

# The Ordering of Experimental Designs

## A Hilbert Space Approach

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The Hilbert space methods are used to study the designs of experiments with uncorrelated observations in a general case, including infinite dimensional models. The generalization of the D-optimality criterion of the optimality of designs for the infinite dimensional case is presented.

### 1. INTRODUCTION

A systematic theoretical study of experimental designs for finite dimensional regression experiments with uncorrelated observations began with the paper [4]. Since then the properties and the methods of construction of optimal experimental designs have been studied in several papers using methods of linear algebra, the approximation of functions and the theory of games. However it seems that all the obtained results remain within the limits of the finite dimensional model. The difficulty of proceeding to the general case lies perhaps in the fact that the most reasonable criterion for optimality of experimental designs, the criterion of the D-optimality [4], is based on the determinant of the matrix of information, a quantity which is difficult to deal with in the infinite dimensional case.

The aim of this paper is to consider the ordering of experimental designs with uncorrelated observations in the general case (including the infinite dimensional model of regression).

We shall present now the formal description of the studied model of an experiment and after that we shall state the main results of the paper.

We shall consider a set  $A$  (called *the set of regulating points*), a set  $\Theta$  of real functions on  $A$  (called *the set of response levels on  $A$* ) and a positive real function  $w$  on  $A$ . ( $w$  is called *the efficiency function*.)  $\theta \in \Theta$ ,  $w, w^{-1}$  will be bounded functions on  $A$ .

We shall use the topology  $\tau$  on  $A$  induced by the functions  $w$  and  $\theta \in \Theta$ , i.e. the

374 minimal topology which ensures the continuity of  $w$  and of  $\theta \in \Theta$ . We shall denote by  $\mathcal{A}$  the  $\sigma$ -algebra of subsets of  $A$  generated by  $\tau$ .

**Definition 1.** Let  $\xi$  be an arbitrary probability measure on  $(A, \mathcal{A})$ . Then a *variant of the experiment which corresponds to the design*  $\xi$  is a class of orthogonal random set functions

$$(1) \quad \mathcal{E}_\xi = \{ \{X_\theta(F) : F \in \mathcal{A}, \xi(F) > 0\}; \theta \in \Theta \}$$

where each orthogonal random set function

$$(2) \quad \{X_\theta(F) : F \in \mathcal{A}, \xi(F) > 0\}$$

is a set of random variables with finite means

$$(3) \quad EX_\theta(F) = \int_F \theta \, d\xi,$$

finite covariances

$$(4) \quad \text{cov} [X_\theta(F), X_\theta(F')] = \int_{F \cap F'} w^{-1} \, d\xi$$

such that

$$X_\theta\left(\bigcup_{i=1}^n F_i\right) = \sum_{i=1}^n X_\theta(F_i); F_i \cap F_j = \emptyset, i, j = 1, \dots, n, \quad i \neq j$$

(consistency condition).

**Definition 2.** An *experiment*  $\mathcal{E}$  is the class of all its variants:

$$(5) \quad \mathcal{E} = \{ \mathcal{E}_\xi : \xi \text{ is a probability measure on } (A, \mathcal{A}) \}.$$

Two points  $a_1, a_2 \in A$  will be considered as equivalent with respect to  $\Theta$  and  $w$  if  $w(a_1) = w(a_2)$  and  $\theta(a_1) = \theta(a_2)$  for every  $\theta \in \Theta$ .

We can now show the correspondence rules between the given formal description of an experiment and a real experiment. The experimenter investigates the state of a measured object, which is described by one of the functions  $\theta \in \Theta$ , observing directly the values of  $\theta$  at different points from  $A$ . The observation at a point  $a \in A$  gives random data, corresponding to a random variable with the mean  $\theta(a)$  and the variance  $w^{-1}(a)$ . If  $a_1, \dots, a_n$  are (nonequivalent) points of observations and  $N_i$  is the number of independent observations at  $a_i$ , then we may associate the measure  $\xi(\{a_i\}) = N_i / \sum_{j=1}^n N_j$  with the equivalence class  $\{a_i\}$  of the points from  $A$  containing  $a_i$ . The obtained probability measure  $\xi$  on  $(A, \mathcal{A})$  is a design of the experiment following definition 1, and it is clear that it describes the strategy of the experimenter in preparing the experiment. If we take the sum of all data obtained by observations

at the point  $a_i$  then this sum is the realisation of the random variable  $\sum_{j=1}^n N_j X_{\theta}(\{a_i\})$ . The variant of the experiment corresponding to the design  $\xi$  is then a class of  $n$ -vectors of independent random variables

$$\mathcal{E}_{\xi} = \{(X_{\theta}(\{a_1\}), \dots, X_{\theta}(\{a_n\})) ; \theta \in \Theta\}$$

with the means

$$EX_{\theta}(\{a_i\}) = \theta(a_i) N_i / \sum_{j=1}^n N_j$$

and the variances

$$DX_{\theta}(\{a_i\}) = w^{-1}(a_i) N_i / \sum_{j=1}^n N_j .$$

Definition 1 enlarges the notions of the design and the variant of the experiment from the described case of discrete designs on  $A$  to a more general case of arbitrary design measures on  $(A, \mathcal{A})$ . This generalization is useful for theoretical considerations even in the simplest case of finite dimensional regression experiments [4].

In the following sections we shall first recapitulate some basic properties of the Hilbert spaces with reproducing kernels which will be often used later (section 2). In section 3 the Hilbert space technique is used to state five equivalent conditions under which a function on  $\Theta$  has the best linear unbiased estimate (Theorem 4). In section 4 different designs are compared. The construction in sections 3 and 4 is the following: The information kernel  $M_{\xi}(\theta, \theta') = \int_A \theta \theta' d\xi$  which is a function on  $\Theta \times \Theta$ , is the reproducing kernel of a Hilbert space  $H(M_{\xi})$ , containing exactly those functions on  $\Theta$  which are linearly estimable under  $\xi$ . On a subset  $G$  of  $H(M_{\xi})$  (the set of useful variables) we define the Hilbert space  $H(D_{\xi})$  of functions on  $G$  with the reproducing kernel  $D_{\xi}$ , where  $D_{\xi}(g, g')$  is the covariance of the best linear estimates of two functions  $g, g' \in G$ . If  $\xi_0$  is an "a priori design" and  $\xi$  is any design of the form  $\xi = \alpha \xi_0 + (1 - \alpha) \xi'$  where  $\alpha \in (0, 1)$  and  $\xi'$  is an arbitrary design, then  $D_{\xi}(g, g')$  is the kernel of an operator in  $H(D_{\xi_0})$  which we denote by  $\bar{D}_{\xi}$ . In Theorem 7 it is proved that  $\bar{D}_{\xi}$  is equivalent to an operator in  $L_2(A, \mathcal{A}, \xi_0)$  composed of suitably chosen projection operators and operators of multiplication. This allows to maintain the whole problem of comparing designs in the space  $L_2(A, \mathcal{A}, \xi_0)$ . Finally it is shown in a very special case that the generalization of the criterion of D-optimality of designs leads to the *I-divergence* (generalized entropy) of  $\xi$  and  $\xi_0$ .

## 2. PRELIMINARIES REGARDING HILBERT SPACES

The aim of this section is to present a short recapitulation of some basic properties of Hilbert spaces (in the following H-spaces).

We shall consider here only real H-spaces, i.e. complete inner product spaces with real inner products.

Let  $S$  be a set,  $\mathcal{S}$  a  $\sigma$ -algebra of subsets of  $S$  and  $\mu$  a probability measure defined on  $\mathcal{S}$ . By  $L_2(S, \mathcal{S}, \mu)$  we denote the H-space with the following properties:

- i) the elements of  $L_2(S, \mathcal{S}, \mu)$  are all equivalence classes of almost equal square integrable real functions on  $S$ .
- ii) the inner product of two equivalence classes  $\{f\}$  and  $\{g\}$  containing the functions  $f, g$  is

$$(6) \quad (\{f\}, \{g\})_\mu = \int_S fg \, d\mu.$$

In the following we shall omit the square brackets when denoting equivalence classes; i.e.  $f$  may denote the function  $f$  but also the class  $\{f\}$ .

Let  $S$  be a set and let  $K$  be a symmetric, nonnegative definite real function defined on  $S \times S$ . By  $H(K)$  we denote the H-space (the H-space with the reproducing kernel  $K$ ) having the following properties:

- i) the elements of  $H(K)$  are real functions defined on  $S$ ,
- $$(7) \quad \text{ii) } K(\cdot, s) \in H(K); s \in S,$$
- $$(8) \quad \text{iii) } f(s) = (f, K(\cdot, s))_K; f \in H(K), s \in S,$$

where  $(\cdot, \cdot)_K$  is the inner product in  $H(K)$ .

The existence and the uniqueness of  $H(K)$  for any set  $S$  and any symmetric, nonnegative definite function  $K$  is proved in [1].  $H(K)$  is the set of all real functions on  $S$  satisfying (8). The set  $\{K(\cdot, s); s \in S\}$  spans  $H(K)$ .

If  $S$  is a set and  $H$  is an H-space of real functions on  $S$ , then a reproducing kernel  $K$  in  $H$  exists (i.e.  $H = H(K)$ ) iff for every  $s \in S$  we can find a number  $\gamma_s > 0$  such that

$$(9) \quad |f(s)| \leq \gamma_s \|f\|; f \in H,$$

where  $\|\cdot\|$  is the norm in  $H$  [1].

An isomorphism  $\psi$  of an H-space  $H_1$  with the inner product  $(\cdot, \cdot)_1$  onto an H-space  $H_2$  with the inner product  $(\cdot, \cdot)_2$  is a unitary operator, i.e. a one-to-one inner product preserving linear mapping of  $H_1$  onto  $H_2$ :

$$(10) \quad \psi : H_1 \xrightarrow{\text{onto}} H_2,$$

$$\psi(\alpha f_1 + \beta f_2) = \alpha \psi(f_1) + \beta \psi(f_2); \quad \alpha, \beta \in \mathbb{R}, f_1, f_2 \in H_1,$$

$$(\psi(f_1), \psi(f_2))_2 = (f_1, f_2)_1; \quad f_1, f_2 \in H_1.$$

We then say that  $H_1$  and  $H_2$  are isomorphic H-spaces.

**Lemma 1.** Let  $H$  be an H-space with the inner product  $(\cdot, \cdot)$  and let  $G$  be a subset of  $H$ . Denote by  $H_G$  the (closed) subspace of  $H$  spanned by  $G$ . Then the H-space

$$K_G(f, f') = (f, f') ; f, f' \in G$$

is the restriction to the set  $G$  of all bounded linear functionals on  $H_G$ . This restriction is an isomorphism of the set  $B_G$  of all bounded linear functionals on  $H_G$  onto  $H(K_G)$ .

Proof.  $K_G$  is a symmetric, nonnegative definite real function on  $G \times G$ , hence a unique H-space  $H(K_G)$  with the reproducing kernel  $K_G$  does exist. From the Riesz representation theorem for bounded linear functionals [3] it follows that

$$B_G = \{(\cdot, g); g \in H_G\}$$

and that  $B_G$  is an H-space with the natural inner product

$$(11) \quad ((\cdot, g), (\cdot, g'))_{K_G} = (g', g).$$

Denote  $\varrho$  the restriction of elements from  $B_G$  to the set  $G$ . The restriction is a one-to-one, since  $G$  spans  $H_G$  and the elements of  $B_G$  are continuous linear functions on  $H_G$ . Obviously,  $\varrho$  maps  $B_G$  linearly onto  $\varrho B_G$ . It is now sufficient to prove that  $\varrho B_G$  with the inner product  $(\varrho(\cdot, f), \varrho(\cdot, f'))' = (f, f'); f, f' \in H_G$ , is identical with  $H(K_G)$ .

Evidently

$$K_G(\cdot, f) = (\cdot, f) \in \varrho(B_G); f \in G.$$

Further we have from (6)

$$(\varrho(\cdot, g), K_G(\cdot, f))' = (f, g); g, f \in G,$$

hence  $K_G$  has the reproducing property (8) in  $B_G$ . From the remarks following (8) we obtain the needed conclusion.  $\square$

**Lemma 2.** Let  $H_1, H_2$  be two H-spaces which are spanned by the sets  $G_1 \subset H_1$  and  $G_2 \subset H_2$ . Let  $\psi$  be a one-to-one mapping of  $G_1$  onto  $G_2$ , which preserves the inner product, i.e.

$$(12) \quad (\psi(h_1), \psi(h_2))_2 = (h_1, h_2)_1 ; h_1, h_2 \in H_1.$$

Then  $\psi$  is an isomorphism of  $H_1$  onto  $H_2$ .

The proof (which is almost evident) is performed in [7].

### 3. BEST LINEAR ESTIMATES

In this section we shall give an H-space description of linear and the best linear estimates for functions defined on  $\Theta$  (compare with [7]).

Throughout this section  $\xi$  will be a given design of the experiment and  $g$  will be a given (not necessarily linear) function on  $\Theta$ .

Let us fix  $\theta \in \Theta$  and let us denote by  $(\Omega, \mathcal{B}, \mathbf{P})$  the probability space on which the random variables  $X_\theta(F); F \in \mathcal{A}, \xi(F) > 0$ , are defined (i.e.  $X_\theta(F) \in L_2(\Omega, \mathcal{B}, \mathbf{P})$ ). Two subspaces of the H-space  $L_2(\Omega, \mathcal{B}, \mathbf{P})$  are important for us.

a) The subspace  $\mathcal{X}_\theta$  spanned by the set of random variables

$$\{X_\theta(F); F \in \mathcal{A}, \xi(F) > 0\}.$$

b) The subspace  $\mathcal{X}_\theta^*$  spanned by the set of random variables

$$\{X_\theta(F) - EX_\theta(F); F \in \mathcal{A}, \xi(F) > 0\}.$$

We denote by  $\xi^-, \xi^+$  the measures on  $(A, \mathcal{A})$  which are defined by

$$(13) \quad \xi^-(F) = \int_F w^{-1} d\xi, \quad \xi^+(F) = \int_F w d\xi; \quad F \in \mathcal{A}.$$

**Lemma 3.** a) There is an isomorphism  $\varkappa_\theta$  of  $L_2(A, \mathcal{A}, \xi^-)$  onto  $\mathcal{X}_\theta^*$  such that

$$\varkappa_\theta(\chi_F) = X_\theta(F) - EX_\theta(F); \quad F \in \mathcal{A}, \quad \xi(F) > 0.$$

b) There is a one-to-one linear map  $\delta_\theta$  of  $\mathcal{X}_\theta^*$  onto  $\mathcal{X}_\theta$  such that

$$(14) \quad \text{cov} [\delta_\theta(X), \delta_\theta(X')] = EXX' = \int \varkappa_\theta^{-1}(X) \varkappa_\theta^{-1}(X') d\xi$$

and

$$(15) \quad E \delta_\theta(X) = \int \varkappa_\theta^{-1}(X) \theta d\xi.$$

**Proof.** a) The sets

$$\{\chi_F : F \in \mathcal{A}, \xi(F) > 0\}, \quad \{X_\theta(F) - EX_\theta(F) : F \in \mathcal{A}, \xi(F) > 0\}$$

span  $L_2(A, \mathcal{A}, \xi^-)$ ,  $\mathcal{X}_\theta^*$ . Further

$$\begin{aligned} (\chi_F, \chi_{F'})_{\xi^-} &= \text{cov} [X_\theta(F), X_\theta(F')] = (X_\theta(F) - EX_\theta(F), \\ &X_\theta(F') - EX_\theta(F'))_{\theta}. \end{aligned}$$

Therefore the first statement of the Lemma follows from Lemma 2.

b) Denote by  $\mathcal{L}$  (and  $\mathcal{L}^*$ ) the set of all finite linear combinations of random variables from the set  $\{X_\theta(F); F \in \mathcal{A}, \xi(F) > 0\}$  (and from the set  $\{X_\theta(F) - EX_\theta(F); F \in \mathcal{A}, \xi(F) > 0\}$ , respectively). We shall use the notation  $X^* = X - EX$  for  $X \in \mathcal{L}$ . We may prove for finite sums:  $\sum_i \alpha_i X_\theta^*(F_i) = \sum_j \beta_j X_\theta^*(F_j)$  if and only if  $\sum_i \alpha_i X_\theta(F_i) = \sum_j \beta_j X_\theta(F_j)$  (the equalities in the  $L_2(\Omega, \mathcal{B}, \mathbf{P})$  - space). The "if" part

is evident. The "only if" part follows from

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$$\begin{aligned} E \sum_i \alpha_i X_\theta(F_i) &= \int \sum_i \alpha_i \chi_{F_i} \theta \, d\xi = \int \alpha_\theta^{-1} [\sum_i \alpha_i X_\theta^*(F_i)] \theta \, d\xi = \\ &= (\sum_i \alpha_i X_\theta^*(F_i), \alpha_\theta(w \theta))_{\mathbb{P}} = (\sum_j \beta_j X_\theta^*(F_j), \alpha_\theta(w \theta))_{\mathbb{P}} = E \sum_j \beta_j X_\theta(F_j), \end{aligned}$$

where we used part a) of the Lemma. Therefore the mapping  $\delta_\theta : \mathcal{L}^* \xrightarrow{\text{onto}} \mathcal{L}$  such that  $\delta_\theta[X - EX] = X$  is a one-to-one and satisfies (14) and (15).

A sequence  $\{X_n\}_{n=1}^\infty$  of points from  $\mathcal{L}$  is fundamental iff the sequence  $\{X_n^*\}_{n=1}^\infty$  is fundamental. For their limits  $X \in \mathcal{X}_\theta$  and  $X^* \in \mathcal{X}_\theta^*$  we may prove  $EX = \int \alpha_\theta^{-1}(X^*) \theta \, d\xi$ . Indeed, since  $E^2(X_n - X_m) \leq E(X_n - X_m)^2$ , the convergence  $E(X_n - X_m)^2 \rightarrow 0$  implies  $|EX_n - EX_m| \rightarrow 0$  and  $E(X_n^* - X_m^*)^2 = E(X_n - X_m)^2 - E^2(X_n - X_m) \rightarrow 0$ . Hence if  $\{X_n\}_{n=1}^\infty$  is fundamental and has the limit  $X$ , then  $\{X_n^*\}_{n=1}^\infty$  and  $\{EX_n\}_{n=1}^\infty$  are fundamental and have limits which we denote by  $X^*$  and  $\beta$ . We may write:

$$|EX - \beta| \leq |E(X - X_n)| + |EX_n - \beta| \rightarrow 0,$$

therefore

$$\begin{aligned} EX &= \lim_{n \rightarrow \infty} EX_n = \lim_{n \rightarrow \infty} \int \alpha_\theta^{-1}(X_n^*) \theta \, d\xi = \lim_{n \rightarrow \infty} (X_n^*, \alpha_\theta(w \theta))_{\mathbb{P}} = \\ &= \int \alpha_\theta^{-1}(X^*) \theta \, d\xi. \end{aligned}$$

On the contrary, if  $\{X_n^*\}_{n=1}^\infty$  is fundamental, then  $E(X_n^* - X_m^*)^2 \rightarrow 0$  implies

$$\begin{aligned} E^2(X_n - X_m) &= \left[ \int \alpha_\theta^{-1}(X_n^* - X_m^*) \theta \, d\xi \right]^2 = \\ &= (X_n^* - X_m^*, \alpha_\theta(w \theta))_{\mathbb{P}}^2 \leq E(X_n^* - X_m^*)^2 E \alpha_\theta^2(w \theta) \rightarrow 0. \end{aligned}$$

Therefore

$$E(X_n - X_m)^2 = E(X_n^* - X_m^*)^2 + E^2(X_n - X_m) \rightarrow 0$$

and  $\{X_n\}_{n=1}^\infty$  is fundamental.

It is now evident that  $\delta_\theta^{-1}$  defined by  $\delta_\theta^{-1}(X) = X - EX$  for every  $X \in \mathcal{X}_\theta$  is a one-to-one mapping of  $\mathcal{X}_\theta$  onto  $\mathcal{X}_\theta^*$  which satisfies (14) and (15).  $\square$

**Definition 3.** A linear estimate associated with an element  $l \in L_2(\mathcal{A}, \mathcal{A}, \xi^-)$  is the class of random variables

$$Y_l = \{\delta_\theta[\alpha_\theta(l)]; \theta \in \Theta\}.$$

If  $Y_1, Y_2$  are two linear estimates associated with  $l_1, l_2$ , then the covariance

$$(16) \quad \text{cov} [\delta_\theta(x_\theta(l_1)), \delta_\theta(x_\theta(l_2))] = \int l_1 l_2 w^{-1} d\xi$$

is the covariance of  $Y_1$  and  $Y_2$ .

This definition can be interpreted simply if  $\xi$  is a design concentrated in a finite number of equivalence classes in  $A$ :

$$\xi(\{a_i\}) > 0; \quad i = 1, \dots, n, \quad \sum_{i=1}^n \xi(\{a_i\}) = 1.$$

In such a case

$$\delta_\theta x_\theta(l) = \sum_{i=1}^n l(a_i) X_\theta(\{a_i\}) \xi(\{a_i\}); \quad l \in L_2(A, \mathcal{A}, \xi).$$

A linear estimate  $Y_l$  is a *linear unbiased estimate (LUE)* for a function  $g$  on  $\Theta$  if

$$E \delta_\theta(x_\theta(l)) = g(\theta)$$

for every  $\theta \in \Theta$ . It is the *best linear unbiased estimate (BLUE)* for  $g$  if its variance

$$\int l^2 w^{-1} d\xi$$

is the least possible one among all variances of LUE's for  $g$ .

The *information kernel* of the design  $\xi$  is a real function  $M_\xi$  defined on  $\Theta \times \Theta$  as

$$M_\xi[\theta, \theta'] = \int \theta \theta' w d\xi; \quad \theta, \theta' \in \Theta.$$

Denote by  $L_2^{+\xi}(\Theta)$  the subspace of  $L_2(A, \mathcal{A}, \xi^+)$  spanned by  $\Theta$  and by  $L_2^{-\xi}(w\Theta)$  the subspace of  $L_2(A, \mathcal{A}, \xi^-)$  spanned by the set  $\{w\theta : \theta \in \Theta\}$ .

We may write

$$M_\xi(\theta, \theta') = (\theta, \theta')_{\xi^+} = (w\theta, w\theta')_{\xi^-}; \quad \theta, \theta' \in \Theta.$$

Thus, according to Lemma 1 and Lemma 2,  $H(M_\xi)$ ,  $L_2^{+\xi}(\Theta)$  and  $L_2^{-\xi}(w\Theta)$  are isomorphic H-spaces. The correspondences due to the isomorphisms are:  $l \in L_2^{+\xi}(\Theta) \leftrightarrow w^{-1}l \in L_2^{-\xi}(w\Theta) \leftrightarrow (\cdot, w^{-1}l)_{\xi^+} = (\cdot, wl)_{\xi^-} \in H(M_\xi)$ .

**Theorem 4.** *The following five statements are equivalent*

1. *There is a LUE for  $g$ .*
2. *There is a BLUE for  $g$ .*
3.  $g \in H(M_\xi)$ .



4. There is an  $l \in L_2(A, \mathcal{A}, \xi^-)$  such that

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

5. There is an  $l_\theta \in L_2^{\xi^-}(w\Theta)$  such that

$$g(\theta) = \int l_\theta \theta \, d\xi; \quad \theta \in \Theta.$$

The element  $l_\theta$  in 5 is unique. The BLUE is unique and is equal to the linear estimate associated to  $l_\theta$ . Its variance is equal to

$$\int l_\theta^2 \, d\xi^-.$$

Proof. If  $Y_1$  is a LUE for  $g$  then, according to Lemma 3 of this section

$$g(\theta) = E \delta_\theta(x_\theta(l)) = \int l \theta \, d\xi,$$

hence 1 implies 4. The variance of  $Y_1$  is equal to  $\int l^2 \, d\xi^-$ . The projection  $l_\theta$  of  $l$  onto  $L_2^{\xi^-}(w\Theta)$  has the property

$$\int l_\theta \theta \, d\xi = \int (l_\theta - l) w \theta \, d\xi^- + \int l \theta \, d\xi = g(\theta).$$

Thus 4 implies 5. Since  $H(M_\xi)$  is isomorphic to  $L_2^{\xi^-}(w\Theta)$ , we have:  $g \in H(M_\xi)$  iff there is an  $l_\theta \in L_2^{\xi^-}(w\Theta)$  such that  $g(\theta) = (\theta, w l_\theta)_{\xi^-} = \int l_\theta \theta \, d\xi$  for every  $\theta \in \Theta$ . Hence 3 is equivalent to 5. If  $l_\theta, l'_\theta$  both satisfy 5, then  $(l_\theta - l'_\theta, w \theta)_{\xi^-} = 0$  for every  $\theta \in \Theta$  and simultaneously  $l_\theta - l'_\theta \in L_2^{\xi^-}(w\Theta)$ , therefore  $l_\theta = l'_\theta$ . Thus  $l_\theta$  in 5 is unique and  $Y_{l_\theta}$  is the BLUE for  $g$ . Hence 5 implies 2. Obviously 2 implies 1.  $\square$

Note. If we denote  $\bar{\theta} = w^{1/2} \theta$ ;  $\theta \in \Theta$ , and  $\bar{\Theta} = \{\bar{\theta} : \theta \in \Theta\}$ , we may write

$$M_\xi(\theta, \theta') = \int \bar{\theta} \bar{\theta}' \, d\xi$$

and the conditions 4 and 5 in the Theorem can be written as

$$g(\theta) = \int l w^{-1/2} \bar{\theta} \, d\xi; \quad \bar{\theta} \in \bar{\Theta}, l w^{-1/2} \in L_2(A, \mathcal{A}, \xi),$$

$$g(\theta) = \int l_\theta w^{-1/2} \bar{\theta} \, d\xi; \quad \bar{\theta} \in \bar{\Theta}, l_\theta w^{-1/2} \in L_2^{\xi}(\bar{\Theta})$$

and the variance of the BLUE for  $g$  is

$$\int [l_\theta w^{-1/2}]^2 \, d\xi.$$

Therefore as long as we shall study only linear estimates for functions on  $\Theta$  we may suppose without restriction of generality that  $w(a) \equiv 1$ . We shall make this assumption in the next section.

#### 4. ORDERING OF DESIGNS

We shall suppose that the aim of the experimenter is to estimate as precisely as possible the values of some real functions on  $\Theta$ . We shall denote by  $G$  the set of these functions and we shall call the elements of  $G$  "useful variables".

Evidently any two designs  $\xi, \xi_0$  (such that  $G \subset H(M_\xi)$  and  $G \subset H(M_{\xi_0})$ ) must be compared according to the variances and the covariances of the BLUE's for the useful variables.

From the Theorem 4 it follows that we can define an isometric operator  $V_\xi$  of  $H(M_{\xi_0})$  onto  $L_2^{\xi}(\Theta)$  such that

$$h(\theta) = (V_\xi h, \theta)_\xi; \quad \theta \in \Theta, h \in H(M_{\xi_0})$$

and the covariance of the BLUE's for  $h, h' \in H(M_\xi)$  under the design  $\xi$  is equal to

$$(V_\xi h, V_\xi h')_\xi = (h, h')_{M_{\xi_0}}.$$

We shall denote by  $D_\xi$  the covariance function of the BLUE's for the useful variables:

$$D_\xi(g, g') = (g, g')_{M_\xi}; \quad g, g' \in G.$$

We say that a design  $\xi$  is *uniformly better* (strictly uniformly better) than a design  $\xi_0$  if the function  $D_{\xi_0} - D_\xi$  is a nonnegative definite (positive definite) function on  $G \times G$ . Then the variance of the BLUE for any finite linear combination of useful variables under the design  $\xi$  is not larger than the variance of the BLUE under the design  $\xi_0$ . Any other ordering of designs must be an extension of the partial ordering defined by the relation "uniformly better".

In the case when the set  $G$  is finite and the matrix  $\{D_\xi(g, g')\}_{g, g' \in G}$  is nonsingular it is mostly usual to compare the designs according to the value of the generalized variance of the BLUE's for  $G$  which is equal to the determinant

$$(17) \quad \det [\{D_\xi(g, g')\}_{g, g' \in G}].$$

This value can be well interpreted in many senses: it is proportional to the volume of the ellipsoid of dispersion [6]; if the data obtained from the experiment are normally distributed, the obtained ordering of designs coincides with the ordering according to the Shannon measure of information about  $G$  contained in the experimental data [10]; it gives the same optimal design as the minimax ordering of designs for the interpolation [4]. Therefore we shall restrict ourselves to the ordering of designs according to the generalized variance of the BLUE's for  $G$  and to its generalization in the case of  $G$  being infinite.

If the set  $G \in H(M_\xi)$  remains finite but the matrix  $\{D_\xi(g, g')\}_{g, g' \in G}$  is singular, a natural generalization of (17) is the product of all nonzero proper values of  $D_\xi$  (respecting their multiplicities). However an extension of this definition of the generalized variance to the case of an infinite  $G$  needs to specify the  $H$ -space in which the spectral values of  $D_\xi$  are to be computed and to replace the product of the proper values by a suitably chosen integral.

We shall denote by  $\mathcal{L}[G]$  the set of all finite linear combinations of elements from  $G$  and by  $H_G(M_\xi)$  the subspace of  $H(M_\xi)$  spanned by  $G$ .

**Definition 4.** A design  $\xi$  is  $G$ -dominated by a design  $\xi_0$  if

- a)  $G \subset H(M_{\xi_0}) \subset H(M_\xi)$
- b) there is a number  $c$  such that

$$\|h\|_{M_\xi}^2 \leq c \|h\|_{M_{\xi_0}}^2 \quad \text{for every } h \in \mathcal{L}[G].$$

**Lemma 5.** If  $\xi$  is  $G$ -dominated by  $\xi_0$ , then

a)  $H_G(M_{\xi_0})$  is a dense subset of the  $H$ -space  $H_G(M_\xi)$  and  $\|h\|_{M_\xi}^2 \leq c \|h\|_{M_{\xi_0}}^2$  for every  $h \in H_G(M_{\xi_0})$ .

b)  $H(D_\xi) \subset H(D_{\xi_0})$  and  $\|v\|_{D_{\xi_0}}^2 \leq c \|v\|_{D_\xi}^2$  for every  $v \in H(D_\xi)$ .

*Proof.* a) If  $h_0 \in H_G(M_{\xi_0})$ , then there is a sequence  $\{h_n\}_{n=1}^\infty$  of elements of  $\mathcal{L}[G]$  such that  $\|h_n - h_0\|_{M_{\xi_0}} \rightarrow 0$ . The sequence  $\{h_n\}_{n=1}^\infty$  is fundamental with respect to the norm  $\|\cdot\|_{M_{\xi_0}}$  and also to the norm  $\|\cdot\|_{M_\xi}$ . Denote by  $h$  the limit of this sequence in the norm  $\|\cdot\|_{M_\xi}$ . We may write:

$$|h_n(\theta) - h_0(\theta)| = |(h_n - h_0, M_{\xi_0}(\cdot, \theta))_{M_{\xi_0}}| \leq \|h_n - h_0\|_{M_{\xi_0}} M_{\xi_0}^{1/2}(\theta, \theta)$$

and

$$|h_n(\theta) - h(\theta)| = |(h_n - h, M_\xi(\cdot, \theta))_{M_\xi}| \leq \|h_n - h\|_{M_\xi} M_\xi^{1/2}(\theta, \theta)$$

for every  $\theta \in \Theta$ . Therefore  $h(\theta) = h_0(\theta)$  and  $H_G(M_{\xi_0}) \subset H_G(M_\xi)$ . Further

$$\|h\|_{M_\xi}^2 = \lim_{n \rightarrow \infty} \|h_n\|_{M_\xi}^2 \leq c \lim_{n \rightarrow \infty} \|h_n\|_{M_{\xi_0}}^2 = \|h\|_{M_{\xi_0}}^2.$$

The subspace  $H_G(M_{\xi_0})$  is dense in  $H_G(M_\xi)$ , since it contains the dense set  $\mathcal{L}[G]$ .

b) According to the Lemma 1 there is an isometric operator  $S_\xi$  of  $H(D_\xi)$  onto  $H_G(M_\xi)$  such that

$$(18) \quad v(g) = (g, S_\xi v)_{M_\xi}; \quad g \in G.$$

From a) we obtain

$$|v(g)| \leq \|g\|_{M_\xi} \|S_\xi v\|_{M_\xi} \leq c \|S_\xi v\|_{M_{\xi_0}} \|g\|_{M_{\xi_0}},$$

384 hence  $v$  can be extended to a bounded linear functional on  $H_G(M_{\xi_0})$ . From the Riesz representation theorem [3] we obtain

$$v(g) = (g, h)_{M_{\xi_0}}; \quad g \in G$$

for some  $h \in H_G(M_{\xi_0})$ . Hence  $v \in H(D_{\xi_0})$  and

$$(19) \quad v(g) = (g, S_{\xi_0} v)_{M_{\xi_0}}; \quad g \in G.$$

Comparing (18) and (19) we obtain

$$(h, S_{\xi} v)_{M_{\xi}} = (h, S_{\xi_0} v)_{M_{\xi_0}}; \quad h \in H_G(M_{\xi_0}), v \in H(D_{\xi}).$$

Therefore

$$\begin{aligned} \|S_{\xi_0} v\|_{M_{\xi_0}}^2 &= (S_{\xi_0} v, S_{\xi_0} v)_{M_{\xi_0}} = \\ &= (S_{\xi_0} v, S_{\xi} v)_{M_{\xi}} \leq c^{1/2} \|S_{\xi_0} v\|_{M_{\xi_0}} \|S_{\xi} v\|_{M_{\xi}}, \end{aligned}$$

which implies

$$\|v\|_{D_{\xi_0}}^2 = \|S_{\xi_0} v\|_{M_{\xi_0}}^2 \leq c \|S_{\xi} v\|_{M_{\xi}}^2 = c \|v\|_{D_{\xi}}^2. \quad \square$$

A direct corollary of the Lemma 5 is that if  $\xi$  is  $G$ -dominated by  $\xi_0$ , then the covariance function  $D_{\xi}$  induces an operator  $\mathbf{D}_{\xi}$  in  $H(D_{\xi_0})$  defined in the following way

$$(20) \quad [\mathbf{D}_{\xi} v](g) = (D_{\xi}(\cdot, g), v)_{D_{\xi_0}}; \quad g \in G, v \in H(D_{\xi_0}).$$

We may compute the spectral values of  $\mathbf{D}_{\xi}$  and use them to compare different designs dominated by the same design  $\xi_0$ . It is easy to prove that the spectrum of  $\mathbf{D}_{\xi}$  is contained in the interval  $\langle 0, c \rangle$ .

**Lemma 6.** *A design  $\xi_0$  is absolutely continuous with respect to a design  $\xi$  ( $\xi_0 \ll \xi$ ) and the Radon derivative  $d\xi_0/d\xi$  is bounded on  $A$  if and only if there is a design  $\xi'$  and a number  $\alpha \in (0, 1)$  such that*

$$\xi = \alpha \xi_0 + (1 - \alpha) \xi'.$$

*Proof.* 1. Suppose that  $d\xi_0/d\xi \leq c < \infty$ . We may assume that  $c > 1$ . We define

$$\xi'(F) = (1 - 1/c)^{-1} \int_F [1 - (1/c)(d\xi_0/d\xi)] d\xi; \quad F \in \mathcal{A}.$$

Evidently  $\xi'$  is a design,  $\xi' \ll \xi$  and

$$\xi = 1/c \xi_0 + (1 - 1/c) \xi'.$$

2.  $\xi = \xi_0 + (1 - \alpha) \xi'$  and  $\alpha \in (0, 1)$  imply

$$\xi_0 \ll \xi, \quad \xi' \ll \xi$$

and

$$1 = \alpha(d\xi_0/d\xi) + (1 - \alpha)(d\xi'/d\xi) \geq \alpha(d\xi_0/d\xi), \text{ a.c.}$$

Therefore  $d\xi_0/d\xi$  is bounded on  $A$ .  $\square$

We shall denote by  $L_2^{\xi_0}$  the subspace of  $L_2(A, \mathcal{A}, \xi_0)$  defined by  $L_2^{\xi_0} = V_{\xi_0} H_G(M_{\xi_0})$ .

**Theorem 7.** *If  $G \in H(M_{\xi_0})$ ,  $\xi_0 \ll \xi$  and  $\xi_0/d\xi \leq c < \infty$ , then*

a)

$$L_2(A, \mathcal{A}, \xi) \subset L_2(A, \mathcal{A}, \xi_0),$$

$$\|l\|_{\xi_0}^2 \leq c \|l\|_{\xi}^2; \quad l \in L_2(A, \mathcal{A}, \xi)$$

and  $L_2^{\xi}(\Theta)$  is a dense subset of  $L_2^{\xi_0}(\Theta)$ ;

b)  $\xi$  is  $G$ -dominated by  $\xi_0$ ;

c) the operator  $\mathbf{D}_{\xi}$  in  $H(D_{\xi_0})$  is equivalent to the operator  $\mathbf{P}_G^0 \mathbf{T} \mathbf{P}_{\Theta} \mathbf{T}^* \mathbf{P}_G^0$  in  $L_2^{\xi_0}$  where  $\mathbf{T}$  maps every  $l \in L_2(A, \mathcal{A}, \xi)$  onto  $l \in L_2(A, \mathcal{A}, \xi_0)$ ,  $\mathbf{T}^*$  is the adjoint of  $\mathbf{T}$ ,  $\mathbf{P}_{\Theta}$  is the projection of  $L_2(A, \mathcal{A}, \xi)$  onto  $L_2^{\xi}(\Theta)$  and  $\mathbf{P}_G^0$  is the projection of  $L_2(A, \mathcal{A}, \xi_0)$  onto  $L_2^{\xi_0}$ .

Proof. a) If  $l \in L_2(A, \mathcal{A}, \xi)$ , then

$$\int l^2 d\xi_0 = \int l^2 \frac{d\xi_0}{d\xi} d\xi \leq c \int l^2 d\xi < \infty,$$

hence  $l \in L_2(A, \mathcal{A}, \xi_0)$  and  $\|l\|_{\xi_0}^2 \leq c \|l\|_{\xi}^2$ . If  $l \in L_2^{\xi}(\Theta)$ , then there is a sequence  $\{l_n\}_{n=1}^{\infty}$  of vectors from  $\mathcal{L}[\Theta]$  (the set of all finite linear combinations of elements from the set  $\Theta$ ) which converges to  $l$  in the norm  $\|\cdot\|_{\xi}$ .

Therefore

$$\lim_{n \rightarrow \infty} \|l_n - l\|_{\xi_0}^2 \leq c \lim_{n \rightarrow \infty} \|l_n - l\|_{\xi}^2 = 0$$

and  $l \in L_2^{\xi_0}(\Theta)$ .  $L_2^{\xi}(\Theta)$  is dense in  $L_2^{\xi_0}(\Theta)$  since it contains the dense set  $\mathcal{L}[\Theta]$ .

b) Denote by  $\mathbf{T}$  the operator from  $L_2(A, \mathcal{A}, \xi)$  into  $L_2(A, \mathcal{A}, \xi_0)$  defined by

$$\mathbf{T}l = l; \quad l \in L_2(A, \mathcal{A}, \xi).$$

We assert that  $\mathbf{T}^*$ , the adjoint of  $\mathbf{T}$ , is a multiplicative operator from  $L_2(A, \mathcal{A}, \xi_0)$  into  $L_2(A, \mathcal{A}, \xi)$  with the multiplicative function  $d\xi_0/d\xi$ . Indeed

$$\int \left[ \frac{d\xi_0}{d\xi} l \right]^2 d\xi \leq c \int l^2 d\xi_0 < \infty; \quad l \in L_2(A, \mathcal{A}, \xi_0)$$

and

$$(\mathbf{T}^*l, h)_{\xi} = (l, \mathbf{T}h)_{\xi_0} = \int \left[ \frac{d\xi_0}{d\xi} l \right] h d\xi; \quad l, h \in L_2(A, \mathcal{A}, \xi_0).$$

386 For any  $h \in H(M_{\xi_0})$  we may write

$$(21) \quad h(\theta) = (\mathbf{V}_{\xi_0} h, \theta)_{\xi_0} = (\mathbf{V}_{\xi_0} h, \mathbf{T}\theta)_{\xi_0} = (\mathbf{P}_\theta \mathbf{T}^* \mathbf{V}_{\xi_0} h, \theta)_\xi; \quad \theta \in \Theta.$$

Hence  $h \in H(M_\xi)$ . We shall denote by  $\mathbf{U}$  the operator from  $H(M_{\xi_0})$  into  $H(M_\xi)$  defined by

$$\mathbf{U}h = h; \quad h \in H(M_{\xi_0}).$$

(21) implies that

$$(22) \quad \mathbf{V}_\xi \mathbf{U}h = \mathbf{P}_\theta \mathbf{T}^* \mathbf{V}_{\xi_0} h; \quad h \in H(M_{\xi_0}).$$

Finally for  $h \in H(M_{\xi_0})$  we have

$$\|h\|_{M_\xi}^2 = \|\mathbf{V}_\xi \mathbf{U}h\|_\xi^2 = \|\mathbf{P}_\theta \mathbf{T}^* \mathbf{V}_{\xi_0} h\|_\xi^2 \leq c \int (\mathbf{V}_{\xi_0} h)^2 d\xi_0 = c \|h\|_{M_{\xi_0}}^2.$$

Thus  $\xi$  is  $G$ -dominated by  $\xi_0$ .

c) For every  $h, h' \in H_G(M_{\xi_0})$  we may write using the equality (22)

$$(23) \quad \begin{aligned} (\mathbf{U}h, \mathbf{U}h')_{M_\xi} &= (\mathbf{V}_\xi \mathbf{U}h, \mathbf{V}_\xi \mathbf{U}h')_\xi = \\ &= (\mathbf{P}_\theta \mathbf{T}^* \mathbf{P}_G^0 \mathbf{V}_{\xi_0} h, \mathbf{P}_\theta \mathbf{T}^* \mathbf{P}_G^0 \mathbf{V}_{\xi_0} h')_\xi = \\ &= (h, \mathbf{V}_{\xi_0}^* \mathbf{P}_G^0 \mathbf{T} \mathbf{P}_\theta \mathbf{T}^* \mathbf{P}_G^0 \mathbf{V}_{\xi_0} h')_{M_{\xi_0}}. \end{aligned}$$

Let  $v_1, v_2$  be two arbitrary vectors from  $H(D_{\xi_0})$ . We may write

$$v_1(g) = (g, S_{\xi_0} v_1)_{M_{\xi_0}}, \quad v_2(g) = (g, S_{\xi_0} v_2)_{M_{\xi_0}}; \quad g \in G.$$

From the definition (20) of the operator  $\bar{\mathbf{D}}_\xi$  we have

$$(24) \quad \begin{aligned} (\bar{\mathbf{D}}_\xi v_1)(g) &= ((\cdot, g)_{M_\xi}, (\cdot, S_{\xi_0} v_1)_{M_{\xi_0}})_{D_{\xi_0}} = \\ &= ((\cdot, \mathbf{U}^* g)_{M_{\xi_0}}, (\cdot, S_{\xi_0} v_1)_{M_{\xi_0}})_{D_{\xi_0}} = \\ &= (\mathbf{U}^* g, S_{\xi_0} v_1)_{M_{\xi_0}} = (g, \mathbf{U} S_{\xi_0} v_1)_{M_\xi}. \end{aligned}$$

Thus using (23) we obtain

$$\begin{aligned} (v_2 \bar{\mathbf{D}}_\xi v_1)_{D_{\xi_0}} &= ((\cdot, S_{\xi_0} v_2)_{M_{\xi_0}}, (\cdot, \mathbf{U} S_{\xi_0} v_1)_{M_\xi})_{D_{\xi_0}} = \\ &= (S_{\xi_0} v_2, \mathbf{U}^* \mathbf{U} S_{\xi_0} v_1)_{M_{\xi_0}} = (\mathbf{U} S_{\xi_0} v_2, \mathbf{U} S_{\xi_0} v_1)_{M_\xi} = \\ &= (v_2, S_{\xi_0}^* \mathbf{V}_{\xi_0}^* \mathbf{P}_G^0 \mathbf{T} \mathbf{P}_\theta \mathbf{T}^* \mathbf{P}_G^0 \mathbf{V}_{\xi_0} S_{\xi_0} v_1)_{D_{\xi_0}}. \end{aligned}$$

$\bar{\mathbf{D}}_\xi$  is equivalent with  $\mathbf{P}_G^0 \mathbf{T} \mathbf{P}_\theta \mathbf{T}^* \mathbf{P}_G^0$ , since  $S_{\xi_0}$  and  $\mathbf{V}_{\xi_0}$  are isometric operators.  $\square$

**Corollary.** Let us consider the special case when  $\Theta$  spans  $L_2(A, \mathcal{A}, \xi_0)$  and  $L_G^{\xi_0}$  is the set of all functions from  $L_2(A, \mathcal{A}, \xi_0)$  measurable with respect to a  $\sigma$ -algebra

$\mathcal{B} \subset \mathcal{A}$ . For any  $l \in L_G^{\xi_0}$  we may then write

$$P_G^0 \mathbf{TP}_\theta \mathbf{T}^* P_G^0 l = P_G^0 \left[ \frac{d\xi_0}{d\xi} l \right] = E_{\xi_0} \left[ \frac{d\xi_0}{d\xi} l \mid \mathcal{B} \right] = E_{\xi_0} \left[ \frac{d\xi_0}{d\xi} \mid \mathcal{B} \right] l,$$

where  $E_{\xi_0} [\cdot \mid \mathcal{B}]$  is the conditional mean with respect to  $\xi_0$  under the  $\sigma$ -algebra  $\mathcal{B}$ . In this special case  $\mathbf{D}_\xi$  is equivalent to the operator of multiplication by the function

$$E_{\xi_0} \left[ \frac{d\xi_0}{d\xi} \mid \mathcal{B} \right] \in L_G^{\xi_0}.$$

Returning to the general case we can now propose a generalization of (17) at least for the case of  $d\xi_0/d\xi$  being bounded also from below, i.e. when  $0 < d \leq (d\xi_0)/d\xi \leq c < \infty$  for some  $c, d$ . Then for any  $l \in L_G^{\xi_0}$  we may prove that  $\|P_G^0 \mathbf{TP}_\theta \mathbf{T}^* P_G^0 l\|_{\xi_0}^2 \geq d \|l\|_{\xi_0}^2$ , and the spectrum of the operator  $P_G^0 \mathbf{TP}_\theta \mathbf{T}^* P_G^0$  is a subset of  $\langle d, c \rangle$ . By the spectral theorem for Hermitian operators [3] we can define an operator

$$\int_{\mathcal{A}} \ln \lambda \, d\mathbf{P}(\lambda),$$

where  $\mathbf{P}(\cdot)$  is the spectral measure of the operator  $P_G^0 \mathbf{TP}_\theta \mathbf{T}^* P_G^0$ . Then there corresponds to the value of the logarithm of the determinant (17) the value of the integral

$$(25) \quad \int_{\mathcal{A}} \ln \lambda \, d(f, \mathbf{P}(\lambda) f)_{\xi_0},$$

where  $f$  is a properly chosen element of  $L_G^{\xi_0}$ .

In the special case, under the assumption of the Corollary to the Theorem, for  $f(a) = 1; a \in \mathcal{A}$ , we obtain from (25) the following expression

$$(26) \quad \int_{\mathcal{A}} \ln E_{\xi_0} \left[ \frac{d\xi_0}{d\xi} \mid \mathcal{B} \right] d\xi_0.$$

In the case when  $G$  spans  $H(M_{\xi_0})$ , (26) is the *I-divergence* (or the *generalized entropy*) of  $\xi_0$  and  $\xi$ , [5].

In the general case we may use (25) to compare designs from the set

$$\mathcal{E} = \left\{ \xi : \xi_0 \ll \xi, 0 < \inf_{a \in \mathcal{A}} \frac{d\xi_0}{d\xi}(a) \leq \sup_{a \in \mathcal{A}} \frac{d\xi_0}{d\xi}(a) < \infty \right\},$$

where the fixed design  $\xi_0$  and the function  $f \in L_G^{\xi_0}$  may correspond to the apriori knowledge of the experimenter about the useful variables. For a finite set  $G$  it has been shown [2; 8; 9; 11], that, if we follow a recurrent formula

$$\xi_n = \alpha_n \xi_{n-1} + (1 - \alpha_n) \xi^{(n)}; \quad n = 1, 2, \dots$$

388 with properly chosen numbers  $\alpha_n \in (0, 1)$  and simple designs  $\xi^{(n)}$ , we shall obtain a sequence  $\{\xi_n\}_{n=0}^{\infty}$  of designs from  $\Xi$  (due to the Lemma 6), which may be considered as approximately optimal with respect to the ordering defined by (17). The aim of a later paper will be to construct a similar procedure also for the infinite dimensional case.

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