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COMPUTATION OF THE OPTIMUM DESIGNS UNDER SINGULAR INFORMATION MATRICES

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The main result of this paper is that g-inverses are not needed for computing optimum designs when the singularity of the information matrix is unavoidable. They are, of course, needed for the analysis. It will be shown that it is possible to augment the experimental region so that procedures for computing optimum designs for s out k parameters ($s < k$) which are developed for the nonsingular case may also be used for the singular case.

1. Introduction. Let us start with the following design problem (cf. Karlin–Studden (1966)). We are given a vector $\theta = (\theta_1, \cdots, \theta_k)'$ of unknown parameters and a vector $f(x) = (f_1(x), \cdots, f_k(x))'$ of the regression functions, all defined on a given set $\mathscr{X}$. It is assumed that the information matrix

$$M(\xi) = \int_{x \in \mathscr{X}} f(x)f'(x)\xi(dx)$$

is singular for any design measure ξ on $\mathscr{X}$. However, some of the parameters, say $\theta_1, \cdots, \theta_s$ ($s < k$) are assumed to be estimable for some (not further specified) design.

The standard iterative methods for computing the optimal designs are necessarily starting from an initial design having a nonsingular information matrix. Hence, they cannot be used directly in the present setting. Moreover, similarly to the problems of parameter estimation (Rao (1971)), the use of the g-inverses seems to be unavoidable.

The aim of this paper is to show that a simple improvement of the existing standard algorithm leads to a computation procedure which does not make use of g-inverses.

2. Estimates and g-inverses. A function $h(\theta) = p'\theta$ is estimable if and only if $p \in \mathscr{U}(M(\xi))$, the range of the information matrix $M(\xi)$ (cf. Karlin–Studden (1966)). The variance of the best linear estimate for h is given by

$$\text{Var}_\xi\, h = p'M^-(\xi)p \tag{1}$$

where $M^-(\xi)$ is a solution of the equation

$$M(\xi)M^-(\xi)M(\xi) = M(\xi)\,. \tag{2}$$

This statement is a special case of Theorem 3.1 in Rao (1971). It may be obtained also from the expression (cf. Karlin–Studden (1966), Theorem 2.1):

$$\text{Var}_\xi\, h = \sup\left\{\frac{(p'd)^2}{d'M(\xi)d} : d \in \mathscr{U}(M(\xi)),\, d \neq 0\right\}$$

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(the supremum is attained for $d = M^{-}(\xi)p$). Finally (2) may be obtained also as a consequence of Theorem 1.1.3 in Fellman (1974).

One solution of (1) which will be used later, may be described as follows: $M^{-}(\xi)g$ is the unique vector $h \in \mathscr{U}(M(\xi))$ such that $M(\xi)h = g$ for $g \in \mathscr{U}(M(\xi))$, otherwise, for $g \in \mathscr{U}^{\perp}(M(\xi))$, $M^{-}(\xi)g$ is the zero vector.

3. Optimum designs. In what follows we shall deal with the optimality criteria of the form $\Phi[D(\xi)]$, $D(\xi)$ being the covariance matrix of the estimates of $\theta_1, \cdots, \theta_s$, Φ having the property $\Phi(A) \leqq \Phi(B)$ for $A \ll B$. Some well-known examples are the following ones:

$$\begin{aligned}\Phi[D(\xi)] &= \det D(\xi) \quad (D_s\text{-optimality}),\\ &= \operatorname{tr} D(\xi)\,,\\ &= \sup\{D_{ii}(\xi),\ 1 \leqq i \leqq s\}\,, \quad \text{etc.}\end{aligned}$$

The dimension of $\mathscr{U}(M(\xi))$ will be denoted by r. Let

$$f(z_j) = (f_1(z_j), \cdots, f_k(z_j))'\,, \qquad j = r+1, \cdots, k$$

be arbitrary vectors with the property that

$$f(z_{r+1}) \perp \{f(x) : x \in \mathscr{X}\}$$

and

$$f(z_j) \perp \{f(x); x \in \mathscr{X}\} \cup \{f(z_{r+1}), \cdots, f(z_{j-1})\} \qquad j = r+2, \cdots, k\,.$$

By adding the "points" $z_{r+1}, \cdots, z_k$ to $\mathscr{X}$ we obtain an extended experiment with the regression functions defined on the set

$$\mathscr{X}^{\mathscr{X}} = \mathscr{X} \cup \{z_{r+1}, \cdots, z_k\}\,.$$

PROPOSITION. *Let ξ be a design measure supported by a subset of $\mathscr{X}^{\mathscr{X}}$. Denote by μ the restriction of ξ to the set $\mathscr{X}$,* i.e.,

$$\mu(\cdot) = \xi(\cdot)/\xi(\mathscr{X})\,.$$

Then the inequality

$$\Phi[D(\mu)] \leqq \Phi[D(\xi)]$$

is valid.

PROOF. The matrix $M(\xi)$ can be expressed in terms of the matrix $M(\mu)$ and the vectors $f(z_j)$ chosen above:

$$M(\xi) = (1 - \textstyle\sum_{j=r+1}^{k} \xi(z_j))M(\mu) + \sum_{j=r+1}^{k} f(z_j)f'(z_j)\xi(z_j)\,.$$

Let us consider the g-inverse $M^{-}(\mu)$ of the matrix $M(\mu)$, as described in Section 2. The formula

$$M^{-}(\xi) = \frac{M^{-}(\mu)}{1 - \sum_{j=r+1}^{k} \xi(z_j)} + \sum_{j=r+1}^{k} \frac{1}{\xi(z_j)} \frac{f(z_j)f'(z_j)}{[f'(z_j)f(z_j)]^2}$$

then established a g-inverse of the matrix $M(\xi)$ of the same type, too. If $h(\theta) = p'\theta$ is estimable in the experiment with the experimental region $\mathscr{X}$ then, $p \in \mathscr{U}(M(\xi))$, that means that

$$p \perp f(z_{r+1}), \cdots, f(z_k)\,,$$

hence

$$\mathrm{Var}_\xi h = p'M^-(\xi)p = \frac{\mathrm{Var}_\mu h}{1 - \sum_{j=r+1}^{k} \xi(z_j)} \geqq \mathrm{Var}_\mu h .$$

Consequently, $\Phi[D(\xi)] \geqq \Phi[D(\mu)]$. The proposition is proved.

The important consequence of the latter statement is that a Φ-optimal design (i.e., design minimizing $\Phi[D(\xi)]$) is not supported by points from the set $\{z_{r+1}, \cdots, z_k\}$. This in turn implies that the standard computation procedures apply for the extended experiment. The resulting nearly optimal design is to be merely restricted from $\mathscr{X}^{\mathscr{X}}$ to $\mathscr{X}$. Following this manner a nearly optimal design is obtained in the original experiment. Hence the use of g-inverses may be avoided.

To finish the paper let us note that the method was essentially based on the Hilbert space structure of a regression experiment. Hence similar ideas are available even in a more complicated (infinite-dimensional) setting (cf. Pázman (1974)).

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REFERENCES

[1] FELLMAN, J. (1974). On the allocation of linear observations. *Comment. Phys.-Math. (Helsinki)* **44** 27–78.

[2] KARLIN, S. and STUDDEN, W. J. (1966). Optimal experimental designs. *Ann. Math. Statist.* **37** 738–815.

[3] PÁZMAN, A. (1974). The ordering of experimental designs. A Hilbert space approach. *Kybernetika (Prague)* **10** 373–388.

[4] RAO, C. R. (1971). Unified theory of linear estimation. *Sankhyā* (A)**33** 371–394.

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