LINEAR OPTIMAL DESIGNS FOR A FINITE FAMILY OF LINEAR MODELS

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1. INTRODUCTION

First of all, we develop notation and terminology before stating the problem that is tackled in this paper.

Let X be a Tychonoff topological space. We call X a design space. Let *B* be the Baire σ-field on X, i.e., the smallest σ- field on X containing all zero-sets of X. A subset Z of X is said to be a zero - set if we can write $Z = f^{-1}$ ({O}). for some real valued continuous function f on X. For topological notions, we refer to Gillman and Jerison[3]. In optimal design problems, it is normally assumed that X is a compact subset of some Euclidean space.

Let $f_{(m)}^T = (f_{mi}, f_{m2}, \ldots, f_{m\,n(m)})$, m= 1 to k, be a row vector of bounded real valued continuous functions on X. (T stands for transpose of a matrix.) For each xE X, we have a randon variable Y(x) having the following properties.

(i) E $Y(x) = f_{(m)}^T(x)\ \beta\ (m)$, for some m E j 1, 2, . . . , k[independent of x, where $P_{(m)}^T$ $ER^n<^m>$ is a vector of n(m) unknown parameters.

(u) Variance of $Y(x) = \sigma^2 > 0$.

For each xEX, we have a random phenomenon typified by the random variable Y(x) with expectation $f_{(m)}^T\ p_{(m)}$, for m E {1, 2,. . .,k}.

This is a multipurpose design model and the set {1, 2, 3,. . . ,k} corresponds to k different linear models all related to the same random variable. Finding optimal designs for each model would involve collecting a large amount of data on Y(x)'s and the basic idea in this paper is to find one universal design optimal in some sense for all the models. We will then use the data collected according to this universal design for the estimation of the unknown parameters in all the models simultaneously. This set-up could also be used to discriminate between several rival models and then follow it up with the estimation of the parameters of the chosen model.

Let ξ be a probability measure on *B*. We call probability measures on *B* as designs. Let.

$$M_m(\xi) = \int_X f_{(m)}(x) f_{(m)}^T(x)\ \xi(dx),\ m = 1 \text{ to } k.$$

$M_m(\xi)$ is called information matrix of order $n(m) \chi n(m)$ associated with the m^{th} model corresponding to the design ξ. $M_m(4)$ is obviously a positive semi - definite matrix. If ξ is the probability measure assigning mass 1/n to some η points Xj, x_2,. . .,Xn in X, $Y(x_1), Y(x_2)$, . . ., $Y(x_n)$ are η uncorrelated random variables m^{th} model is the true model, and $M_m(\xi)$ is nonsingular, then $\beta_{(m)}$ admits best linear unbiased estimator with dispersion matrix $\frac{1}{\eta}\ \sigma^2\ Mm^{-1}(\xi)$. In optimal designs we are mainly concerned with the selection of points x_1, x_2,. . ., χ_η such that $Mm^{-1}(\xi)$ is small in some acceptable sense.

Let L_m, m = 1 to k, be a real function defined on the linear space of all matrices of order $n(m)\ \chi\ n(m)$ satisfying the following properties.

(a) $L_m(A+B) = L_m(A)+L_m(B)$.

(β) $Lm(\lambda A) = \lambda L_m(A)$, λ real.

(γ) If A is positive semi-definite, $L_m(A) >0$. (If A is positive semi - definite, we use the notation A>0.)

Let Ξ_I denote the collection of all probability measures ξ on *B* for which $|Mm(\xi)$: 0 for every m= 1 to k, and Ξ the collection of all probability measures *on B*. For notational convenience, we let $D_m(\xi) = Mm^{-1}(\xi)$ for $\xi E \Xi_\iota$

For $\xi \in \Xi_1$ we define

(a) $F(\xi) = \sum_{m=1}^{k} \omega(m) \; L_m(D_m(\xi))$, where $\omega(1), \omega(2), \ldots, \omega(k)$

ar($\sum_{m=1}^{k} \omega(m) = 1.$ ghts with each $\omega(m)$ 0 and

(b) $\phi(\xi) = \sup_{x \in X} \sum_{m=1}^{k} \omega(m)\varphi_m(x,\xi)$, where

$$\varphi_m(\chi, \xi) = L_m(D_m(\xi) f_{(m)}(x) \; f_{(m)} \tau (\chi) \; D_m(\xi) \;), \; x \in X, \; \xi \in \Xi_1.$$

One may note that $\varphi_m(\cdot,\xi)$ is a bounded continuous function on X, and consequently, the supremum in (b) is finite.

D e f i n i t i o n 1.1. An element $\xi^* \in \Xi_1$ is said to be F - optimal if

$$F(\xi^*) = \min_{\xi \in \Xi_1} F(\xi).$$

D e f i n i t i o n 1.2. An element $\xi_0 \in \Xi_1$ is said to be φ - optimal if

$$\phi(\xi_0) = \min_{\xi \in \Xi_1} \phi(\xi).$$

This paper is aimed at studying these optimal measures. Lauter[5] studied this problem with respect to a different optimality criterion based on determinants of the information matrices. This paper could be regarded as complementary to that of Lauter's[5]. Fedorov [2, 2.9, 2.10 and 2.11, pp. 122 - 142] studied this problem in the case when there is only one model.

An F-optimal probability measure could be regarded as a good one minimising some function of all $D_m(\xi)$.

2. OPTIMAL MEASURES

$$\text{Let } \Xi_2 = \{ \xi^* \in \Xi_1 : F(\xi^*) = \min_{\xi \in \Xi_1} F(\xi) \}$$

$$\Xi_3 = \{\xi_0 \in \Xi_1 : \phi(\xi_0) = \min_{\xi \in \Xi_1} \phi(\xi), \}, \text{ and}$$

$$\Xi_4 = \{\xi' \in \Xi_1 : \sup_{x \in X} \sum_{m=1}^{k} \omega(m) \varphi_m(\chi, \xi'))$$

$$= F(\xi') \}.$$

First, we note that Ξ_1 is a convex set, i.e., if $\xi_1, \xi_2 \in \Xi_1$ and $0 \quad \lambda \quad 1$, then $\lambda\xi_1$ +

We begin with a Lemma.

L e m m a 2.1. F is a convex function on Ξ_1

P r o o f. Each L_m is a convex function on Ξ_1. See Fedorov [2, Lemma 2.9.1, p. 123]. Consequently., F is a convex function *on* Ξ_1.

T h e o r e m 2.2. Assume $\Xi_2 \quad 0$. The following statements are equivalent for $\xi^* \in \Xi_1$.

(ι) ξ^* is F-optimal,

(ii) ξ^* is φ-optimal.

$$\text{(iii)} \quad \sup_{x \in X} \sum_{m=1}^{k} \omega(m)\varphi_m(x, \xi^*) = F(\xi^*) = \phi(\xi^*).$$

Equivalently, $\Xi_2 = \Xi_3 = \Xi_4$.

P r o o f. (i) (ii). Suppose ξ^* is F - optimal. Consider the design $\tilde{\xi}(\alpha) = (1-\alpha)\,\xi^* + \alpha\xi$, O $\alpha < 1$ and $\xi \mathrm{E}\, \Xi$ be fixed. Note that $\tilde{\xi}(\alpha)\ \mathbf{E}\ \Xi_1$ for 0 $\alpha < 1$. Now,

$$\frac{\partial}{\partial \alpha} F(\tilde{\xi}(\alpha))\Big]_{\alpha = o} = \frac{\partial}{\partial \alpha} \sum_{m=1}^{k} \omega(m)\, L_m(D_m(\tilde{\xi}(\alpha)))\Big]_{\alpha = 0}$$

$$= \sum_{m=1}^{k} \omega(m)\, L_m\left\{ \frac{\partial}{\partial \alpha} D_m(\tilde{\xi}(\alpha))\Big]_{\alpha = 0}\right\}$$

$$= \sum_{m=1}^{k} \omega(m)\, L_m\{-D_m(\tilde{\xi}(\alpha))\,[M_m(\xi) - M_m(\xi^*)]\, D_m(\tilde{\xi}(\alpha))\}\,]_{\alpha=o}$$

(See Fedorov [2, Lemma 2.9.2, p. 124]).

$$= \sum_{m=1}^{k} \omega(m)\, L_m(D_m(\xi^*)) - \sum_{m=1}^{k} \omega(m)\, L_m\,[D_m(\xi^*) M_m(\xi)\, D_m(\xi^*)]$$

$$= F(\xi^*) - \sum_{m=1}^{k} \omega(m)\, L_m[D_m(\xi^*)\, M_m(\xi)\, D_m(\xi^*)] \qquad (2.2.1)$$

Alternatively, we note

$$\frac{\partial}{\partial \alpha} F(\tilde{\xi}(\alpha))\Big]_{\alpha = 0} = \lim_{\alpha \downarrow 0} \frac{F[(1-\alpha)\,\xi^* + \alpha\xi] - F(\xi^*)}{\alpha} \geqslant 0 \qquad (2.2.2)$$

since ξ^* is F-optimal.

From (2.2.1) and (2.2.2) we get

$$F(\xi^*) \geqslant \sum_{m=1}^{k} \omega(m)\, L_m[D_m(\xi^*)\, M_m(\xi)\, D_m(\xi^*)].$$

This inequality is valid whatever design ξ we choose. In particular, if ξ is degenerate at $x \in X$, we have

$$F(\xi^*) \geqslant \sum_{k=1}^{k} \omega(m)\, L_m[D_m(\xi^*) f_{(m)}(x)\, f^T_{(m)}(x)\, D_m(\xi^*)]$$

valid for every $x \in X$.

Consequently,

$$F(\xi^*) \geqslant \sup_{x \in X} \sum_{m=1}^{k} \omega(m)\, L_m[D_m(\xi^*) f_{(m)}(x)\, f_{(m)}^T(x)\, D_m(\xi^*)]$$

$$= \sup_{x \in X} \sum_{m=1}^{k} \omega(m) \varphi_m(x, \xi^*) = \phi(\xi^*). \tag{2.2.3}$$

On the other hand, let $\xi \in \Xi_1$.

$$= \sum_{m=1}^{k} \omega(m) \int_X L_m[D_m(\xi)\, f_{(m)}(x)\, f_{(m)}^T(x)\, D_m(\xi)]\; \xi(dx)$$

$$= \sum_{m=1}^{k} \omega(m)\, L_m\left[D_m(\xi) \left(\int_X f_{(m)}(x) f_{(m)}^T(x)\; \xi(dx) \right) D_m(\xi)\right]$$

by Lebesgue dominated convergence theorem.

$$= \sum_{m=1}^{k} \omega(m) L_m[D_m(\xi) M_m(\xi) D_m(\xi)]$$

$$= \sum_{m=1}^{k} \omega(m) L_m(D_m(\xi)) = F(\xi).$$

Now,

$$\sup_{x \in X} \sum_{m=1}^{k} \omega(m) \varphi_m(x,\xi) = \phi(\xi) \geqslant \int_X \sum_{m=1}^{k} \omega(m)\varphi_m(x,\xi)\,\xi(dx)$$

$$= F(\xi)$$

In particular, $\varphi(\xi^*)$ $F(\xi^*)$. This, in conjunction with (2.2.3) gives $\varphi(\xi^*) =$ *¥(ξ*)*. This equality, incidentally, proves (iii). Also $\varphi(\xi)$ *F(ξ)* *F(ξ*)* for every $\xi \in \Xi_1$ Consequently, $\varphi(\xi^*)$ $\operatorname{Inf}_{\in \Xi_1}$ $\varphi(\xi)$ $F(\xi^*)$. Hence equality must prevail

throughout. Thus

$$\phi(\xi^*) = \operatorname*{Inf}_{\xi \in \Xi_1} \phi(\xi) = \min_{\xi \in \Xi_1} \phi(\xi).$$

This proves (i) (ii).

Let us prove now (ii) (i)

Let ξ_0 be φ-optimal. Since Ξ_2 0, choose any $\xi_1 \in \Xi_2$. By the argument given in proving (i) (ii) and (iii), $F(\xi_1) = \varphi(\xi_1)$. Note that $F(\xi) < \varphi(\xi)$ is always true for any $\xi \in \Xi_1$ The following inequalities $F(\xi) < F(\xi_0) < \varphi(\xi_0) < \Phi(\xi_1)$ are now obvious. Thus equality prevails everywhere and hence ξ_0 is F—optimal.

Incidentally, the proof presented here provides a simple proof of Fedorov's Theorem 2.9.2 [2, p. 125-127] for the implication (2) (1).

Now we prove (iii) (i). Suppose ξ^* satisfies $P(\xi^*) = \varphi(\xi^*)$. Suppose ξ^* is not F-optimal. Let $\xi_2 \in \Xi_2$ be any design. Consider $\xi(\alpha) = (1-\alpha)\xi^* + \alpha\xi_2$, $0 < \alpha < 1$.

$$\frac{\partial}{\partial\alpha} \tilde{F}(\xi(\alpha))\Big]_{\alpha=0} = \lim_{\alpha \downarrow 0} \frac{\tilde{F}(\xi(\alpha)) - F(\xi^*)}{\alpha}$$

$$\begin{aligned}\tilde{F}(\xi(\alpha)) &\leqslant (1-\alpha)\, F(\xi^*) + \alpha F(\xi_2) \text{ by Lemma 2.1} \\ &= F(\xi^*) + \alpha[F(\xi_2) - F(\xi^*)]\end{aligned}$$

$$\frac{\tilde{F}(\xi(\alpha)) - F(\xi^*)}{\alpha} \leqslant F(\xi_2) - F(\xi^*) < 0 \text{ for every } \alpha \in (0,1)$$

Consequently, $\frac{\partial}{\partial\alpha} \tilde{F}(\xi(\alpha))\Big]_{\alpha=0} < 0.$

From (2.2.1)

$$\frac{\partial}{\partial\alpha} \tilde{F}(\xi(\alpha))\Big]_{\alpha=0} = F(\xi^*) - \sum_{m=1}^{k} \omega(m)\, L_m[D_m(\xi^*)\, M_m(\xi_2) D_m(\xi^*)]$$

$$= F(\xi^*) - \int_X \sum_{m=1}^{k} \omega(m)\, L_m[D_m(\xi^*)\, f_{(m)}(x)\, f_{(m)}^T(x)\, D_m(\xi^*)]\; \xi_2(dx)$$

$$\geqslant F(\xi^*) - \sup_{x \in X} \sum_{m=1}^{k} \omega(m)\varphi_m(x, \xi^*) \quad \xi_2(dx)$$

$= F(\xi^*) - \varphi(\xi^*) = 0.$

This contradiction proves (iii) (i). The proof is complete.

3. PROPERTIES OF F-OPTIMAL DESIGNS

We establish below some properties of F - optimal designs.

Proposition 3.1. Let ξ_1^* and ξ_2^* be two F - optimal designs. Then any $\tilde{\xi} = \lambda\xi_1^* + (1-\lambda)\xi_2^*$, $0<\lambda<1$, is also F - optimal.

Proof. This follows from the convexity of F.

Proposition 3.2. Let ξ_1^* and ξ_2^* be two F—optimal designs. Let $L_m(A)>0$ whenever A is a positive semi - definite matrix of rank at least 1 for some fixed $m \in \{1, 2, 3, \ldots, k\}$. Suppose $\omega(m)>0$.

Then

$$M_m(\xi_1^*) = M_m(\xi_2^*).$$

Proof. Suppose that $M_m(\xi_1^*)$ $M_m(\xi_2^*)$. It is known that

$$(1-\alpha)[M_m(\xi_1^*)]^{-1} + \alpha[M_m(\xi_2^*)]^{-1} - [(1-\alpha) M_m(\xi_1^*) + \alpha M_m(\xi_2^*)]^{-1}$$

is positive semi - definite of rank at least 1 for each $0<\alpha<1$. See Moore [6, p. 409] Consequently

$$L_m([(1-\alpha)M_m(\xi_1^*) + \alpha M_m(\xi_2^*)]^{-1}) < (1-\alpha) L_m(D_m(\xi_1^*)) + \alpha L_m(D_m(\xi_2^*)),$$

for each $0<\alpha<1$. Let $\tilde{\xi} = (1-\alpha)\xi_1^* + \alpha\xi_2^*$ for some fixed $0<\alpha<1$. By Proposition 3.1, $\tilde{\xi}$ is F – optimal. However,

$$F(\tilde{\xi}) = \sum_{j=1}^{k} \omega(j)\, L_j(D_j(\tilde{\xi})) < \sum_{j=1}^{k} \omega(j)(1-\alpha)\, L_j(D_j(\xi_1^*))$$

$$+ \sum_{j=1}^{k} \omega(j)\,\alpha\, L_j(D_j(\xi_2^*)) = (1-\alpha)\, F(\xi_1^*) + \alpha\, F(\xi_2^*) = F(\xi_1^*).$$

This is a contradiction.

R e m a r k : The linear functional L defined on the space of all nxn matrices A by L(A) = Tr. (A) satisfies the property that if A is positive semi-definite of rank at least 1, L(A)>0.

4. DESIGNS WITH FINITE SUPPORT.

For $\xi \in \Xi$, define

$$M(\xi) = \begin{pmatrix} M_1(\xi) & 0 & 0 & \dots & 0 \\ 0 & M_2(\xi) & 0 & \dots & 0 \\ 0 & 0 & M_3(\xi) & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & M_k(\xi) \end{pmatrix}$$

This is a block diagonal matrix of order $\left(\sum_{m=1}^{k} n(m)\right) \times \left(\sum_{m=1}^{k} n(m)\right)$.

We call $M(\xi)$ as the class-information matrix corresponding to the design ξ.

P r o p o s i t i o n 4.1. $\{M(\xi)\ ;\ \xi \in \Xi\}$ is a convex set.

P r o o f. It is obvious that $\{M_m(\xi) : \xi \in \Xi\}$ is convex for each m.

P r o p o s i t i o n 4.2. $\{M(\xi)\ ;\ \xi \in \Xi\}$ is the convex hull of the set of class - information matrices corresponding to one - point designs.

P r o o f. First, note that the collection of all designs ξ in Ξ with finite spectrum is dense in Ξ under weak topology, i.e., given any $\xi \in \Xi$, we can find a net $\{\xi_\alpha\}$ in Ξ, each ξ_α having finite spectrum, and

$$\int f d\xi_a \quad \text{converges to} \quad \int f d\xi$$

for each bounded continuous function f on X. See Varadarajan [7, Theorem 10, p. 187]. Consequently, the collection of all class - information matrices $M(\xi)$, with ξ having a finite spectrum, is dense in $\{ M(\xi) : \xi E \Xi\}$. But $\{M(\xi) ; \xi E \Xi$ with finite spectrum$\}$ is convex. By Caratheodory's Theorem, by viewing $M(\xi)$ as an element in R^{τ}, where $\tau =$

$\sum_{m=1}^{k} \frac{n(m)[n(m)+1]}{2}$, we can write $M(\xi)$ as a convex combination of at most

$\tau+1$ class - information matrices each of which corresponds to one-point designs. For this, we observe $\{M(\xi) ; \xi E \Xi\}$ = closure of the convex hull of $\{M(\eta) ; \eta E \Xi$, η is a one -point design$\}$.

Corollary 4.3. Let ξ be any design. Then there exists a design ξ_1 with finite spectrum and the spectrum containing no more than $\tau+1$ points such that

$$M(\xi)=M(\xi_1).$$

Theorem 4.4. Let ξ^* be any F - optimal design. Then there exists a design ξ_1 with finite spectrum and the spectrum containing no more than τ points such that

$$M(\xi^*)=M(\xi_1).$$

Proof. In view of Caratheodory's Theorem, it suffices to show $M(\xi^*)$ is a boundary point of the set $\{M(\xi) ; \xi E \Xi, \xi$ has a finite spectrum$\}$. See Fedorov [2. Theorem 2.1.1, p. 66]. In view of Corollary 4,3, we can assume ξ^* to have a finite spectrum with the spectrum containing no more than $\tau+1$ points. Suppoce $M(\xi^*)$ is not a boundary point. Then it is an interior point. We can find $a>0$ such that $M(\xi^*)+\alpha M(\xi^*) E \{M(\xi) ; \xi E \Xi, \xi$ has a finite spectrum$\}$. Consequently, there exists ξ such that $(1+\alpha) M(\xi^*)=M(\xi^*)$. Now, we claim that $F(\xi) < F(\xi^*)$.

$$\tilde{F}(\xi) = \sum_{m=1}^{k} \omega(m)\ L_m(D_m(\tilde{\xi})) = \sum_{m=1}^{k} \omega(m) L_m \left(\frac{1}{1+\alpha}\ D_m(\xi^*)\right)$$

$$= \frac{1}{1+\alpha} \sum_{m=1}^{k} \omega(m)\ L_m(D_m(\xi^*)) = \frac{1}{1+\alpha}\ F(\xi^*) < F(\xi^*).$$

This contradiction shows that $M(\xi^*)$ is a boundary point. Now, Caratheodory's Theorem completes the proof.

5. AN ALGORITHM

Before we give an iterative procedure for the construction of F - optimal designs we give some preliminary lemmas.

Lemma 5.1. **For $\tilde{\xi}(\alpha) = (1-\alpha)\xi + \alpha\xi_x$, $\alpha \in [0,1$, $\xi \in \Xi_1$,**

$$\frac{\partial}{\partial \alpha} \tilde{F}(\xi(\alpha)) = \frac{1}{(1-\alpha)^2} F(\xi) - \sum_{m=1}^{k} \omega(m)\varphi_m(x,\xi) \frac{1-\alpha^2+\alpha^2 d_m(x,\xi)}{(1-\alpha)^2(1-\alpha+a d_m(x,\xi))^2} \tag{5.1.1}$$

$$\frac{\partial^2}{\partial \alpha^2} \tilde{F}(\xi(\alpha)) = \frac{2}{(1-\alpha)^3} F(\xi)$$

$$-2 \sum_{m=1}^{k} \omega(m)\ \varphi_m(x,\xi) \frac{1+(3\alpha-1)[d_m(x,\xi)-1]+\alpha^3[d_m(x,\xi)-1]^2}{(1-\alpha)^3\ [1-\alpha+a d_m(x,\xi)]^3} \tag{5.1.2}$$

where $d_m(\chi,\xi) = f_{(m)}^T(x)\ D_m(\xi)\ f_{(m)}(\chi)$, $\chi \in X$, $\xi \in \Xi_1$

Proof. We first prove that

$$\tilde{F}(\xi(\alpha)) = \frac{1}{1-\alpha}\left\{ F(\xi) - \sum_{m=1}^{k} \omega(m) \frac{\alpha\varphi_m(x,\xi)}{1-\alpha+\alpha d_m(x,\xi)} \right\} \tag{5.1.3}$$

In fact, we have from Fedorov [2, Theorem 2.6.1, p. 106],

$$\tilde{D}_m(\xi(\alpha)) = \frac{1}{1-\alpha}\left\{ I_{a(m)} - \frac{\alpha D_m(\xi)\, f_{(m)}(x)\, f_{(m)}^T(x)}{1-\alpha+\alpha d_m(x,\xi)} \right\} D_m(\xi).$$

Applying L_m throughout and summing it over m = 1 to k after weighting it $\omega(m)$, we obtain the equation (5.1.3). A direct differentiation of (5.1.3) yields (5.1.1) and from this (5.1.2).

In what follows, we shall assume that X is a compact Hausdorff space.

Lemma 5.2. If

$$\sup_{\xi \in \Xi_1,\ \chi \in X} f^T(x)\ D^2(\xi)\ f(x) < \ , \tag{5.2.1}$$

then

$$\sup_{\substack{\xi \in \Xi_1 \\ \chi \in X}} f^T(x)\ D(\xi)\ f(x) < \ . \tag{5.2.2}$$

(Here $D(\xi)$ stands for $D_m(\xi)$ and $f(x)$ for $f_{(m)}(x)$ for any fixed m.)

Proof. Consider the spectral decomposition of

$$\underset{n x n}{D(\xi)} = \sum_{i=1}^{n} \lambda_i(\xi)\, x_i(\xi)\, x_i^T(\xi)$$

$$D^2(\xi) = \sum_{j=1}^{n} \lambda_i^2(\xi)\ x_i(\xi) x_i^T(\xi), \text{ where}$$

$\lambda_i(\xi)$, i= 1,2,. . ., η are the eigenvalues of $D(\xi)$ and $X_i(\xi)$ i= 1, 2,. . .,n constitute an orthonormal basis. First, note that the double supremum is equal to repeated supremums taken in any order.

$$\text{(5.2.1)} \qquad \sup_{\xi E \Xi_1} \max_{\chi E X} \sum_{i=1}^{n} \lambda_i^2(\xi)\, f^T(x)\, x_i(\xi) x_i^T(\xi)\, f(x) < \infty,$$

from which we obtain

$$\sup_{\xi E \Xi_1} \max_{\chi E X} \lambda_i^2(\xi) f^T(\chi)\, x_i(\xi)\, X_i^T(\xi)\, f(x) < \quad , \quad i= 1,2,. . .,n$$

Define the

$$g_i(\xi) = \begin{cases} 1, \text{ if } \lambda_i(\xi) < 1 \\ \lambda_i^2(\xi), \text{ if } \lambda_i(\xi) \geqslant 1, i = 1,2,. . .,n. \end{cases}$$

Now,

$$\lambda_i^2(\xi \leqslant \begin{cases} f^T(x)\, x_i(\xi)\, x_i^T(\xi)\, f(x), \text{ if } \lambda_i(\xi) < 1 \\ \lambda_i^2(\xi)\, f^T(x)\, x_i(\xi)\, x_i^T(\xi)\, f(x), \text{if } \lambda_i\,(\xi) \geqslant 1. \end{cases}$$

We claim that

$$\sup_{\xi E \Xi_1} \max_{x E X} g_i(\xi)\, f^T(x) x_i(\xi)\, x_i^T(\xi)\, f(x) < \infty \qquad (5.2.3)$$

Note that

$$\sup_{\xi E \Xi_1} \max_{x E X} f^T(x)\, x_i(\xi)\, x_i^T(\xi) f(x) < \infty, \text{ as}$$

$X_i(\xi)$'s are vectors of unit legth and the functions are bounded.

Let this supremum be C_1.

Let $\sup_{\xi \in \Xi_1} \max_{\chi \in X} \lambda_i^2(\xi)\ f^T(\chi)\ \chi_i(\xi)\ \chi_i^T(\xi)\ f(x) = C_2.$

Let $C = \max \{C_1, C_2\}$.

Observe that

$$g_i(\xi)\ f^T(x)\ \chi_i(\xi)\ \chi_i^T(\Xi)\ f(x) < C \text{ for every } \chi \in X, \xi \in \Xi_1.$$

Hence the claim.

Now,

$$\lambda_i^2(\xi)\ f^T(x)\ \chi_i(\xi)\ \chi_i^T(\xi)\ f(x) < g_i(\xi)\ f^T(x)\ \chi_i(\xi)\ \chi_i^T(\xi)\ f(x)$$

for every $\chi \in X$, $\xi \in \Xi_1$.

Hence,

$$\sup_{\xi \in \Xi_1} \max_{x \in X} \lambda_i(\xi)\ f^T(x)\ x_i(\xi)\ x_i^T(\xi)\ f(x) < \infty.$$

This is true for every i. Therefore,

$$\sup_{\xi \in \Xi_1} \max_{x \in X} f^T(x)\ D(\xi)\ f(x) < \infty .$$

L e m m a 5.3. It

$$\sup_{\xi \in \Xi_1} \max_{\chi \in X} f(m)^T(x)\ D_m^2(\xi)\ f_{(m)}(x) < \quad \text{for every } m = 1 \text{ to } k,$$

then

$$\max_{x \in X} \sup_{\xi \in \Xi_0} \sup_{0 \leqslant \alpha \leqslant \alpha_0} \left\{ \frac{2}{(1-\alpha)^3} F(\xi) - 2 \sum_{m=1}^{k} \omega(m) \varphi_m(x,\xi). \right.$$

$$\frac{1+(3\alpha-1)\ [d_m(x,\xi)-1]+\alpha^3[d_m(x,\xi)-1]^2}{(1-\alpha)^3\ [1-\alpha+\alpha d_m(x,\xi)]^3}\ \} < \infty$$

for any fixed $\alpha_0 E\ (0,1)$, where

$\Xi_0 = \{\xi E \Xi_1\ :\ F(\xi) < F(\xi o)$, for some fixed $\xi_0 E \Xi_1\ \}$

Proof. Note that the expression within the flower brackets is $\frac{\partial^2}{\partial\alpha^2} F((1-\alpha)\xi +$ $+\alpha\xi_\chi)$, $\alpha E(O,1)$, $\xi E\Xi_1$ χEX. From the definition of Ξ_0, we have that

$F(\xi)\frac{2}{(1-\alpha)^3}$ is bounded over the set Ξ_0 x $[0, a_0]$

for any fixed $(\alpha_o E(0,l)$.

So if suffices to show that

$$\sum_{m=1}^{k} \omega(m)\varphi_m(x,\xi)\ K_m(\alpha,x,\xi), \text{where}$$

$$K_m(\alpha,x,\xi) = \frac{1+(3\alpha-1)\ [d_m(x,\xi)-1]+\alpha^3\ [d_m(x,\xi)-1]^2}{(1-\alpha)^3\ [1-\alpha+\alpha d_m(x,\xi)]^3},$$

is bounded over the set $[0, \alpha_0]\ \chi\ X\ \chi\Xi_0$. For this it is sufficient to show that $\varphi_m(\chi,\xi)\ K_m\ (\alpha,\chi,\xi)$ is bounded over the set $[0, \alpha_0]\chi\ X\ \chi\ \Xi_0$, for every m = 1, 2,. . ,k.

Let

$$\max_{1\leqslant m\leqslant k}\ \sup_{\xi E\Xi_1}\ \max_{xEX}\ f_{(m)}^T(x)\ D_m^2(\xi)\ f_m(x) = C_1 \text{ and}$$

$$\max_{1\leqslant m\leqslant k}\ \sup_{\xi E\Xi_1}\ \max_{xEX}\ f_{(m)}^T(x)\ D_m(\xi)\ f_{(m)}(x) = C_2.$$

Note that $C_2 <$ by Lemma 5.2.

Now,

$$\varphi_m(x,\xi) = L_m\ [D_m(\xi)\ f_{(m)}(x)\ f_{(m)}^T(x) D_m(\xi)]$$

$$\leqslant \|L_m\| . \|\ D_m(\xi)\ f_{(m)}(x)\ f_{(m)}^T(x)\ D_m(\xi)\ \|$$

$$= \|L_m\|\ [Tr. \{D_m(\xi) f_{(m)}(x) f_{(m)}^T(x) D_m(\xi) D_m(\xi) f_{(m)}(x) f_m T(x) D_m(\xi)\}]^{1/2}$$

$$= \|\ L_m \|\ [Tr. [f_{(m)}^T(x) D_m^2(\xi) f_{(m)}(x)\}^2]^{\frac{1}{2}}$$

$$\leqslant \|\ L_m \|\ C_1 \text{ for every } (x,\xi) E\ X \times \Xi_0 \text{ and } m = 1 \text{ to } k.$$

Also,

$$d_m(x,\xi) = f_m^T(x)\ D_m(\xi)\ f_{(m)}(x) \leqslant C_2, \text{ for every } (x,\xi) E$$

$X \chi \Xi_0$ and $m = 1$ to k. Consequently,

$$|\ d_m(x,\xi) - 1\ | \leqslant C_2+1, \text{ for every } (x,\xi) E\ X \times \Xi_0 \text{ and } m = 1 \text{ to } k.$$

Note that the function

$$g(\omega,\alpha) = \frac{1}{(1-\alpha)^3} - \frac{1+(3\alpha-1)\omega+\alpha^3\omega^2}{(1+\alpha\omega)^3}$$

is bounded over the set $[-1, C_2+1] \times [0, a_0]$, being a continuous function. From this it follows that

$$K_m(\alpha,x,\xi) = \frac{1}{(1-\alpha)^3} - \frac{1+(3\alpha-1)\omega_m+\alpha^3\ \omega_m^2}{(1+\alpha\omega_m)^3}$$

is bounded over the set $[-1, C_2+1]\ \chi\ [0, \alpha_0]$ for every $m = 1$ to k, where $\omega_m = d_m(x,\xi)-1$. This completes the proof.

We are now in a position to give an algorithm.

Assume

$$\sup_{\xi \in \Xi_1} \max_{x \in X} f_m^T(x) D_m^2(\xi) f_m(x) < \infty \quad \text{for every } m = 1,2,\ldots,k.$$

Let ξ_0 be a design for which $|M_m \xi_0)|$ 0 for every m= 1 to k. Now, we shall assume X is a compact Hausdorff space. Note that $\sum_{m=1}^{k} \omega(m.)\ \varphi_m(\cdot, \xi o)$ is a continuous function on X, and consequently it is bounded and the supremum is attained. Let Ξ_0 be the set defined in Lemma 5.3 corresponding to ξ_0.

First Step of Iterative Procedure

Let Xo be a solution satisfying

$$\max_{x \in X} \sum_{m=1}^{k} \omega(m)\varphi_m(x,\xi_0) = \sum_{m=1}^{k} \omega(m)\varphi_m(x_0,\xi_0).$$

Let

$$K_0 = F(\xi_0) - \sum_{m=1}^{k} \omega(m)\varphi_m(x_0, \xi_0).$$

If $K_0 = 0$, by Theorem 2.2, ξ_0 is F - optimal and the procedure is terminated here. If $K_0 < 0$, the second step outlined below is carried out.

Second Step.

Let a_0^* be the smallest positive root satisfying the following equation in $a > 0$.

$$F(\xi_0) - \sum_{m=1}^{k} \omega(m)\varphi_m(x_0,\xi_0)\ \frac{1 - \alpha^2 + \alpha^2 d_m(x_0, \xi_0)}{[1 - \alpha + \alpha d_m(x_0,\xi_0]^2} = 0.$$

Note that $\alpha = 0$ is never a solution of this equation. There are three possibilities.

(i) α_0^* exists and $\in (0,1)$.

(ii) α_0^* exists and $\in [1, \infty)$.

(iii) α_0^* does not exist.

In cases (ii) and (iii) define $\alpha_0^* = 0.99$.

Let $\bar{\alpha} \in (0,1)$ be fixed. Let $\gamma > \frac{1}{\bar{\alpha}}$ be a fixed constant

Define $\alpha_0 = \frac{1}{\gamma} \alpha_0^*$. Note that $\alpha_0 < \alpha_0^*$. Now, construct the design

$$\xi_1 = (1 - \alpha_0) \xi_0 + \alpha_0 \xi_{x_0},$$

where ξ_{x_0} is the design degenerated at x_0.
Let x_1 be any solution satisfying

$$\max_{x \in X} \sum_{m=1}^{k} \omega(m)\varphi_m(x,\xi_1) = \sum_{m=1}^{k} \omega(m) \varphi_m(x_1,\xi_1).$$

Let

$$K_1 = F(\xi_1) - \sum_{m=1}^{k} \omega(m)\varphi_m(x_1,\xi_1)$$

If $K_1 = 0$, ξ_1 is F- optimal and we terminate the procedure here.

If $K_1 < 0$, the next step is carried out.

The n th. step is modelled after the second one.

L e m m a 5.4. Suppose the iterative procedure described above never terminates.

Let ξ_n, n>0 be the sequence of designs obtained by the above procedure. Then.

$$F(\xi n) > F(\xi_{n+1}) \quad \text{for every } n>0.$$

P r o o f. Let $\xi E \Xi_1$ be any design and xEX any point. Consider $\xi(\alpha) = (1-\alpha)\xi +$ $+ \alpha\xi_\chi$, $\alpha E[0,1)$. Using Lemma 5.1,

$$\frac{\partial}{\partial\alpha} \tilde{F}(\xi(\alpha)) \Big|_{\alpha=0} = F(\xi) - \sum_{m=1}^{k} \omega(m)\varphi_m(x,\xi).$$

In our case, when $\xi = \xi_n$ and $\chi = x_n$, we have

$$\frac{\partial}{\partial\alpha} \tilde{F}(\xi_n(\alpha)) \Big|_{\alpha=0} = F(\xi_n) - \sum_{m=1}^{k} \omega(m)\ \varphi_m(x_n,\xi_n) = K_n < 0,$$

by hypothesis.

Since $\frac{\partial}{\partial\alpha}$ $\tilde{F}(\xi_n(\alpha))$ is a continuous function in [0,1), we can find a number O < 0 < 1

such that $\frac{\partial}{\partial\alpha}\tilde{F}(\xi_n(\alpha))<0$ ifas[0,c). Ifa$_n$*is the smallest positive root E (0,1) of

$\frac{\partial}{\partial\alpha}\tilde{F}(\xi_n(\alpha))=0$, then it follows that $\frac{\partial}{\partial\alpha}\tilde{F}(\xi_n(\alpha))<0$ if $\alpha\varepsilon[0,En^*)$. If a_n^* does

not satisfy the above condition, then $\frac{\partial}{\partial\alpha}\tilde{F}(\xi_n(\alpha))$ must be of the same sign in (0,1)

Consequently, in any case we have

$$\frac{\partial}{\partial \alpha} \tilde{F}(\xi_n(\alpha)) < 0, \text{ if } \alpha \varepsilon [0, \alpha_n^*).$$

This implies that $\tilde{F}(\xi_n(\alpha))$ is a strictly decreasing function in αE[0,α* j). Since a_nE[0,a_n*), we have $F(\xi_n(0)) = F(\xi_n) > \tilde{F}(\xi_n(\alpha_n)) = F(\xi_{n+1})$. This completes the proof.

The following is an important result in showing that the iterative procedure gives an F-optimal design in the limit.

Lemma 5.5. Let $\xi_i(\alpha) = (1 - \alpha)\, \xi_i + \alpha \xi_{\chi_i}$, αE[0,1), i>0.

Then

$$\lim_{i \to \infty} \frac{\partial}{\partial \alpha} \tilde{F}(\xi_i(\alpha)) \Big|_{\alpha = 0} = 0,$$

where ξ_i, χ_i are obtained by the algorithm.

Proof. Suppose the assertion is not true. Then there exists an e > 0 such that

$$\frac{\partial}{\partial \alpha} \tilde{F}(\xi_i(\alpha)) \Big|_{\alpha = 0} < -e$$

for infinitely many i's. Let B be the set of those i's. By Lemma 5.4 it follows that ξ_nE Ξ_0 for every n>0. Let the second derivative of $\tilde{F}(\xi(\alpha))$ be uniformly bounded by a constant C>0 over the set [0,α]χ X χ Ξ_0, w $\tilde{\xi}(\alpha) = (1-\alpha)\, \xi + \alpha\, \xi_x$, e Lemma 5.3. Take a in the place of a_0).

in particular, we have

$$\frac{\partial^2}{\partial\alpha^2} \tilde{F}(\xi_i(\alpha)) \leqslant C \text{ for every } \alpha \in [0,\bar{\alpha}] \text{ and } i \in B.$$

We had taken $\gamma > \frac{1}{\bar{\alpha}}$ in the algorithm. Then

$$a_i = \frac{1}{\gamma}\alpha_i^* < \frac{1}{\gamma} < \bar{\alpha} \tag{5.5.1}$$

Case I $\bar{\alpha} \leqslant \frac{\varepsilon}{2C}$. Then

$$\frac{\partial}{\partial\alpha}\tilde{F}(\xi_i(\alpha)) = \frac{\partial}{\partial\alpha}\tilde{F}(\xi_i(\alpha))\Big|_{\alpha=0} + \alpha\frac{\partial^2}{\partial\alpha^2}\tilde{F}(\xi_i(\alpha))\Big|_{\alpha=\alpha_*}$$

for every $\alpha \in (0,1)$ and for some $\alpha_* \in (0,\alpha)$, by Taylor's expansion. So, for every $\alpha \in [0, \bar{\alpha}]$, we have

$$\frac{\partial}{\partial\alpha}\tilde{F}(\xi_i(\alpha)) < -e + \alpha C \leqslant -2C\bar{\alpha} + \bar{\alpha}C = -C\alpha \tag{5.5.2}$$

Now,

$$\tilde{F}(\xi_i(\alpha))\Big|_{\alpha=\alpha_i} = \tilde{F}(\xi_{i+1}) = \tilde{F}(\xi_i(\alpha))\Big|_{\alpha=0} + \alpha_i\frac{\partial}{\partial\alpha}\tilde{F}(\xi_i(\alpha))\Big|_{\alpha=\theta_i}$$

$$\theta_i \in (0,\alpha_i). \tag{5.5.3}$$

From (5.5.2) we have that $\frac{\partial}{\partial\alpha}\tilde{F}(\xi_i(\alpha))$ is bounded away from zero in the interval [O,α] and for any iEB. So there is no root of the equation $\frac{\partial}{\partial\alpha} F(\tilde{\xi}_i(\alpha)) = 0$ in the interval [O,α], which means that the smallest positive root of this equation αï* should be greater than $\bar{\alpha}$. Hence

$$\alpha_i = \frac{1}{\gamma} \alpha_i^* > \frac{1}{\gamma} \bar{\alpha} \tag{5.5.4}$$

From (5.5.2), (5.5.3) and (5.5.4) we obtain

$$F(\xi_{i+1}) \leqslant F(\xi_i) + \frac{1}{\gamma} \bar{\alpha} (-C\bar{\alpha}) = F(\xi_i) - \frac{1}{\gamma} C\bar{\alpha}^2. \tag{5.5.5.}$$

which is a contradiction to the fact that $F(\varsigma_n)$ n>0 converges, being a decreasing sequence of non - negative real numbers.

Case II. $\frac{\varepsilon}{2C} < \bar{\alpha}$.

From (5.5.1), each αi<α. Now, for every $\alpha \in [0, \frac{\varepsilon}{2C}]$ and for every iEB,

$$\frac{\partial}{\partial\alpha} F(\tilde{\xi}_i(\alpha)) = \frac{\partial}{\partial\alpha} F(\tilde{\xi}_i(\alpha)) \Big|_{\alpha=0} + \alpha \frac{\partial^2}{\partial\alpha^2} F(\tilde{\xi}_i(\alpha)) \Big|_{\alpha=\alpha'}$$

for some α'E(O,α).

$$\leqslant -\varepsilon + \alpha C \leqslant -\varepsilon + \frac{\varepsilon}{2} - \frac{\varepsilon}{2}$$

This means that $\frac{\partial}{\partial\alpha} F(\tilde{\xi}_i(\alpha))$, iEB is bounded away from zero. Consequently, there is no root of the equation $\frac{\partial}{\partial\alpha} F(\tilde{\xi}_i(\alpha)) = 0$ in the interval $[0, \frac{\varepsilon}{2C}]$. Hence

$$\alpha_i^* > \frac{\varepsilon}{2C} \quad \text{and}$$

$$\alpha_i = \frac{1}{\gamma}\alpha_i^* > \frac{1}{\gamma}\frac{\varepsilon}{2C} \text{ for each } i \text{ in } B.$$

Proceeding as in Case I, we get

$$F(\xi_{i+1}) < F(\xi_i) - \frac{1}{\gamma}\frac{\varepsilon^2}{4C}, \ i \text{ in } B,$$

which, obviously, contradicts the fact that the sequence $F(\xi_n)$, $n>0$ converges. This completes the proof.

Theorem 5.6. Let ξ_v, $n>0$ be the sequence of designs provided by the above iterative procedure. Assume Ξ_2 0. Then for any F-optimal design ξ^*, we have.

$$\lim_{n\to\infty} F(\xi_n) = F(\xi^*).$$

Proof. Note that

$$\min_{x \in X} \frac{\partial}{\partial\alpha} F[(1-\alpha)\xi_n + \alpha\xi_x]\Big|_{\alpha=0}$$

$$= \min_{x \in X} \left[\frac{1}{(1-\alpha)^2} F(\xi_n) - \sum_{m=1}^{k} \omega(m) \frac{1-\alpha^2+\alpha^2 d_m(x,\xi_n)}{(1-\alpha)^2[1-\alpha+\alpha d_m(x,\xi_n)]^2} \varphi_m(x,\xi_n)\right]_{\alpha=0}$$

$$= \min_{x \in X} [F(\xi_n) - \sum_{m=1}^{k} \omega(m)\varphi_m(x,\xi_n)]$$

$$= F(\xi_n) - \max_{x \in X} \sum_{m=1}^{k} \omega(m)\varphi_m(x,\xi_n)$$

$$= F(\xi_n) - \sum_{m=1}^{k} \omega_{(m)}\varphi_m(x_n,\xi_n), \quad \text{by the } n^{th} \text{ step of the itera-}$$

tive procedure

$$= \frac{\partial}{\partial \alpha} F[(1-\alpha)\xi_n + \alpha\xi_{x_n}]\Big|_{\alpha=0} = \frac{\partial}{\partial \alpha} F(\tilde{\xi}_n(\alpha))\Big]_{\alpha=0}$$

which converges to 0 as n , by Lemma 5.5.

The following inequality is due to Kiefer [4, Equation (6.5) p. 877]. See also Atwood [1, Equation (2.1), p. 1126].

$$\min_{x \in X} \frac{\partial}{\partial \alpha} F[(1-\alpha)\xi_n + \alpha\xi_x]\Big|_{\alpha=0} \leqslant F(\xi^*) - F(\xi_n) \leqslant 0$$

Consequently,

$$\lim_{n \to \infty} F(\xi_n) = F(\xi^*)$$

R e m a r k 5.7. The above algorithm is modelled after Làuter's algorithm [5] which is, in fact, a modification of Fedorov's algorithm [2]. The crucial step in showing convergence of the designs obtained iteratively is the boundedness of the second derivate of $F(\tilde{\xi}(\alpha))$ with respect to α in some interval [O,α]. In the case of determinant criterion, Làuter [5] shows that the derivative is indeed always bounded without any further assumptions. In our case, we assume

$$\sup_{\xi \varepsilon \Xi_1} \max_{x \varepsilon X} f^{T}_{(m)}(x)\, D^2_m(\xi)\, f_{(m)}(x) < \infty$$

for every m= 1 to k in order to show that this second derivative is pounded.

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