A_{\xi_n}$$

$$= \left(\frac{1}{1 - \alpha_n}\right)^r \left\{1 - \frac{\alpha_n}{1 - \alpha_n} \frac{d_G(a_n, \xi_n)}{1 - \alpha_n + \alpha_n \|K(\cdot, a_n)\|_{K_{\xi_n}}^2}\right\}; \quad a_n \in A_{\xi_n}.$$

(The proof follows directly from Proposition 4.8 in Section 4.)

**Theorem 4.9.** Let us suppose that the design  $\xi$  and the set of functionals  $G$  are such that to every  $g \in G$  there is an  $l \in H(K)$  such that  $g[K] = \int \mathbf{K} l d\xi$ . Let  $\mu$  be a design which allows the estimation of every  $g \in G$  and such that  $H(K_\mu) \subset$

232  $\subset [H(K_\zeta)]^k$ . Then

$$\frac{1}{r} \sup_{a \in S_\mu} d_G(a, \zeta) \geq \left[ \frac{\det D(\zeta)}{\det D(\mu)} \right]^{1/r}.$$

As a corollary we obtain:

**Theorem 4.10.** If  $G$  and  $\zeta$  are as in Theorem 4.9, then

$$\frac{1}{r} \sup_{a \in T_\zeta} d_G(a, \zeta) \geq \left[ \frac{\det D(\zeta)}{\inf_{x \in Z} \det D(x)} \right]^{1/r}.$$

It means that the expression  $1/r \sup_{a \in T_\zeta} d_G(a, \zeta)$  may serve as an evaluation of "how far" the design  $\zeta$  is from an  $D$ -optimal design. Every functional  $g$  which is estimable under a design  $\zeta$  is expressible as  $g(\cdot) = \int h \cdot d\zeta$  for some  $h \in [H(K)]^\zeta$ . Hence there is a sequence  $\{l_i\}_{i=1}^\infty$  of elements of  $H(K)$  such that  $\lim_{i \rightarrow \infty} \|l_i - h\|_\zeta = 0$ . It follows that we have a sequence  $\{g_i\}_{i=1}^\infty$  of functionals  $g_i(\cdot) = \int l_i \cdot d\zeta$ ;  $i = 1, 2$ , satisfying the assumptions of Theorem 4.10 and such that

$$\lim_{i \rightarrow \infty} |g_i(\theta) - g(\theta)| = 0; \quad \theta \in \Theta$$

and that

$$\lim_{i \rightarrow \infty} |\text{var}_\zeta g_i - \text{var}_\zeta g| = 0.$$

This allows to use Theorem 4.10 at least in principle to construct a stopping rule for the iterative procedure yielding to a  $\Phi$ -optimum design.

### 3. REPRODUCING KERNEL HILBERT SPACES AND PROBABILITY MEASURES

The aim of this section is to recapitulate some standard properties of a reproducing kernel Hilbert space (RKHS) and to relate the RKHS with a probability measure. The proofs of the statements, which are in Paragraphs 3.1–3.4, may be found in [1].

**3.1.** If  $S$  is a set and  $k$  is a symmetric, nonnegative definite, real function on  $S \times S$  (a kernel), then there is exactly one Hilbert space (called the RKHS with the kernel  $k$  and denoted by  $H(k)$ ) with the following properties:

- i) elements of  $H(k)$  are real functions on  $S$ ,
- ii)  $k(\cdot, s) \in H(k)$  for every  $s \in S$ ,
- iii)  $(f, k(\cdot, s))_k = f(s)$  for every  $f \in H(k)$ ,  $s \in S$ .

The set  $\{k(\cdot, s) : s \in S\}$  spans  $H(k)$ .

Take an arbitrary Hilbert space  $H$  with the inner product denoted by  $\langle \cdot, \cdot \rangle$ . It may be proved (using the Riesz representation theorem) that the set of all bounded linear functionals on  $H$  is an RKHS with the kernel

$$k(h, h') = \langle h, h' \rangle; \quad h, h' \in H.$$

**3.2.** Every set  $V$  which is a closed subspace of  $H(k)$  is an RKHS with the kernel  $k'(s_1, s_2) = [P_V k(\cdot, s_1)](s_2)$ , where  $P_V$  is the projection of  $H(k)$  onto  $V$ . Consider especially the following subspace  $V$ : Take a set  $T \subset S$  and denote  $N(T) = \{f : f \in H(k), f(s) = 0 \text{ for } s \in T\}$ ; denote by  $V$  the orthogonal complement of  $N(T)$  in  $H(k)$ .  $V$  is the subspace of  $H(k)$  which is spanned by the set  $\{k(\cdot, s) : s \in T\}$ . It is an RKHS as mentioned above. The mapping, which maps every  $f \in V$  onto the restriction of  $f$  to the set  $T$ , is a linear isometry of the RKHS  $V$  onto the RKHS  $H(k^T)$ , where  $k^T$  is the restriction of the kernel  $k$  onto  $T \times T$ .

**3.3.** Let  $k_1, k_2$  be two kernels defined both on  $S \times S$ . The function  $k = k_1 + k_2$  is also a kernel and  $H(k) = \{f : f = f_1 + f_2, f_1 \in H(k_1), f_2 \in H(k_2)\}$ . Further

$$(3.1) \quad \|f\|_k^2 = \min \{ \|f_1\|_{k_1}^2 + \|f_2\|_{k_2}^2 : f = f_1 + f_2 \}.$$

The sets  $H(k_1)$  and  $H(k_2)$  are closed subspaces of  $H(k)$ . We have:  $H(k_1) \cap H(k_2) = \{0\}$ , iff  $H(k_1)$  and  $H(k_2)$  are orthogonal in  $H(k)$ . In such a case  $k_1(\cdot, s) = P_1 k(\cdot, s)$ ,  $k_2(\cdot, s) = P_2 k(\cdot, s)$ ;  $s \in S$ , where  $P_i$  is the projection of  $H(k)$  onto  $H(k_i)$ .

$H(k_1)$  is a closed subspace of  $H(k_2)$  iff there is a  $c > 0$  such that  $k_2 - ck_1$  is a kernel. In such a case  $\|f\|_{k_1}^2 \geq c \|f\|_{k_2}^2$  for every  $f \in H(k_1)$ .

**3.4.** Consider a sequence  $\{k_n\}_{n=1}^{\infty}$  of kernels defined on  $S \times S$ .

If

$$\begin{aligned} H(k_n) &\supset H(k_{n+1}); \quad n = 1, 2, \dots, \\ \|f\|_{k_n} &\leq \|f\|_{k_{n+1}}; \quad f \in H(k_{n+1}), \quad n = 1, 2, \dots, \end{aligned}$$

then there is a limit

$$\lim_{n \rightarrow \infty} k_n(s_1, s_2) = k_0(s_1, s_2)$$

and

$$H(k_0) = \{f : f \in \bigcap_{n=1}^{\infty} H(k_n), \lim_{n \rightarrow \infty} \|f\|_{k_n}^2 < \infty\}.$$

Moreover,

$$\|f\|_{k_0}^2 = \lim_{n \rightarrow \infty} \|f\|_{k_n}^2; \quad f \in H(k_0).$$

Similarly, let us suppose that  $H(k_n) \subset H(k_{n+1}); n = 1, 2, \dots$

$$\|f\|_{k_n} \geq \|f\|_{k_{n+1}}; \quad f \in H(k_n), \quad n = 1, 2, \dots,$$

234 and that there is the limit

$$\lim_{n \rightarrow \infty} k_n(s_1, s_2) = k_0(s_1, s_2); \quad s_1, s_2 \in S.$$

Then  $k_0$  is a kernel, the set  $\bigcup_{n=1}^{\infty} H(k_n)$  is dense in  $H(k_0)$ , and

$$\|f\|_{k_0}^2 = \lim_{n \rightarrow \infty} \|f\|_{k_n}^2; \quad f \in \bigcup_{n=1}^{\infty} H(k_n).$$

**3.5.** Suppose now that  $A$  is a compact metric space and  $K$  is a kernel which is continuous on  $A \times A$ . Take a Borel probability measure  $\xi$  on  $A$ .

We have

$$\begin{aligned} \sup_{a \in A} |f_1(a) - f_2(a)| &= \sup_{a \in A} |(K(\cdot, a), f_1 - f_2)_K| \leq \\ &\leq \|f_1 - f_2\|_K \sup_{a \in A} \sqrt{K(a, a)}; \quad f_1, f_2 \in H(K). \end{aligned}$$

It follows that functions which are elements of  $H(K)$  are continuous. Hence  $H(K) \subset L_2(\xi)$  and

$$\|f\|_{\xi}^2 \leq \sup_{a \in A} K(a, a) \|f\|_K^2; \quad f \in H(K).$$

**3.6.** Let  $K_{\xi}$  and  $\mathbf{K}$  be defined as in Section 2.

**Proposition.** The operator  $\mathbf{K}$  maps isometrically  $[H(K)]_{\xi}^{\xi}$  (with the norm  $\|\cdot\|_{\xi}$ ) onto  $H(K_{\xi})$  (with the norm  $\|\cdot\|_{K_{\xi}}$ ).  $H(K_{\xi})$  is a subset of  $H(K)$  and the inner products in  $H(K)$  and  $L_2(\xi)$  are related by the equation

$$(3.2) \quad (f, \mathbf{K}l)_K = (f, l)_{\xi}; \quad f \in H(K), \quad l \in L_2(\xi).$$

*Proof.* As in (2.3) we denote by  $P_{\xi}$  the projection of  $L_2(\xi)$  onto  $[H(K)]_{\xi}^{\xi}$ .  $\mathbf{K}$  maps  $[H(K)]_{\xi}^{\xi}$  onto  $\mathbf{K}L_2(\xi)$ , since  $(\mathbf{K}h)(a) = (K(\cdot, a), h)_{\xi} = (K(\cdot, a), P_{\xi}h)_{\xi} = [\mathbf{K}P_{\xi}h](a)$  for every  $a \in A$ .  $\mathbf{K}$  restricted to  $[H(K)]_{\xi}^{\xi}$  is a bijection, since the equations

$$(K(\cdot, a), P_{\xi}h_1)_{\xi} = \mathbf{K}P_{\xi}h_1 = \mathbf{K}P_{\xi}h_2 = (K(\cdot, a), P_{\xi}h_2)_{\xi}; \quad a \in A$$

imply  $P_{\xi}h_1 = P_{\xi}h_2$  (because the set  $\{K(\cdot, a) : a \in A\}$  spans  $H(K)$ ). We shall prove that the set  $\mathbf{K}[L_2(\xi)]$  with the inner product  $(\cdot, \cdot)$  defined by

$$(3.3) \quad (\mathbf{K}l_1, \mathbf{K}l_2) = (l_1, l_2)_{\xi}; \quad l_1, l_2 \in [H(K)]_{\xi}^{\xi}$$

is equal to  $H(K_{\xi})$ . Indeed, we have  $K_{\xi}(\cdot, a) = \mathbf{K}K(\cdot, a)$ ;  $a \in A$ . Hence from (3.3) it follows that

$$(\mathbf{K}l, K_{\xi}(\cdot, a)) = \int l K(\cdot, a) d\xi = (\mathbf{K}l)(a); \quad l \in L_2(\xi); \quad a \in A.$$

Thus  $\mathbf{K} L_2(\xi)$  with the inner product  $(\cdot, \cdot)$  and the kernel  $K_\xi$  has the properties i, ii, iii, from 3.1. It follows that  $\mathbf{K} L_2(\xi) = H(K_\xi)$ .

From the equality (3.3) we obtain that

$$(3.4) \quad \|\mathbf{K}l\|_{K_\xi} = \|l\|_\xi; \quad l \in [H(K)]^\xi.$$

Let  $\{f_i\}_{i=1}^\infty$  be an orthonormal basis of  $H(K)$ . We have  $K(\cdot, a) = \lim_{n \rightarrow \infty} \sum_{i=1}^n f_i(\cdot) f_i(a)$ ;  $a \in A$  (since  $f_i(a) = (K(\cdot, a), f_i)_K$ ) the convergence being uniform on  $A$ , according to 3.5. It follows that

$$\mathbf{K}h = \sum_{i=1}^\infty \left( \int f_i h \, d\xi \right) f_i(\cdot); \quad h \in L_2(\xi).$$

Further we have

$$\|\mathbf{K}h\|_K^2 = \sum_{i=1}^\infty \left\{ \int f_i h \, d\xi \right\}^2 \leq \|h\|_\xi^2 \int K(a, a) \, d\xi(a) < \infty.$$

This implies first that  $\mathbf{K}h \in H(K)$ , and secondly that, according to (3.4),

$$\|\mathbf{K}h\|_K^2 \leq \|\mathbf{K}h\|_{K_\xi}^2 \int K(a, a) \, d\xi(a); \quad h \in L_2(\xi),$$

that is

$$(3.5) \quad \|\psi\|_K^2 \leq \|\psi\|_{K_\xi}^2 \int K(a, a) \, d\xi(a); \quad \psi \in H(K_\xi).$$

It follows that  $H(K_\xi)$  is a subset of  $H(K)$ .

From the reproducing property of the kernel  $K$  (3.1 point iii) we obtain

$$(K(\cdot, a), \int K(\cdot, b) l(b) \, d\xi(b))_K = \int K(b, a) l(b) \, d\xi(b); \quad a \in A, l \in L_2(\xi),$$

which may be rewritten as

$$(K(\cdot, a), \mathbf{K}l)_K = (K(\cdot, a), l)_\xi; \quad a \in A, \quad l \in L_2(\xi).$$

It follows that (3.2) is valid since  $\{K(\cdot, a) : a \in A\}$  spans  $H(K)$  and since  $\|f\|_\xi^2 \leq \|f\|_K^2 \sup_{a \in A} K(a, a)$  for every  $f \in H(K)$  (Paragraph 3.5). □

**3.7. Proposition.** We may write

a)  $[\mathbf{K} H(K)]^\xi = [H(K_\xi)]^\xi = [H(K)]^\xi$

b)  $[\mathbf{K} H(K)]^K = [H(K_\xi)]^K$

and the latter is the subspace of  $H(K)$  spanned by  $\{K(\cdot, a) : a \in S_\xi\}$ .

Proof. Consider the set  $Q = \{f : \mathbf{K}f = \lambda f, \lambda \neq 0\}$  of proper functions of  $\mathbf{K}$  corresponding to nonzero proper values. If  $[\mathcal{L}(Q)]^\xi \neq [H(K)]^\xi$ , then  $\mathbf{K}$  restricted to the orthogonal complement of  $[\mathcal{L}(Q)]^\xi$  in  $[H(K)]^\xi$  is a bijection onto a nonzero subspace of  $H(K_\xi)$  (see Paragraph 3.6). Such a restricted  $\mathbf{K}$  is a nonzero Hilbert-Schmidt operator, hence it has a proper function  $f \in Q$ . It follows that  $[H(K)]^\xi = [\mathcal{L}(Q)]^\xi$ . Evidently  $[\mathcal{L}(Q)]^\xi \subset [\mathbf{K}H(K)]^\xi \subset [H(K_\xi)]^\xi \subset [H(K)]^\xi$ . Thus a) is true.

We have

$$(3.6) \quad [\mathcal{L}(Q)]^{K_\xi} = H(K_\xi),$$

since  $[\mathcal{L}(Q)]^\xi = [H(K)]^\xi$  (as we have just proved), since  $\mathbf{K} \mathcal{L}(Q) = \mathcal{L}(Q)$  and since  $\mathbf{K}$  restricted to  $[H(K)]^\xi$  is an isometry onto  $H(K_\xi)$  (Paragraph 3.6). From (3.5) and (3.6) we obtain

$$H(K_\xi) = [\mathcal{L}(Q)]^{K_\xi} \subset [\mathcal{L}(Q)]^K.$$

Thus  $[H(K_\xi)]^K \subset [\mathcal{L}(Q)]^K$ . On the other hand,  $[\mathcal{L}(Q)]^K \subset [\mathbf{K}H(K)]^K \subset [H(K_\xi)]^K$ , evidently. Thus  $[\mathbf{K}H(K)]^K = [H(K_\xi)]^K$ .

If  $a \in S_\xi$ , then  $\xi(U) > 0$  for every open set  $U$  containing  $a$ . Denote by  $G_n$  the open sphere in the metric space  $A$ , which has the center  $a$  and the radius  $1/n$ . We write, using (3.2)

$$\begin{aligned} & \left\| \int_{G_n} [K(\cdot, a) - K(\cdot, b)] d\xi(b) \right\|_K^2 = \\ &= \int_{G_n} \left( [K(\cdot, a) - K(\cdot, b)], \int_{G_n} [K(\cdot, a) - K(\cdot, b')] d\xi(b') \right)_K d\xi(b) \leq \\ & \leq \int_{G_n} \|K(\cdot, a) - K(\cdot, b)\|_K d\xi(b) \left\| \int_{G_n} [K(\cdot, a) - K(\cdot, b')] d\xi(b') \right\|_K. \end{aligned}$$

Consequently

$$\begin{aligned} & \left\| K(\cdot, a) - \int K(\cdot, b) \chi_{G_n}(b) d\xi(b) / \xi(G_n) \right\|_K \leq \\ & \leq \int \|K(\cdot, a) - K(\cdot, b)\|_K \chi_{G_n}(b) d\xi(b) / \xi(G_n) \rightarrow 0 \end{aligned}$$

with  $n \rightarrow \infty$ . Thus  $K(\cdot, a) \in [H(K_\xi)]^K$  for every  $a \in S_\xi$ . On the other hand, according to (3.2)

$$(\mathbf{K}h, f)_K = \int hf d\xi = 0; \quad h \in L_2(\xi), \quad f \in N(S_\xi).$$

It follows that  $H(K_\xi) \subset N^\perp(S_\xi)$  and the latter is the span of the set  $\{K(\cdot, a) : a \in S_\xi\}$  in  $H(K)$  (see Paragraph 3.2).  $\square$

**3.8. Proposition.**  $\mathbf{K}$  restricted to  $[\mathbf{K} H(K)]^{\mathbf{K}}$  is a bijection onto  $\mathbf{K} H(K)$ .

*Proof.* Denote by  $P$  the projection of  $H(K)$  onto  $[\mathbf{K} H(K)]^{\mathbf{K}}$ .

Using the statements from 3.2, we obtain  $(Pf)(a) = f(a)$  for every  $f \in H(K)$ ,  $a \in S_{\xi}$ , since  $[\mathbf{K} H(K)]^{\mathbf{K}} = [\mathcal{L}\{K(\cdot, a) : a \in S_{\xi}\}]^{\mathbf{K}}$  (see 3.7). Hence, from the definition of  $\mathbf{K}$  we obtain

$$(3.7) \quad \mathbf{K}f = \mathbf{K}Pf; \quad f \in H(K).$$

that is  $\mathbf{K}$  maps  $[\mathbf{K} H(K)]^{\mathbf{K}}$  onto  $\mathbf{K} H(K)$ .

$\mathbf{K}$  restricted to  $[\mathbf{K} H(K)]^{\mathbf{K}}$  is a bijection, since  $[\mathbf{K} H(K)]^{\mathbf{K}} \subset [H(K)]^{\xi}$  and  $\mathbf{K}$  restricted to  $[H(K)]^{\xi}$  is a bijection (Proposition 3.6).  $\square$

**3.9. Proposition.** The functional  $(\psi, \cdot)_{K_{\xi}}$  defined on  $H(K_{\xi})$  is continuous

- with respect to  $\| \cdot \|_{K_{\xi}}$  if  $\psi \in H(K_{\xi})$
- with respect to  $\| \cdot \|_{\mathbf{K}}$  if  $\psi \in \mathbf{K} H(K)$
- with respect to  $\| \cdot \|_{\xi}$  if  $\psi \in \mathbf{K} H(K_{\xi})$ .

*Proof.* a) is obvious. To prove b) take  $\varphi = \mathbf{K}h$ ,  $\psi = \mathbf{K}f$ , where  $h \in L_2(\xi)$ ,  $f \in H(K)$ . We may write, using (3.4) and (3.2),

$$(3.8) \quad (\psi, \varphi)_{K_{\xi}} = \int f h \, d\xi = (f, \mathbf{K}h)_{\mathbf{K}} = (f, \varphi)_{\mathbf{K}}; \quad \varphi \in H(K_{\xi}).$$

In order to prove c) write  $\psi = \mathbf{K}K h = \int K_{\xi} h \, d\xi$  for some  $h \in L_2(\xi)$ . Using (3.2) (but writing  $K_{\xi}$  instead of  $K$  in (3.2)), we obtain

$$(\psi, \varphi)_{K_{\xi}} = \left( \int K_{\xi} h \, d\xi, \varphi \right)_{K_{\xi}} = (h, \varphi)_{\xi}; \quad \varphi \in H(K_{\xi}). \quad \square$$

**3.10** Consider in more detail the case  $\psi \in \mathbf{K} H(K)$ . According to (3.8), the functional  $(f, \cdot)_{\mathbf{K}}$  restricted to  $[H(K_{\xi})]^{\mathbf{K}}$  is an extension of the functional  $(\psi, \cdot)_{K_{\xi}}$  from  $H(K_{\xi})$  onto  $[H(K_{\xi})]^{\mathbf{K}}$ . We shall denote also this extension by  $(\psi, \cdot)_{K_{\xi}}$ . Hence we may consider the integral

$$\int \mathbf{K}(b, a) (\psi, K(\cdot, a))_{K_{\xi}} \, d\xi(a),$$

since  $K(\cdot, a) \in [H(K_{\xi})]^{\mathbf{K}}$  if  $a \in S_{\xi}$  (Proposition 3.7). Using (3.2) we obtain  $\int \mathbf{K}(b, a) (\psi, K(\cdot, a))_{K_{\xi}} \, d\xi(a) = (f, \int \mathbf{K}(\cdot, a) K(b, a) \, d\xi(a))_{\mathbf{K}} = (\psi, K_{\xi}(\cdot, b))_{K_{\xi}} = \psi(b)$ .

**3.11. Proposition.** A (linear) functional  $g$  defined on  $H(K)$  is continuous with respect to  $\| \cdot \|_{\mathbf{K}}$  iff  $g(K) \in H(K)$ . It is continuous with respect to  $\| \cdot \|_{\xi}$  iff  $g(K) \in H(K_{\xi})$ .

Proof. The functional  $g$  is continuous with respect to  $\|\cdot\|_K$  iff  $g(\cdot) = (\psi, \cdot)_K$  for some  $\psi \in H(K)$ . Evidently  $\psi(a) = (\psi, K(\cdot, a))_K = g[K(\cdot, a)]$ ;  $a \in A$ .

If  $g(K) \in H(K_\xi)$ , then  $g(K) = \mathbf{K}h$  for some  $h \in L_2(\xi)$  (Proposition 3.6). Using (3.2), we obtain

$$g(f) = (\mathbf{K}h, f)_K = (h, f)_\xi; \quad f \in H(K).$$

That means  $g$  is continuous with respect to  $\|\cdot\|_\xi$ . On the other hand, if  $g$  is continuous with respect to  $\|\cdot\|_\xi$ , then there is an  $h \in L_2(\xi)$  such that  $g(\cdot) = (h, \cdot)_\xi$ . Taking  $\psi = \mathbf{K}h$ , we obtain with the use of (3.2):  $g(\cdot) = (\psi, \cdot)_K$ .  $\square$

#### 4. THE PROPERTIES OF ITERATIVE PROCEDURES

**4.1. Theorem.** A functional  $g$  on  $H(K)$  is estimable (i.e. has a linear unbiased estimate) under the design  $\xi$  iff one of the following four equivalent statements is true.

1) There is an  $l \in L_2(\xi)$  such that

$$g(\theta) = \int l \theta \, d\xi; \quad \theta \in H(K).$$

2)  $g[K]$  is in the range of the operator  $\mathbf{K}$  defined in 3.6.

3)  $g[K] \in H(K_\xi)$ .

4)  $g \in H(M_\xi)$ .

$g[K]$  is the unique element of  $H(K)$  with the property  $g(\theta) = (g[K], \theta)_K$ ;  $\theta \in H(K)$ . The variance of the best linear estimate for  $g$  under the design  $\xi$  is equal to

$$(4.1) \quad \text{var}_\xi g = \|g[K]\|_{K_\xi}^2 = \|g\|_{M_\xi}^2 = \|P_\xi l\|_\xi^2$$

Proof. The necessity and the sufficiency of 1. or 3. as well as the equalities

$$\text{var}_\xi g = \|g\|_{M_\xi}^2 = \|P_\xi l\|_\xi^2$$

may be proved by a modification of Parzen's construction (for a detailed proof see [8]).

Obviously 1) implies  $g[K] = \mathbf{K}l$ . From (3.2) in 3.6 there follow the equalities  $\int l \theta \, d\xi = (\mathbf{K}l, \theta)_K$ ;  $\theta \in H(K)$ . Evidently,  $\mathbf{K}l$  is the unique element of  $H(K)$  satisfying these equalities. On the other hand, if  $g[K] = \mathbf{K}l$ , then, again from (3.2), we obtain  $g(\theta) = \int l \theta \, d\xi$ ;  $\theta \in \Theta$ . Thus 2) implies 1) The equivalence of 2) and 3) follows from Proposition 3.6 as well as the equality  $\|P_\xi l\|_\xi^2 = \|g[K]\|_{K_\xi}^2$ .

Using (3.2) several times, we obtain for every  $\theta, \theta' \in H(K)$ :  $(K_\xi(\cdot, a), \theta)_K = (\mathbf{K}K(\cdot, a), \theta)_K = \int K(\cdot, a) \theta \, d\xi = (\mathbf{K}\theta)(a)$ .

Thus

$$(\theta, (K_\xi(\cdot, a))_K)_K = (\theta, \mathbf{K}\theta')_K = \int \theta \theta' \, d\xi = M_\xi(\theta, \theta'); \quad \theta, \theta' \in H(K). \quad \square$$



**4.2. Proposition.** A sequence of designs  $\xi_0, \xi_1, \dots$  is an iterative procedure iff

- a) there is a sequence  $\{c_n\}_{n=0}^{\infty}$  of numbers  $c_n \in (1, \infty)$  such that  $\prod_{n=0}^{\infty} c_n < \infty$ ,  
 b) for  $n = 0, 1, 2, \dots$  there is

$$\xi_n \ll \xi_{n+1} \quad \text{and} \quad d_{\xi_n}^{\xi_n} / d_{\xi_{n+1}}^{\xi_{n+1}} \leq c_n$$

or

$$\xi_{n+1} \ll \xi_n \quad \text{and} \quad d_{\xi_{n+1}}^{\xi_{n+1}} / d_{\xi_n}^{\xi_n} \leq c_n.$$

**Proof.** If  $d_{\xi_n}^{\xi_n} / d_{\xi_{n+1}}^{\xi_{n+1}} \leq c_n$ , we define  $\alpha_n = 1 - 1/c_n$  and  $\varkappa_n = (1/\alpha_n) \xi_{n+1} - [(1 - \alpha_n)/\alpha_n] \xi_n$ . Thus we obtain (2.5) immediately. Conversely, if (2.5) is true, we have  $d_{\xi_n}^{\xi_n} / d_{\xi_{n+1}}^{\xi_{n+1}} \leq 1/(1 - \alpha_n)$ . Further  $\sum_{n=0}^{\infty} \alpha_n < \infty$  iff  $\prod_{n=0}^{\infty} c_n < \infty$ , since for  $\alpha_n < 1/2$  we may write the inequalities

$$\alpha_n \leq -\ln(1 - \alpha_n) \leq 2\alpha_n$$

and since  $c_n = (1 - \alpha_n)^{-1}$ .

We proceed in the same way if  $\xi_{n+1} \ll \xi_n$ . □

**4.3. Theorem.** A sequence of designs  $\{\xi_n\}_{n=0}^{\infty}$ , which is an increasing or a decreasing iterative procedure, is weakly convergent, and

$$(4.2) \quad \Phi^*[\lim_{n \rightarrow \infty} \xi_n] = \lim_{n \rightarrow \infty} \Phi^*[\xi_n]$$

for every optimality criterion  $\Phi$ .

**Proof.** 1) Consider an increasing iterative procedure  $\{\xi_n\}_{n=0}^{\infty}$ . We may write

$$\xi_{n+1} = \sum_{i=0}^n \alpha_i \prod_{j=i+1}^n (1 - \alpha_j) \varkappa_i + \prod_{j=0}^n (1 - \alpha_j) \xi_0.$$

(Conventionally we put  $\prod_{j=k}^m (1 - \alpha_j) = 1$  if  $m < k$ ). We shall denote by  $\xi$  the design

$$\xi = \sum_{i=0}^{\infty} \alpha_i \prod_{j=i+1}^{\infty} (1 - \alpha_j) \varkappa_i + \prod_{j=0}^{\infty} (1 - \alpha_j) \xi_0.$$

The sequence  $\{\xi_n\}_{n=0}^{\infty}$  converges weakly to  $\xi$ , since for every continuous function  $f$  defined on  $A$

$$\begin{aligned} \left| \int f d\xi - \int f d\xi_{n+1} \right| &\leq \max_{a \in A} |f(a)| \left\{ \sum_{i=0}^{\infty} \alpha_i \left| \prod_{j=i+1}^{\infty} (1 - \alpha_j) - \prod_{j=i+1}^n (1 - \alpha_j) \right| + \right. \\ &\quad \left. + \sum_{i=n+1}^{\infty} \alpha_i + \left| \prod_{k=0}^{\infty} (1 - \alpha_k) - \prod_{k=0}^n (1 - \alpha_k) \right| \right\}. \end{aligned}$$

2. We denote  $c_n = (1 - \alpha_n)^{-1}$  and we use Proposition 4.2. We define

$$K_n = \prod_{i=n}^{\infty} c_i K_{\xi_n}; \quad n = 1, 2, \dots$$

The equality

$$(4.3) \quad \sum_{i,j=1}^m \beta_i [c_n K_{\xi_n}(a_i, a_j) - K_{\xi_{n+1}}(a_i, a_j)] \beta_j = \\ = \int \left[ \sum_{i=1}^m \beta_i K(\cdot, a_i) \right]^2 \left( c_n - \frac{d\xi_{n+1}}{d\xi_n} \right) d\xi_n \geq 0$$

which is valid for any reals  $\beta_1, \beta_2, \dots$ , implies  $K_n \geq K_{n+1}$ . Hence from Paragraph 3.3 we obtain  $H(K_{n+1}) \subset H(K_n)$  and  $\| \cdot \|_{K_n} \geq \| \cdot \|_{K_{n+1}}$  on  $H(K_{n+1})$ . From the first part of Paragraph 3.4 we have

$$(4.4) \quad \lim_{n \rightarrow \infty} \| \psi \|_{K_{\xi_n}}^2 = \lim_{n \rightarrow \infty} \prod_{i=n}^{\infty} c_i \| \psi \|_{K_n}^2 = \| \psi \|_{K_{\xi}}^2; \quad \psi \in \bigcap_{n=0}^{\infty} H(K_{\xi_n})$$

and

$$H(K_{\xi}) = H(\lim_{n \rightarrow \infty} K_n) = \bigcap_{n=0}^{\infty} H(K_{\xi_n}).$$

3) Consider now the case of a decreasing iterative procedure  $\{\xi_n\}_{n=0}^{\infty}$ . We may write for every  $p > n$

$$\xi_n = \prod_{i=n}^{p-1} (1 - \alpha_i) \xi_p + \sum_{i=n}^{p-1} \alpha_i \prod_{j=n}^{i-1} (1 - \alpha_j) \xi_i.$$

Hence for a function  $f$ , which is continuous on  $A$ , we have

$$\left| \int f d\xi_n - \int f d\xi_p \right| \leq \max_{a \in A} |f(a)| \left\{ 1 - \prod_{i=n}^{p-1} (1 - \alpha_i) + \sum_{i=n}^{p-1} \alpha_i \right\}.$$

It follows that  $\{\xi_n\}_{n=0}^{\infty}$  is a Cauchy sequence in the (weakly) compact metric space  $\Xi$ , hence it converges (weakly). We have

$$\lim_{n \rightarrow \infty} K_{\xi_n}(a, a') = K_{\xi}(a, a'); \quad a, a' \in A,$$

since  $K$  is continuous and since  $K_{\xi_n}(a, a') = \int K(\cdot, a) K(\cdot, a') d\xi_n$ .

4. Define now

$$K_n = \prod_{i=1}^{n-1} c_i K_{\xi_n}; \quad n = 1, 2, \dots$$

From an inequality similar to (4.3) we obtain that  $K_{n+1} \geq K_n$ , hence  $H(K_{n+1}) \supset H(K_n)$  and  $\|f\|_{K_{n+1}} \leq \|f\|_{K_n}$  for every  $f \in H(K_n)$ . Further

$$\lim_{n \rightarrow \infty} K_n(a, a') = \prod_{i=1}^{\infty} c_i K_{\xi}(a, a'); \quad a, a' \in A,$$

thus, according to the second part of Paragraph 3.4,

$$(4.5) \quad \|\psi\|_{K_\xi}^2 = \lim_{n \rightarrow \infty} \|\psi\|_{K_{\xi_n}}^2; \quad \psi \in \bigcup_{n=0}^{\infty} H(K_{\xi_n})$$

and the set  $\bigcup_{n=1}^{\infty} H(K_{\xi_n})$  is dense in  $H(K_\xi)$ .

5) The equality (4.2) for both, the increasing and the decreasing cases, follows now from the continuity of  $\Phi$ , from (4.4) and (4.5) and from the equality

$$(\psi, \varphi)_{K_\xi} = \frac{1}{2} \{ \|\psi + \varphi\|_{K_\xi}^2 - \|\psi - \varphi\|_{K_\xi}^2 \}; \quad \varphi, \psi \in H(K_\xi). \quad \square$$

**4.4. Theorem.** If  $\Phi$  is an optimality criterion which is such that  $\Phi^*$  is convex on  $\Xi$ , then there is a decreasing iterative procedure weakly converging to a  $\Phi$ -optimum design.

**Proof.** Take a sequence of designs  $\{\varkappa_n\}_{n=0}^{\infty}$  so that  $\{\Phi^*(\varkappa_n)\}_{n=0}^{\infty}$  converges monotonely to the inf  $\Phi(\xi)$ . Take a sequence of reals  $\alpha_0, \alpha_1, \dots \in (0, 1)$  such that  $\sum_{i=0}^{\infty} \alpha_i < \infty$ .

Define

$$(4.6) \quad \xi_n = \sum_{k=n}^{\infty} \alpha_k \prod_{l=n}^{k-1} (1 - \alpha_l) \varkappa_k$$

Evidently  $\xi_n = (1 - \alpha_n) \xi_{n+1} + \alpha_n \varkappa_n$ , hence  $\{\xi_n\}_{n=1}^{\infty}$  is a decreasing iterative procedure. Denote by  $\xi^*$  its weak limit. From the convexity of  $\Phi^*$  and from (4.6) we obtain

$$\Phi^*(\xi_n) \leq \max_{k \geq n} \Phi^*(\varkappa_k) = \Phi^*(\varkappa_n),$$

hence

$$\Phi^*(\xi^*) = \lim_{n \rightarrow \infty} \Phi^*(\xi_n) = \inf_{\xi \in \Xi} \Phi^*(\xi). \quad \square$$

**4.5. Proposition.** Let  $\xi, \mu$  be designs allowing the estimation of every  $g \in G$  and let  $\varkappa$  be a design defined by

$$\mu(T_\xi) \varkappa(\cdot) = \mu(\cdot \cap T_\xi).$$

Then

$$\text{var}_\varkappa g \leq \text{var}_\mu g; \quad g \in G.$$

**Proof.** We repeat that  $T_\xi$  is the set  $\{a : a \in A, K(\cdot, a) \in [H(K_\xi)]^K\}$ . For any  $b \in A$  we denote by  $H_b$  the span of  $K(\cdot, b) : H_b = \mathcal{L}\{K(\cdot, b)\}$ . By  $P_b$  we denote the projection of  $H(K)$  onto  $H_b$ , and by  $P$  the projection of  $H(K)$  onto  $[H(K_\xi)]^K$ . The space  $[H(K_\xi)]^K$  is an RKHS with the kernel  $[PK(\cdot, a)](a')$  and  $H_b$  is an RKHS with the kernel  $[P_b K(\cdot, a)](a')$  (see Paragraph 3.2). Take  $b \in A - T_\xi$ . Since  $H_b \cap [H(K_\xi)]^K = \{0\}$ , we know (Paragraph 3.3) that  $H_b$  is orthogonal to  $[H(K_\xi)]^K$  in the RKHS

242  $[H(K_\xi)]^K \oplus H_b$ , which has the reproducing kernel  $[(P + P_b)K(\cdot, a)](a')$ . Hence  $b \in A - T_\xi$  implies that  $K(\cdot, b)$  is orthogonal to  $[H(K_\xi)]^K$  (in  $H(K)$ ). As a consequence

$$(4.7) \quad K(a, b) = 0; \quad a \in T_\xi, \quad b \in A - T_\xi.$$

Take  $g \in G$ . As  $g$  is estimable under the designs  $\xi, \mu$ , we may write

$$(4.8) \quad g[K(\cdot, a)] = \int K(a, \cdot) l d\xi = \int K(a, \cdot) h d\mu; \quad a \in A$$

for some  $l \in [H(K)]^\xi, h \in [H(K)]^\mu$ . If  $a \in A - T_\xi$ , then (4.7) implies that  $g[K(\cdot, a)] = \int K(\cdot, a) l d\xi = 0 = \int_{T_\xi} K(\cdot, a) h d\mu$  (since  $S_\xi \subset T_\xi$ ). If  $a \in T_\xi$ , then (4.7) implies  $g[K(\cdot, a)] = \int K(a, \cdot) h d\mu = \int_{T_\xi} K(a, \cdot) h d\mu$ . Thus  $g[K(\cdot, a)] = \mu(T_\xi) \int K(a, \cdot) h d\mu; a \in A$ . It follows (Theorem 4.1) that

$$\text{var}_x g = \int \mu^2(T_\xi) [P_x h]^2 dx \leq \int h^2 d\mu = \text{var}_\mu g. \quad \square$$

**4.6. Theorem.** The iterative procedure  $\{\xi_n\}_{n=0}^\infty$  described in Section 2 converges to a design  $\xi^*$  such that

$$\Phi^*(\xi^*) \leq \inf_{\xi \in \Xi} \Phi^*(\xi) + \varepsilon.$$

*Proof.* From the equality

$$\left[ \bigcup_{i=1}^{\infty} \Theta_i \right]^K = H(K)$$

stated in Section 2, we obtain

$$(4.9) \quad \left[ \bigcup_{i=1}^{\infty} \Theta_i \right]^\xi = \left\{ \left[ \bigcup_{i=1}^{\infty} \Theta_i \right]^K \right\}^\xi = [H(K)]^\xi; \quad \xi \in \Xi$$

since  $\|f\|_\xi^2 \leq \sup_{a \in A} K(a, a) \|f\|_K^2$  for every  $f \in H(K)$  (see Paragraph 3.5). Let us denote by  $P_\xi^{(k)}$  the projection of  $L_2(\xi)$  onto  $[\Theta_k]^\xi$  ( $P_\xi$  remains the projection of  $L_2(\xi)$  onto  $[H(K)]^\xi$ ).

From (4.9) we obtain (see [4] § 28)

$$(4.10) \quad \lim_{k \rightarrow \infty} \|(P_\xi - P_\xi^{(k)})h\|_\xi = 0; \quad h \in L_2(\xi), \quad \xi \in \Xi.$$

If  $g \in G$  is estimable under a design  $\xi$ , then it may be expressed as

$$g(\theta) = \int h\theta d\xi; \quad \theta \in H(K)$$

for some  $h \in [H(K)]^{\xi}$ . Hence the restriction  $g^{(k)}$  of  $g$  to  $\Theta_k$  is also estimable under  $\xi$  (statement 1, in Theorem 4.1) and vice versa as may be shown by the use of (4.9). From the formula (4.1) we obtain

$$(4.11) \quad \text{var}_{\xi} g^{(k)} = \|P_{\xi}^{(k)} h\|_{\xi}^2 \leq \text{var}_{\xi} g^{(k+1)} (= \|P_{\xi}^{(k+1)} h\|_{\xi}^2) \leq \\ \leq \text{var}_{\xi} g (= \|P_{\xi} h\|_{\xi}^2)$$

and, according to (4.10),

$$\lim_{k \rightarrow \infty} \text{var}_{\xi} g^{(k)} = \text{var}_{\xi} g.$$

It follows that

$$\lim_{k \rightarrow \infty} D^{(k)}(\xi) = D(\xi); \quad \xi \in \Xi_G.$$

Thus

$$(4.12) \quad \lim_{k \rightarrow \infty} \Phi_k^*(\xi) = \Phi^*(\xi); \quad \xi \in \Xi_G.$$

Moreover the sequence  $\{\Phi_k^*(\xi)\}_{k=0}^{\infty}$  is increasing, according to (4.11) and to the property  $c$  of optimality criteria (see Section 2).

The set  $\Xi^* = \{\xi^*, \xi_0, \xi_1, \dots\} \subset \Xi_G$  is compact in the weak topology of  $\Xi$  and, according to Theorem 4.3,  $\Phi^*(\cdot)$  and  $\Phi_k^*(\cdot)$ ;  $k = 0, 1, 2, \dots$  are continuous functions on  $\Xi^*$ . By the use of Dinni's theorem we obtain that the convergence in (4.12) is uniform on  $\Xi^*$ . As a consequence there is a limit

$$(4.13) \quad \lim_{k \rightarrow \infty} \inf_{\xi \in \Xi^*} \Phi_k^*(\xi) = \inf_{\xi \in \Xi^*} \Phi^*(\xi).$$

Further, from (2.7), we obtain

$$(4.14) \quad \inf_{\xi \in \Xi} \Phi_k^*(\xi) \leq \inf_{\xi \in \Xi^*} \Phi_k^*(\xi) \leq \Phi_k^*(\xi_k) \leq \\ \leq \inf_{\xi \in \Xi} \Phi_k^*(\xi) + \varepsilon_k; \quad k = 0, 1, 2, \dots$$

The limit  $\lim_{k \rightarrow \infty} \inf_{\xi \in \Xi} \Phi_k^*(\xi)$  does exist, because the sequence  $\{\Phi_k^*(\xi)\}_{k=0}^{\infty}$  is increasing for every  $\xi \in \Xi_G$ .

The formulae (4.13) and (4.14) imply

$$(4.15) \quad \inf_{\xi \in \Xi^*} \Phi^*(\xi) = \lim_{k \rightarrow \infty} \inf_{\xi \in \Xi^*} \Phi_k^*(\xi) \leq \lim_{k \rightarrow \infty} \inf_{\xi \in \Xi} \Phi_k^*(\xi) + \varepsilon$$

Since  $\Phi_k^*(\xi) \leq \Phi^*(\xi)$ ;  $\xi \in \Xi_G$ , we may write

$$(4.16) \quad \lim_{k \rightarrow \infty} \inf_{\xi \in \Xi} \Phi_k^*(\xi) \leq \inf_{\xi \in \Xi} \Phi^*(\xi)$$

244 Taking both (4.15) and (4.16), we obtain

$$(4.17) \quad 0 \leq \inf_{\xi \in \Xi} \Phi^*(\xi) - \lim_{k \rightarrow \infty} \inf_{\xi \in \Xi} \Phi_k^*(\xi) < \varepsilon$$

Since the convergence in (4.12) is uniform on  $\Xi^*$ , we have the limit

$$(4.18) \quad \lim_{k \rightarrow \infty} \Phi_k^*(\xi_k) = \lim_{n \rightarrow \infty} \lim_{k \rightarrow \infty} \Phi_k^*(\xi_n) = \Phi^*(\xi^*).$$

From (4.14) we obtain further

$$(4.19) \quad 0 \leq \lim_{k \rightarrow \infty} \Phi_k^*(\xi_k) - \lim_{k \rightarrow \infty} \inf_{\xi \in \Xi} \Phi_k^*(\xi) < \varepsilon.$$

By a comparison of (4.17), (4.18) and (4.19) we obtain finally

$$\Phi^*(\xi^*) - \inf_{\xi \in \Xi} \Phi^*(\xi) < \varepsilon. \quad \square$$

4.7. Take a design  $\xi \in \Xi$ , a point  $b \in A$  and a number  $\alpha \in (0, 1)$ . Denote  $\varkappa = (1 - \alpha)\xi + \alpha\chi_{\{b\}}$ . As in 3.9,  $A_\xi$  is the set  $\{a : a \in A, K(\cdot, a) \in H(K_\xi)\}$ .

**Proposition.** For every  $\varphi, \psi \in H(K_\xi)$

$$(4.20) \quad (\varphi, \psi)_{K_\varkappa} = \frac{(\varphi, \psi)_{K_\xi}}{1 - \alpha}; \quad \text{if } b \notin A_\xi,$$

$$= \frac{(\varphi, \psi)_{K_\xi}}{1 - \alpha} - \frac{\alpha}{1 - \alpha} \frac{(\varphi, K(\cdot, b))_{K_\xi} (\psi, K(\cdot, b))_{K_\xi}}{1 - \alpha + \alpha \|K(\cdot, b)\|_{K_\xi}^2}; \quad \text{if } b \in A_\xi.$$

**Proof.** Since

$$(4.21) \quad K_\varkappa(a, a') = (1 - \alpha)K_\xi(a, a') + \alpha K(a, b)K(b, a')$$

we may write, according to Paragraph 3.3,

$$(4.22) \quad H(K_\varkappa) = \{f : f = f_1 + f_2, f_1 \in H(K_\xi), f_2 \in H_b\}$$

where  $H_b$  is the one-dimensional space spanned by  $K(\cdot, b)$ . If  $K(\cdot, b) \notin H(K_\xi)$ , then  $H_b \cap H(K_\xi) = \{0\}$ , hence (see Paragraph 3.3),  $H_b$  and  $H(K_\xi)$  are orthogonal subspaces of  $H(K_\varkappa)$ . The equality (4.20) follows directly from (3.1) in 3.3 and from the formula

$$(\varphi, \psi)_{K_\varkappa} = \frac{1}{2} \{ \|\varphi + \psi\|_{K_\varkappa}^2 + \|\varphi - \psi\|_{K_\varkappa}^2 \}.$$

If  $K(\cdot, b) \in H(K_\xi)$ , then (4.22) implies  $H(K_\varkappa) = H(K_\xi)$ . From (4.21) we obtain

$$\|K_\varkappa(\cdot, a)\|_{K_\xi}^2 = (1 - \alpha)K_\varkappa(a, a) + \alpha K(a, b)(K_\varkappa(\cdot, a), K(\cdot, b))_{K_\xi}$$

and

$$(K_\varkappa(\cdot, a), K(\cdot, b))_{K_\xi} = (1 - \alpha + \alpha \|K(\cdot, b)\|_{K_\xi}^2).$$

Thus

$$(4.23) \quad \begin{aligned} \|K_x(\cdot, a)\|_{K_\xi}^2 &= (1 - \alpha) \|K_x(\cdot, a)\|_{K_x}^2 + \\ &+ \alpha \frac{(K_x(\cdot, a), K(\cdot, b))_{K_\xi}^2}{1 - \alpha + \alpha \|K(\cdot, b)\|_{K_\xi}^2}; \quad a \in A. \end{aligned}$$

As a consequence we have

$$\|K_x(\cdot, a)\|_{K_\xi}^2 \leq \frac{1 - \alpha}{\alpha} \frac{\|K(\cdot, b)\|_{K_\xi}^2}{\|K(\cdot, b)\|_{K_\xi}^2} \|K_x(\cdot, a)\|_{K_x}^2.$$

It implies that the set  $\{K_x(\cdot, a) : a \in A\}$  spans  $H(K_\xi)$  (since it spans  $H(K_x)$ ). Using this we may prove without difficulty that (4.20) is true, since (4.23) is the equality (4.20) taken for  $\varphi = \psi = K_x(\cdot, a)$ .  $\square$

**4.8. Proposition.** If  $g_1, \dots, g_r$  are estimable under the design  $\xi$  then

$$\begin{aligned} \frac{\det D(\alpha)}{\det D(\xi)} &= \left(\frac{1}{1 - \alpha}\right)^r; \quad \text{if } b \notin A_\xi \\ &= \left(\frac{1}{1 - \alpha}\right)^r \left\{ 1 - \frac{1}{1 - \alpha} \frac{\sum_{i,j=1}^r (g_i[K], K(\cdot, b))_{K_\xi} \{D^{-1}(\xi)\}_{ij} (g_j[K], K(\cdot, b))_{K_\xi}}{1 - \alpha + \alpha \|K(\cdot, b)\|_{K_\xi}^2} \right\} \end{aligned}$$

if  $b \in A_\xi$ .

**Proof.** We know that  $\text{cov}_\xi(g_i, g_j) = (g_i[K], g_j[K])_{K_\xi}$  (Theorem 4.1). We use the Proposition 4.7 for  $\varphi, \psi \in \{g_i[K] : i = 1, \dots, r\}$ . Finally we use the matrix formula

$$\det \{B + cc'\} = \det B \{1 - c'B^{-1}c\},$$

which is valid for every nonsingular matrix  $B$  and every vector  $c$ .  $\square$

**4.9. Theorem.** Suppose that the design  $\xi$  and the set of functionals  $G$  are such that to every  $g \in G$  there is an  $l \in H(K)$ , so that

$$g[K] = \int \mathbf{K}l \, d\xi.$$

Then

$$(4.24) \quad \frac{1}{r} \sup_{a \in \mathcal{S}_\mu} d_a(a, \xi) \geq \left[ \frac{\det D(\xi)}{\det D(\mu)} \right]^{1/r}$$

for every design  $\mu$ , which allows the estimation of every  $g \in G$  and such that  $H(K_\mu) \subset [H(K_\xi)]^K$ .

**Remarks.** We have  $S_\mu \subset T_\mu \subset T_\xi$ , since  $H(K_\mu) \subset [H(K_\xi)]^K$ . Hence  $d_G(\cdot, \xi)$  is continuous on  $S_\mu$  and the sup  $d_G(a, \xi)$  is well defined.

Further the expression  $\det \{D(\xi)/D(\mu)\}$  does not depend on the choice of the linear basis of  $G$ , hence the right side of (4.24) is well defined.

**Proof.** Let  $q_1, \dots, q_r$  be a linear basis of  $G$ . Denote by  $\tilde{D}(\mu)$  (by  $\tilde{D}(\xi)$ ) the covariance matrix of the best linear estimates for  $q_1, \dots, q_r$ , under the design  $\mu$  (the design  $\xi$ ). The functionals  $q_1, \dots, q_r$  may be chosen so that  $\tilde{D}(\mu)$  is the unit  $r \times r$  matrix  $I$ . Further there is an orthogonal matrix  $C$  (such that  $CC' = I$ ) so that

$$\sum_j \{\tilde{D}(\xi)\}_{ij} C_{js} = \lambda_s C_{is}; \quad i, s = 1, \dots, r$$

for some reals  $\lambda_1, \dots, \lambda_r$ .

We define  $g_1, \dots, g_r$  by

$$g_s = \sum_i C_{is} q_i; \quad s = 1, \dots, r.$$

Evidently  $g_1, \dots, g_r$  is a basis of  $G$ . We may check directly that for such a choice of  $g_1, \dots, g_r$ , we have  $D(\mu) = I$  and  $D(\xi)$  is a diagonal matrix:  $D_{ii}(\xi) = \lambda_i$ . From the assumption of the theorem it follows that there are  $h_1, \dots, h_r \in [H(K)]^n$  and  $l_1, \dots, l_r \in H(K)$ , so that

$$g_i(\theta) = \int l_i \theta \, d\xi = \int h_i \theta \, d\mu; \quad i = 1, \dots, r, \quad \theta \in H(K).$$

Thus we may write

$$\lambda_i = D_{ii}(\xi) = \int l_i^2 \, d\xi = g_i(l_i) = \int l_i h_i \, d\mu; \quad i = 1, \dots, r.$$

We now proceed to the proof of (4.24). We have

$$\begin{aligned} \sup_{a \in S_\mu} \frac{1}{r} \sum_{i,j=1}^r l_i(a) \{D^{-1}(\xi)\}_{ij} l_j(a) &\geq \int \frac{1}{r} \sum_{i=1}^r \frac{l_i^2(a)}{\lambda_i} \, d\mu \geq \frac{1}{r} \sum_{i=1}^r \frac{1}{\lambda_i} \left[ \int l_i h_i \, d\mu \right]^2 = \\ &= \frac{1}{r} \sum_{i=1}^r \lambda_i \geq \left[ \prod_{i=1}^r \lambda_i \right]^{1/r} = \left[ \frac{\det D(\xi)}{\det D(\mu)} \right]^{1/r}. \quad \square \end{aligned}$$

**4.10. Theorem.** If  $G$  and  $\xi$  are as in Theorem 4.9, then

$$\frac{1}{r} \sup_{a \in T_\xi} d_G(a, \xi) \geq \left[ \frac{\det D(\xi)}{\inf_{x \in \mathcal{E}} \det D(x)} \right]^{1/r}.$$



Proof. From the Proposition 4.5 and Theorem 4.4 it follows that there is a design  $\xi^*$  such that  $\det D(\xi^*) = \inf_{\xi \in \mathcal{E}} \det D(\xi)$ , and such that  $S_{\xi^*} \subset T_{\xi^*}$ . Hence using the statement b) of Proposition 3.7 we obtain

$$\begin{aligned} [H(K_{\xi^*})]^K &= [\mathcal{L}\{K(\cdot, a) : a \in S_{\xi^*}\}]^K \subset \\ &\subset [\mathcal{L}\{K(\cdot, a) : a \in T_{\xi^*}\}]^K = [H(K_{\xi^*})]^K. \end{aligned}$$

Thus the assumptions of Theorem 4.9 are satisfied if we take  $\xi^*$  instead of  $\mu$ .  $\square$

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*RNDr. Andrej Pázman, C.Sc., Ústav merania a meracej techniky SAV (Institute of Measurement and Measuring Technic — Slovak Academy of Sciences), Dúbravská cesta, 885 27 Bratislava, Czechoslovakia.*