OPTIMAL DESIGNS FOR THE ESTIMATION OF LINEAR FUNCTIONS OF PARAMETERS

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I. INTRODUCTION

Let the design space X be a compact Hausdorff topological space and let B be the Baire σ -field on X. Let $f_i^T = (f_{i_1}, \ f_{i_2}, \dots, f_{i_n})$ be a vector of continuous real valued functions on X for i=1 to q for some $q \ge 1$. For each $x \in X$, Y (x) stands as a generic random valiable with

$$EY(x) = f_{i}^{T}(x) \beta_{i}, i = 1 \text{ to } q, \text{ and } Var(Y(x)) = \sigma^{2},$$

where,

 $\beta \stackrel{T}{_{i}} \in R^{ni}$ is the vector of unknown parameters in the i-th model.

Let A_i , i=1 to q, be a given family of matrices, where the order of A_i is $n_i x s_i$ 148

and is of foull rank $s_i \le n_i$. We are primarily interested in estimating $A_i^T \beta_i$ simultaneously for i=1 to q using the same set of uncorrelated random variables $Y(x_1)$, $Y(x_2)$,..., $Y(x_n)$. The choice of x_1, x_2, \ldots, x_n is governed by some optimality criterion and is tantamount to choosing a design, i. e. a probability measure ξ on B. Let ξ be a design and M_i (ξ) the corresponding information m atrix. It can be verified that $A_i^T \beta_i$ is estimable if and only if $R(A_i) \subseteq R(M_i(\xi))$ where R(A) denotes the Range of A, and that in such a case dispersion matrix of $\widehat{A_i}\beta_i$ is proportional to $A_i^T M_i(\xi) A_i$, where M+ denotes the Moore Penrose Inverse of M. Consequently, when we look for a design for the above problem, first of all, we must make sure that the given design satisfies $R(A_i) \subseteq R(M_i(\xi))$ for each i=1 to q. Let Ξ be the class of all designs.

Define
$$\Xi_1 = \{ \xi \in \Xi : R(A_i) \subseteq R(M_i(\xi)), i=1 \text{ to } q \}.$$

The optimality criterion we are interested in is the following:

$$F(\xi) = \sum_{i=1}^{q} w_i Tr. (A_i^T M_i^+(\xi) A_i),$$

where

 w_i , i = 1 to q, are preassigned weights, all positive and $\sum\limits_{i=1}^q w_i = 1$.

The purpose of this paper is to find an optimal design according to the above criterion. Fellman^[7] considered the above problem when q = 1 and the design

space X is finite. In this paper, we will employ simpler and more direct methods to show the existence of optimal designs according to the above criterion. We will also give some characterizations of these optimal designs.

2. OPTIMAL DESIGNS

As usual, we define a design $\xi_o \in \Xi_1$ optimal if $F(\xi_o) = Inf \ F(\xi) = \xi \in \Xi_1$ min $F(\xi)$. The following series of results are designed to establish the existence $\xi \in \Xi_1$ of ξ_0 .

Lemma 2.1.

 Ξ_1 is a convex set.

Proof. Let $\xi_1, \xi_2 \in \Xi_1$ and $0 \le \lambda \le 1$, we shall prove that $\xi(\lambda) = \lambda \xi_1 + (1 - \lambda) \xi_2 \in \Xi_1$. The cases $\lambda = 0$ or = 1 are obvious. Let $0 < \lambda < 1$. Note that M_i $[\xi(\lambda)] = \lambda M_i(\xi_1) + (1 - \lambda) M_i(\xi_2)$. Observe that M_i $[\xi(\lambda)] \ge \lambda M_i$ (ξ_1) . (P $\ge Q \Leftrightarrow P - Q$ is positive semi - de finite). It easily follows that $R[M_i(\xi_1)] \subset R[M_i(\xi(\lambda))]$. See, for example, Fellman [7, Lemma 1.1.5, p. 34]. As $R(A_i) \subset R[M_i(\xi_1)]$, it follows that $R(A_i) \subset R[M_i(\xi_1)]$. And this is true for every i = 1 to q.

Lemma 2.2.

The function F is convex on Ξ_1 .

Proof. Fellman [7, Lemma 3.1.1., p. 45] proved that the function $\operatorname{Tr.}(A_i^T \operatorname{M}_i^+(\xi) A_i) \text{ is convex on the set } \{\xi \in \Xi; R(A_i) \subset R [\operatorname{M}_i(\xi)] \}.$

The next result is fundamental in proving the existence of optimal designs.

Theorem 2.3.

Let B_n , $n \ge 1$ be a sequence of positive semidefinite matrices of order qxq converging to B_0 . Let c be a fixed qx1 vector. We can prove that

(i) If
$$c \in \bigcap_{n \geqslant 0} R(B_n)$$
, then $\lim_{n \to \infty} c^T B_n^+ c = c^T B_0^+ c$

(ii) If $c \in \bigcap_{n \geqslant 1} R(B_n)$, but c does not belong to $R(B_0)$, then $\limsup_{n \to \infty} c^{\mathrm{T}} B_n^+ c = \infty$.

Proof. See Kaffes [8].

If Ξ_1 is a strict subset of Ξ , we can always find a boundary point of Ξ_1 not belonging to Ξ_1 . For such points, the following is true

Theorem 2.4.

Let ξ_0 be a boundary point of Ξ_1 not belonging to Ξ_1 . Then $\limsup_{\xi \to \xi_0} F(\xi) = \infty$. $\xi \to \xi_0$ $\xi \in \Xi_1$

 $(\xi \to \xi_0)$ is understood in the sense of weak convergence).

Proof. Since $\xi_0 \notin \Xi_1$, there exists $i \in \{1, 2, 3, ..., q\}$, such that $R(A_i)$ is not a subset of $R[M_i(\xi_0)]$. Consequently, there is a column vector c of A_i such that $c \notin R[M_i(\xi_0)]$. Let ξ_n , $n \ge 1$ be any sequence in Ξ_1 converging to ξ_0 weakly. It then follows that $M_i(\xi_n)$, $n \ge 1$ converges to $M_i(\xi_0)$. By theorem 2.3.,

$$\label{eq:constraints} \underset{n\to\infty}{\text{limsup}} \ c^T \ M_{\hat{1}}^+(\xi_n) \ c = \infty \,.$$

Consequently, $\limsup_{n\to\infty}$ Tr. $(A_i^T\ M_i^+(\xi_n)\ A_i)=\infty$. Since each $w_i>0,$ it

follows that $\limsup_{n\to\infty} F(\xi_n) = \infty$. This completes the proof.

Theorem 2.5.

F is continuous on Ξ_1 .

Proof. This is a simple consequence of the first part of theorem 2.3. Theoreme 2.4 and 2.5 combined will now give us the existence theorem of an optimal design.

Theorem 2.6.

There always exists an optimal design $\xi_0 \in \Xi_1$.

Proof. Let $\beta = \inf_{\xi \in \Xi_1} F(\xi)$. Obviously, β is finite. We can find a sequence ξ_n , $\xi \in \Xi_1$ $n \ge 1$, such that $\xi_n \in \Xi_1$ and $\lim_{n \to \infty} F(\xi_n) = \beta$.

Since X is compact, Ξ is compact under weak topology. (Ξ consists of all regular probability measures on the Baire σ - field of X). See Varadarajan [12].

Consequently, we can find a subnet $\{\xi_a\}$ of ξ_n , $n\geqslant 1$ converging to some element $\xi_0\in\Xi$. If $\xi_0\in\Xi_1$, since F is continuous, $\lim_a F(\xi_a)=F(\xi_0)=\lim_{n\to\infty} F(\xi_n)=\beta$.

Hence ξ_0 is optimal. If $\xi_0 \notin \Xi_1$, then ξ_0 is a boundary point of Ξ_1 not belonging to Ξ_1 . Consequently, limsup $F(\xi) = \infty$, by theorem 2.4. This then would imply $\xi \to \xi_0, \xi \in \Xi_1$

that $\beta = \infty$, a contradiction. This completes the proof.

3. SOME CHARACTERIZATIONS OF OPTIMAL DESIGNS

Some of the results in this section could be used in developing an algorithm for the above situation. We begin with a lemma.

Lemma 3.1.

Let M_1 and M_2 be two given positive semi-definite matrices. For every $\alpha \in (0, 1)$, define $M(\alpha) = (1 - \alpha)M_1 + \alpha M_2$. Then

$$\frac{d}{d\alpha}M^{+}(\alpha) = -M^{+}(\alpha)\left(\frac{d}{d\alpha}M(\alpha)\right)M^{+}(\alpha) \tag{3.1.1.}$$

P r o o f. This result is well known when M_1 and M_2 are just nonsingular matrices. See Fedorov [6, Lemma 2.9.2., p. 124]. See also Decell [5, Introduction, p. 357].

We first have to show that $M^+(\alpha)$ is differentiable in α . For this we need the following result of Cline [4].

$$(UU^{T} + VV^{T})^{+} = (I - C^{+T} V^{T}) U^{+T}K U^{+} (I - VC^{+}) + (CC^{T})^{+},$$

where

$$K = I - U^{+}V (I - C^{+}C) M (U^{+}V)^{T}$$
, with $C = (I - UU^{+}) V$ and

$$M = (I + (I-C+C) V^{T}U^{+T} U + V (I-C+C))^{-1}$$

In our case, we can write $(1 - \alpha) M_1 + \alpha M_2 = (1 - \alpha) AA^T + \alpha BB^T$. Let $U = \sqrt{1-\alpha} A$ and $V = \sqrt{\alpha} B$. I can easily check that $I - C^+C$ is independent of α . From this the desired conclusion follows.

Now, using a result of Decell [5, Theorem, p. 358], we obtain

$$\frac{d}{d\alpha}M^{+}(\alpha) = -M^{+}(\alpha)\left[\frac{d}{d\alpha}M(\alpha)\right]M^{+}(\alpha) + \left[\frac{d}{d\alpha}M(\alpha)\right]M^{+}(\alpha)M^{+}(\alpha) + \frac{d}{d\alpha}M(\alpha)$$

$$M+(\alpha)\ M+(\alpha)\ [\frac{d}{d\alpha}M\ (\alpha)\]-M^+(\alpha)M(\alpha)\ \{\frac{d}{d\alpha}M\ (\alpha)\]M^+(\alpha)M^+(\alpha)+$$

$$M^{+}(\alpha)M^{+}(\alpha) = \{-\frac{d}{d\alpha} M(\alpha)\} \} M(\alpha)M^{+}(\alpha).$$

Note that
$$\begin{bmatrix} \frac{d}{d\alpha}M(\alpha) = M_2 - M_1, & \text{and } R(M_i) \subseteq R(M(\alpha)) \text{ for } i = 1, 2. \end{bmatrix}$$

By lemma 2.2.4. of Rao and Mitra [11, p. 21], a necessary and sufficient condition for B $A^-A = B$ is that $R(B^T) \subset R(A^T)$, where A and B are any two matrices, A^- being a g-inverse of A. Similarily, $AA^-B = B$ is true if and only if $R(B) \subset R(A)$. Using this result and the fact that $M(\alpha)$ is symmetric, we obtain

$$M^{+}(\alpha)M(\alpha)(M_2-M_1) = M(\alpha)M^{+}(\alpha)M_2-M(\alpha)M^{+}(\alpha)M_1 = M_2-M_1 =$$

$$\frac{d}{d\alpha}$$
 $M(\alpha)$ and

$$[\ \, -- M(\alpha) \,] M(\alpha) M^+(\alpha) = M_2 M^+(\alpha) M(\alpha) - M_1 M^+(\alpha) \, M(\alpha) = M_2 - M_1 = \frac{d}{d\alpha} \, M(\alpha).$$

Consequently, (3.1.1) is true.

Theorem 3.2.

The following conditions are equivalent

(α) ξ* is optimal

(b)
$$\sum_{i=1}^{q} w_i Tr. \{ A_i^T [M_i (\xi^*) M_i^+ (\xi) M_i (\xi^*)]^+ A_i \} \le F (\xi^*)$$

for every $\xi \in \Xi_1$ satisfying $R(M_i(\xi^*)) \subseteq R(M_i(\xi))$ for all i=1 to q.

Proof. This result is similar to theorem 1(a) of Läuter [10, p. 54], in spirit.

(a)
$$\Rightarrow$$
 (b). For $\xi \in \Xi_1$ satisfying R $(M_i(\xi^*)) \subseteq R(M_i(\xi))$ for every $i=1$ to q and $\alpha \in [0, 1)$, let $\xi(\alpha) = (1-\alpha) \xi^* + \alpha \xi$. Then

$$\frac{d}{d\alpha} F(\widetilde{\xi}(\alpha)) \Big]_{\alpha = 0} = \sum_{i=1}^{q} w_i \operatorname{Tr.} \left\{ A_i^T \left[\frac{d}{d\alpha} M_i^+(\widetilde{\xi}(\alpha)) \right] A_i \right\} \Big]_{\alpha = 0}$$

$$= -\sum_{i=1}^{q} w_{i} \operatorname{Tr.} \{ A_{i}^{T} M_{i}^{+} (\widetilde{\xi}(\alpha)) [M_{i}(\xi) - M_{i}(\xi^{*})] M_{i}^{+} (\widetilde{\xi}(\alpha)) A_{i} \}]_{\alpha = 0}$$
(By Lemma 3.1)

$$=\sum_{i=1}^{q}\,w_{i}\,\text{Tr.}\,\left\{\,A_{i}^{T}M_{i}^{+}\,\left(\,\widetilde{\xi}\,(\alpha)\right)\!M_{i}\,(\xi^{*})\!M_{i}^{+}\,\left(\,\widetilde{\xi}\,(\alpha)\,A_{i}\right\}\,\right]_{\,\alpha\,=\,0}$$

$$-\sum_{i=1}^{q} w_{i} \operatorname{Tr.} \left\{ A_{i}^{T} M_{i}^{+} \left(\widetilde{\xi} \alpha \right) \right\} M_{i} \left(\xi \right) M_{i}^{+} \left(\widetilde{\xi} \left(\alpha \right) \right) A_{i} \left\{ \right\} \right]_{\alpha = 0}$$

Note that

$$\lim_{\alpha\downarrow 0}\ A_{i}^{T}\ M_{i}^{+}\ (\widetilde{\xi}\ (\alpha))M_{i}\ (\xi^{*})M_{i}^{+}\ (\ \widetilde{\xi}\ (\alpha)\)\ A_{i}=A_{i}^{T}M_{i}^{+}\ (\xi^{*})\ A_{i},\quad \text{and}\quad$$

$$\lim_{\alpha \downarrow 0} A_{i}^{T} M_{i}^{+} (\widetilde{\xi}(\alpha)) M_{i} (\xi) M_{i}^{+} (\widetilde{\xi}(\alpha)) A_{i}$$

$$= \! A_i^T \ M_i^+ \ (\xi^*) \ M_i^{\frac{1}{2}}\!(\xi) \ P \\ R \! \left\{\! [M_i^{-\frac{1}{2}}\!(\xi)] \! + \! M_i(\xi^*) \! \right\} \! M_i^{-\frac{1}{2}}\!(\xi) M_i^+ \ (\xi^*) \ A_i$$

See Läuter [10, Theorem 1 (a), p. 55]. Here Ps denotes the projection operator onto the subspace S. Now,

$$M_{i}^{\frac{1}{2}}(\xi) P$$
 $R^{\frac{1}{2}}(\xi)]^{+}M_{i}(\xi^{*})$
 $M_{i}^{\frac{1}{2}}(\xi)$

$$= M_{i}^{\frac{1}{2}}(\xi)[M_{i}^{\frac{1}{2}}(\xi)]^{+} M_{i}(\xi^{*})[M_{i}(\xi^{*})]M_{i}^{\frac{1}{2}}(\xi)]^{+} \{M_{i}^{\frac{1}{2}}(\xi)\}^{+} M_{i}(\xi^{*})]^{+} M_{i}(\xi^{*})[M_{i}^{\frac{1}{2}}(\xi)]^{+} M_{i}^{\frac{1}{2}}(\xi)$$

Note that for any matrix M, $P_{R(M)} = M (M^TM)^+ M^T$. See Boullion and Odell [3, Theorem 7, p. 7).

Now, we observe that

$$M_{i}^{\frac{1}{2}}(\xi) [M_{i}^{\frac{1}{2}}(\xi)]^{+} M_{i}(\xi^{*}) = M_{i}(\xi^{*}), \text{ as } R[M_{i}(\xi^{*})] \subset R[M_{i}(\xi)] \subset R[M_{i}(\xi)],$$

by hypothesis, and, by a similar argument,

$$M_{i}(\xi^{*})[M_{i}^{\frac{1}{2}}(\xi)]^{+}M_{i}^{\frac{1}{2}}(\xi)=M_{i}(\xi^{*}).$$

It is also true that $R \{ [M_i(\xi^*) M_i^+(\xi) | (\xi^*)]^+ \} \subset R [M_i(\xi^*)].$

Now, it is not difficult to see that

$$M_{i}^{+}(\xi^{*})\,M_{i}^{1/2}(\xi)\,P R_{i}^{1/2}(\xi)]^{+}\,M_{i}(\xi^{*}) M_{i}^{1/2}(\xi)\,M_{i}^{+}(\xi^{*}) = [M_{i}(\xi^{*})M_{i}^{+}(\xi)\,M_{i}^{+}(\xi^{*})]^{+}\,M_{i}(\xi^{*})]^{+}$$

Thus we have

$$\frac{d}{d\alpha}F(\stackrel{\sim}{\xi}(\alpha))]_{\alpha=0} = F(\xi^*) - \sum_{i=1}^{q} w_i Tr. \left\{A_i^T[M_i(\xi^*)M_i^+(\xi)M_i(\xi^*)]A_i\right\}$$

Since
$$\xi^*$$
 is optimal we have $\frac{d}{d\alpha} F(\xi(\alpha)) = 0$.

This proves (b).

(b) = (a). Suppose ξ^* satisfies (b) but not (a). So we can find $\xi_1 \in \Xi_1$ such that $F(\xi_1) < F(\xi^*)$. We can assume that $|M_1(\xi_1)| \neq 0$ for every i = 1 to q. If not, we can always find $\xi_1^* \in \Xi_1$ with $|M_1(\xi_1^*)| \neq 0$ for every i = 1 to q and $M_1(\xi_1)$ and $M_1(\xi_1^*)$ are as close as you please for every i = 1 to q. Since F is continuous on Ξ_1 , we can choose the above ξ_1^* to satisfy $F(\xi_1^*) < F(\xi^*)$ as well. Now, we consider the design.

 \approx $\xi(\alpha) = (1-\alpha)\xi^* + \alpha\xi_1$ for $\alpha\epsilon(0,1)$. By an argument similar to the one used in proving the implication (a) = (b), we have

$$\frac{d}{d\alpha} F(\overset{\thickapprox}{\xi}(\alpha)) \Big]_{\alpha = 0} = F(\xi^*) - \sum_{i=1}^q w_i \operatorname{Tr.} \big\{ A_i^T \big[M_i(\xi^*) M_i^+ (\xi_i) M_i(\xi^*) \big]^+ A_i \big\}$$

 ≥ 0 , by condition (b).

On the other hand, by the convexity of F, we have

$$\frac{\mathrm{d}}{\mathrm{d}\alpha} F \stackrel{\approx}{(\xi} (\alpha))]_{\alpha = 0} < 0.$$

This is a contradiction. This completes the proof.

Lemma 3.3.

Let $\Xi_2 = \{ \xi \epsilon \Xi_1; R [M_i(\xi)) \} \subseteq R [M_i(\xi^*)] \text{ for all } i = 1 \text{ to } q \},$

Where $\xi^+ \in \Xi_1$ is some fixed design. Then

$$\min_{x \in X} \frac{d}{d\alpha} F [(1-\alpha) \xi + \alpha \xi_x)] \underset{\alpha = 0}{\leqslant} F (\xi^*) - F (\xi)$$

for every $\xi \in \Xi_2$, where ξ_x is the one point design associated with $x \in X$.

Proof. Let $\xi \in \Xi_2$ and consider the designs $\widetilde{\xi}(\alpha) = (1-\alpha)\xi + \alpha\xi^*$, $\alpha \in (0,1)$. Since F is convex on Ξ_1 , we have,

$$\frac{d}{d\alpha} F(\widetilde{\xi}(\alpha)) \right]_{\alpha = 0} \le F(\xi^*) - F(\xi).$$

On the other hand, by an argument used in the proof of theorem 3.2,

$$\frac{d}{d\alpha} F(\widetilde{\xi}(\alpha))]_{\alpha=0} = \sum_{i=1}^{q} w_i \operatorname{Tr.} \{A_i^T M_i^+ (\xi) A_i \}$$

$$- \sum_{i=1}^{q} \ w_i \ \mathrm{Tr.} \ \big\{ \ A_i^T \ M_i^{\ +} \ (\xi) \ M_i^{\ 1/2} (\xi^*) \ P_{R[\{M_i^{\ 1/2} \ (\xi^*) \ \} \ + \ M_i \ (\xi)]}^{\ 1/2} \ M_i^{\ 1/2} \ (\xi^*) \big\}$$

$$\begin{split} M_{i}^{+} & (\xi) \, A_{i} \, \big\} \! \geqslant \! F (\xi) - \sum_{i=1}^{q} w_{i} \, Tr. \, \big\{ A_{i}^{T} \, M_{i}^{+} \, (\xi) \, M_{i}^{1/2} \! (\xi^{*}) \, P_{R \, \big\{ [M_{i} \, (\xi^{*})]^{+} \, \big\}} \\ M_{i}^{1/2} \! (\xi^{*}) \, M_{i}^{+} & (\xi) A_{i}) \end{split}$$

(it is known that $P_{R(A)} \leq P_{R(B)}$ if $R(A) \subseteq R(B)$. See Ben-Israel and Creville [2, Exercise 54, p. 71].

$$= F(\xi) - \sum_{i=1}^{q} w_i^{Tr} \cdot \{A_i^T M_i^+ (\xi) M_i(\xi^*) M_i^+(\xi) A_i \}.$$

(see the proof of theorem 3.2.).

Thus we have

$$\begin{split} &\frac{d}{d\alpha} F\left(\xi^{*}\left(\alpha\right)\right) \right] \\ &\geqslant F\left(\xi\right) - \int_{X}^{\infty} \sum_{i=1}^{q} w_{i} \, Tr. \left\{A_{i}^{T} M_{i}^{+} \left(\xi\right) f_{i}\left(x\right) f_{i}^{T}\left(x\right) M_{i}^{+} \left(\xi\right) A_{i} \right\} \, \xi^{*}\left(dx\right) \\ &\geqslant F\left(\xi\right) - \max_{x \in X} \sum_{i=1}^{q} w_{i} \, Tr. \left\{A_{i}^{T} M_{i}^{+} \left(\xi\right) f_{i}\left(x\right) f_{i}^{T}\left(x\right) M_{i}^{+} \left(\xi\right) A_{i} \right\}. \end{split}$$

It is true that

$$\begin{split} &\frac{d}{d\alpha}F\left[\left(l-\alpha\right)\xi+\alpha\xi_{x}\right]\bigg]_{\alpha=0} = F\left(\xi\right) - \sum_{i=1}^{q} w_{i} Tr.\left\{A_{i}^{T}M_{i}^{+}\left(\xi\right)f_{i}\left(x\right)\right\} \\ &f_{i}^{T}(x) M_{i}^{+}\left(\xi\right)A_{i}\right\}. \end{split}$$

The above is a modified version of what Läuter [10, p. 56) proved.

Consequently,

$$\min_{x \in X} \frac{d}{d\alpha} F \left[\begin{array}{c} (1-\alpha) \, \xi + \alpha \xi_x \end{array} \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, \operatorname{Tr.} \left[A_i^T \, M_i^+(\xi) f_i(x) \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, \operatorname{Tr.} \left[A_i^T \, M_i^+(\xi) f_i(x) \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, \operatorname{Tr.} \left[A_i^T \, M_i^+(\xi) f_i(x) \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, \operatorname{Tr.} \left[A_i^T \, M_i^+(\xi) f_i(x) \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, \operatorname{Tr.} \left[A_i^T \, M_i^+(\xi) f_i(x) \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, \operatorname{Tr.} \left[A_i^T \, M_i^+(\xi) f_i(x) \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, \operatorname{Tr.} \left[A_i^T \, M_i^+(\xi) f_i(x) \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, \operatorname{Tr.} \left[A_i^T \, M_i^+(\xi) f_i(x) \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, \operatorname{Tr.} \left[A_i^T \, M_i^+(\xi) f_i(x) \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, \operatorname{Tr.} \left[A_i^T \, M_i^+(\xi) f_i(x) \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, \operatorname{Tr.} \left[A_i^T \, M_i^+(\xi) f_i(x) \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, \operatorname{Tr.} \left[A_i^T \, M_i^+(\xi) f_i(x) \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, \operatorname{Tr.} \left[A_i^T \, M_i^+(\xi) f_i(x) \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, \operatorname{Tr.} \left[A_i^T \, M_i^+(\xi) f_i(x) \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, \operatorname{Tr.} \left[A_i^T \, M_i^+(\xi) f_i(x) \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, f_i^T(x) \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, f_i^T(x) \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, f_i^T(x) \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, f_i^T(x) \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{i=1}^q w_i \, f_i^T(x) \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{x \in X} \sum_{x \in X} \sum_{x \in X} \left[A_i \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \sum_{x \in X} \sum_{x \in X} \left[A_i \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \left[A_i \, f_i^T(x) \right] \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \left[A_i \, f_i^T(x) \right] \bigg|_{\alpha = 0} \bigg|_{\alpha = 0} = F(\xi) - \max_{x \in X} \left[A_i \, f_i$$

$$M_{i}^{+}(\xi) A_{i} \leqslant \frac{d}{d\alpha} F(\widetilde{\xi}(\alpha))] = 0 \leqslant F(\xi^{*}) - F(\xi).$$

This completes the proof.

The following is an important consequence of the above.

Theorem 3.4.

Let $\xi^* \in \Xi_1$ be optimal. Then,

$$\min_{x \in X} \ \frac{d}{d\alpha} \ F\left[(1-\alpha) \ \xi + \alpha \xi_x \ \right] \bigg]_{\alpha = 0} \leqslant F\left(\xi^* \right) - F(\xi) \ \text{for every } \xi \in \Xi_1.$$

Proof. By Lemma 3.3, for $\xi_1 \in \Xi_1$

$$\min_{x \in X} \frac{d}{d\alpha} F \left[(1-\alpha) \xi + \alpha \xi_x \right]_{\alpha = 0} \leq F(\xi_1) - F(\xi)$$

for every $\xi \in \Xi_2 = \{ \xi \in \Xi_1; R[M_i(\xi)] \subseteq R(M_i(\xi_1) \text{ for every } i=1 \text{ to } q \}.$

If $\xi_1 \in \Xi_1$ is such that $M_i(\xi_1) \neq 0$ for every i = 1 to q, then $\Xi_2 = \Xi_1$. Let $\Xi_3 = \{\xi \in \Xi; |M_i(\xi)| \neq 0 \text{ for every } i = 1 \text{ to } q \}$. Then

$$\min_{\mathbf{x} \in \mathbf{X}} \frac{d}{d\alpha} F \left[(1-\alpha) \xi + \alpha \xi_{\mathbf{x}} \right] \Big|_{\alpha=0} \leqslant \inf_{\xi_1 \in \Xi_3} F(\xi_1) - F(\xi)$$

for every $\xi \mathbf{E} \Xi_1$. As Ξ_3 is dense in Ξ_1 and F is continuous on Ξ_1 , we have

$$\min_{x\in X}\frac{d}{d\alpha}\;F\;\left[\left(1-\alpha\right)\xi+\alpha\xi_{x}\right]\bigg]_{\alpha\;=\;0}\leqslant \inf_{\xi_{1}\in\Xi_{1}}F\;(\xi_{1})-\;F(\xi)=F\;(\xi^{*})-F\;(\xi)$$

for every $\xi \in \Xi_1$. This completes the proof.

Remark 3.5. Kiefer [9, Equation 6.5, p. 877] proved a result similar to the above. See also Arwood [1, Equation 2.1., p. 1126]. Their inequality is for general convex criterion and in our special case, the above inequality is more informative.

Theorem 3.6.

For $\xi^* \in \Xi_1$, the following are equivalent.

(a) 5* is optimal.

(b)
$$\max_{x \in X} \sum_{i=1}^{q} w_i \text{ Tr.} \{A_i^T M_i^+ (\xi^*) f_i(x) f_i^T M_i^+ (\xi^*) A_i \} = F(\xi^*).$$

Proof. Let us denote Tr. $\{A_i^T M_i^+ (\xi) f_i(x) f_i^T(x) M_i^+ (\xi) A_i\}$ by $\phi_i(x,\xi)$

for i = 1 to q and $\xi \in \Xi_1$.

(a) \Rightarrow (b). Consider the design $\widetilde{\xi}(\alpha) = (1-\alpha) \xi^* + \alpha \xi_x, x \in X, \alpha \in [0,1)$.

Then

$$F\left(\widetilde{\xi}(\alpha)\right) = \frac{1}{1-\alpha} \sum_{i=1}^{q} w_i \operatorname{Tr.} \left\{ A_i^{\mathrm{T}} M_i^{+} (\xi^*) A_i \right\}$$

$$-\sum_{i=1}^{q} w_{i} \frac{\alpha}{(1-\alpha)[1-\alpha+\alpha d_{i}(x,\xi^{*})]} Tr. \{A_{i}^{T} M_{i}^{+} (\xi^{*}) f_{i}(x) f_{i}^{T}(x) M_{i}^{+} (\xi^{*}) A_{i}\}$$

$$= \frac{1}{1-\alpha} F(\xi^*) - \frac{\alpha}{1-\alpha} \sum_{i=1}^{q} w_i \frac{\phi_i(x, \xi^*)}{1-\alpha+\alpha d_i(x, \xi^*)},$$

where

$$d_{i}(x, \xi^{*}) = f_{i}^{T}(x) M_{i}^{+}(\xi^{*}) f_{i}(x).$$

The above identities are derived based on the identities given by Läuter [10 p. 56].

Now, from the above, we derive

$$\frac{d}{d\alpha}F\left(\widetilde{\xi}\left(\alpha\right)\right)\Big|_{\alpha=0} = F\left(\xi^*\right) - \sum_{i=1}^{q} w_i \, \varphi_i\left(x, \, \xi^*\right) \tag{3.6.1}$$

for every $x \in X$. See also the proof of Lemma 3.3.

Thus, since ξ^* is optimal,

$$F(\xi^*) \ge \max_{x \in X} \sum_{i=1}^{q} w_i \phi_i(x, \xi^*)$$
 (3.6.2.)

On the other hand, for every $\xi \in \Xi_1$

$$\int \sum_{i=1}^{q} w_{i} \, \phi_{i} \, (x,\xi)) \, \xi \, (dx) \, = \!\!\!\!\!\!\! \sum_{i=1}^{q} w_{i} \, Tr. \, \big\{ A_{i}^{T} \, M_{i}^{+} \, (\xi) \, M_{i} \, (\xi) \, M_{i}^{+} \, (\xi) \, A_{i} \, \big\} = F \, (\xi),$$

from which it follows that

$$\max_{\mathbf{x} \in \mathbf{X}} \sum_{i=1}^{q} w_{i} \, \varphi_{i} (\mathbf{x}, \boldsymbol{\xi}) \geq F \, (\boldsymbol{\xi}) \tag{3.6.3}.$$

Now, (3.6.2.) and (3.6.3) together establish (b).

(b) \Rightarrow (a). Suppose ξ^* is not optimal. Let $\xi_1 \in \Xi_1$ be any optimal design. By Theorem 3.4

$$\min_{x \in X} \frac{d}{d\alpha} F \left[(1-\alpha) \xi^* + \alpha_x \right] \Big]_{\alpha=0} \leq F (\xi_1) - F (\xi^*) < 0$$

On the other hand,

$$\min_{x \in X} -\frac{d}{d\alpha} F\left[(1-\alpha) \xi^* + \alpha \xi_x \right] \bigg|_{\alpha=0} = F\left(\xi^*\right) - \max_{x \in X} \sum_{i=1}^{q} w_i \phi_i \left(x,\xi\right) = 0,$$

as we assumed (b) and in view of the identity (3.6.1). This is a contradiction and completes the proof.

Now, let us specialise to the case q = 1. Write $A_1 = A_1 f_1 = f$ $M_1 = M_2$. A result similar to the following one can be found in Fedorov [6, Corrolary 1, p. 128] for the case of non - singular linear optimal designs.

Corrolary 3.7.

Let the design space X be compact Hausdorff and let Y (x) be a random variable with EY (x) = $f^T(x) \beta$ and Var (Y (x)) = σ^2 for every x \in X, where $f^T: X \to R^n$ is a continuous function and $\beta^T \in R^n$, is the unknown vector 1xn

of parameters. Let $\Xi = \{\xi ; \xi \text{ is a regular probability measure of the Baire } \sigma \text{-field}$

of X}. let
$$\Xi_1 = \{\xi \epsilon \Xi; R(A) \subseteq R(M(\xi))\}$$
, where $M(\xi) = \int_{\mathbf{X}} f(x) f^T(x) \xi(dx)$ is

the information matrix associated with ξ and A is a matrix of full rank s.

Let $F(\xi) = Tr. \{A^TM^+(\xi) A\}, \xi \in \Xi_1$. If a finite design

$$\xi^*: \left\{ \begin{array}{cccc} x_1 & x_2 & \dots & x_r \\ & & & & \\ p_1 & p_2 & \dots & p_r \end{array} \right\}$$

with $p_1, p_2, ..., p_r$ all positive and $\xi^* \in \Xi_1$ is F - optimal, then

$$f^{T}(x_{i}) M^{+}(\xi^{*}) A A^{T} M^{+}(\xi^{*}) f(x_{i}) = F(\xi^{*})$$

for every i = 1 to r.

Proof. Suppose ξ^* is F-optimal but $f^T(x_i)M^+$ (ξ^*) AA^TM^+ (ξ^*) $f(x_i)$ $< F(\xi^*)$ for some $i \ni \{1, 2, ..., r\}$. Note that $\sum_{j=1}^r p_j f^T(x_j) M^+$ (ξ^*) AA^TM^+ (ξ^*) $f(x_j) = Tr. \{A^TM^+$ (ξ^*) $A \} = F(\xi^*).$

Since ξ^* is optimal, by Theorem 3.6.,

$$f^{T}(x) M^{+}(\xi^{*}) AA^{T}M^{+}(\xi^{*}) f(x) \leq F(\xi^{*})$$
 for every $x \ni X$.

Therefore,

$$F\left(\xi^{*}\right) = \sum_{j=1}^{r} \; p_{j} \; f^{T}\left(x_{j}\right) M^{+} \; (\xi^{*}) \; AA^{T} \, M^{+} \; (\xi^{*}) \; f\left(x_{j}\right) < \sum_{j=1}^{r} \; p_{j} \; F\left(\xi^{*}\right) = F\left(\xi^{*}\right),$$

a contradiction. This proves the result.

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