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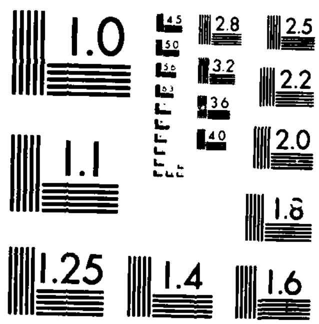

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THE SEQUENTIAL GENERATION OF MULTIRESPONSE D-OPTIMAL DESIGNS WHEN THE VARIANCE-COVARIANCE MATRIX IS NOT KNOWN

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This paper discusses the sequential generation of a D-optimal design for a linear multiresponse model when the variance-covariance matrix of the responses is not known.

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Key Words and Phrases: multiresponse design; D-optimality; sequential generation.

ABSTRACT

The construction of D-optimal designs for multiresponse experiments was considered ~~by~~ Fedorov (1972, Ch. 5). His algorithm required that the variance-covariance matrix, Σ, of the responses be known. This is rarely the case in practice. The primary objective of this paper is to develop a sequential procedure for the construction of multiresponse designs when Σ is not known. Several numerical examples are given to illustrate this procedure.

Sigma

1. MODEL AND NOTATION

We consider a situation in which observations are made on $r(>2)$ responses at N experimental runs (not necessarily all distinct) such that the ith response is represented by the linear model

$$y_{ui} = \underset{\sim}{f}_i'(\underset{\sim}{x}_u)\underset{\sim}{\beta}_i + \varepsilon_{ui}, \quad i = 1,2,\ldots,r; \; u = 1,2,\ldots,N. \tag{1}$$

Here y_{ui} *is the observation* on the ith response at the uth design setting; $\underset{\sim}{\beta}_i$ ($i = 1,2,\ldots,r$) is a vector of p_i unknown parameters associated with the ith response model; ε_{ui} is a random error in the ith response value at the uth experimental run; $\underset{\sim}{x}_u = (x_{u_1}, x_{u_2}, \ldots, x_{u_k})'$ represents the uth design settings of k controllable variables ($u=1,2,\ldots,N$) within some experimental region, χ, considered to be a compact subset in the k-dimensional Euclidean space and, $\underset{\sim}{f}_i(\underset{\sim}{x})$ is a $p_i \times 1$ vector whose elements are known functions of the controllable variables assumed to be continuous within χ. The set of points $\underset{\sim}{x}_1, \underset{\sim}{x}_2, \ldots, \underset{\sim}{x}_N$ (not necessarily distinct) form an N-point design which we denote by D_N. Using matrix notation, model (1) can be written as

$$\underset{\sim}{Y}_i = \underset{\sim}{F}_i\underset{\sim}{\beta}_i + \underset{\sim}{\varepsilon}_i, \quad i = 1,2,\ldots,r, \tag{2}$$

where $\underset{\sim}{Y}_i$ is the $N\times 1$ vector of observations on the ith response, $\underset{\sim}{F}_i$ is an $N\times p_i$ matrix of full column rank whose uth row contains the elements of $\underset{\sim}{f}_i'(\underset{\sim}{x}_u)$ ($u=1,2,\ldots,N$), and $\underset{\sim}{\varepsilon}_i$ is an $N\times 1$ vector of random errors associated with the ith response ($i=1,2,\ldots,r$) with the assumption that $E(\underset{\sim}{\varepsilon}_i)=\underset{\sim}{0}$ and $E(\underset{\sim}{\varepsilon}_i\underset{\sim}{\varepsilon}_j') = \sigma_{ij}\underset{\sim}{I}_N$ ($i,j=1,2,\ldots r$), where $\underset{\sim}{I}_N$ is the identity matrix of order $N\times N$. Thus, the variance-covariance matrix of the $Nr\times 1$ vector $\underset{\sim}{\varepsilon}=(\underset{\sim}{\varepsilon}_1', \underset{\sim}{\varepsilon}_2', \ldots, \underset{\sim}{\varepsilon}_r')'$ is given by the direct product

$$\mathrm{var}(\underset{\sim}{\varepsilon}) = \underset{\sim}{\Sigma} \otimes \underset{\sim}{I}_N, \tag{3}$$

where $\underset{\sim}{\Sigma}=(\sigma_{ij})$ is the variance-covariance matrix for the r responses. The r models in (2) can be written as

$$\underset{\sim}{Y} = \underset{\sim}{F}_{D_N}\,\underset{\sim}{\beta} + \underset{\sim}{\varepsilon}, \tag{4}$$

where

$$\underset{\sim}{Y}' = [\underset{\sim}{Y}_1', \underset{\sim}{Y}_2', \ldots, \underset{\sim}{Y}_r'] \;,\; \underset{\sim}{\beta}' = [\underset{\sim}{\beta}_1', \underset{\sim}{\beta}_2', \ldots, \underset{\sim}{\beta}_r'] \;,\; \underset{\sim}{\varepsilon}' = [\underset{\sim}{\varepsilon}_1', \underset{\sim}{\varepsilon}_2', \ldots, \underset{\sim}{\varepsilon}_r'],$$

and $\underset{\sim}{F}_{D_N}$ is the block-diagonal matrix diag$(\underset{\sim}{F}_1, \underset{\sim}{F}_2, \ldots, \underset{\sim}{F}_r)$. Thus, the total number of unknown parameters in the system is $p = \sum_{i=1}^{r} p_i$. Since each $\underset{\sim}{F}_i$ is of full column rank, $\underset{\sim}{F}_{D_N}$ is also of full column rank equal to p. The best linear unbiased estimator of $\underset{\sim}{\beta}$ is then given by

$$\hat{\underset{\sim}{\beta}} = [\underset{\sim}{F}_{D_N}'(\underset{\sim}{\Sigma}^{-1} \otimes \underset{\sim}{I}_N)\underset{\sim}{F}_{D_N}]^{-1}\underset{\sim}{F}_{D_N}'(\underset{\sim}{\Sigma}^{-1} \otimes \underset{\sim}{I}_N)\underset{\sim}{Y}. \tag{5}$$

The variance-covariance matrix of $\hat{\underset{\sim}{\beta}}$ is

$$\text{var}(\hat{\underset{\sim}{\beta}}) = [\underset{\sim}{F}_{D_N}'(\underset{\sim}{\Sigma}^{-1} \otimes \underset{\sim}{I}_N)\underset{\sim}{F}_{D_N}]^{-1}. \tag{6}$$

At a point $\underset{\sim}{x} = (x_1, x_2, \ldots, x_k)'$ in the experimental region χ, the vector of predicted responses, $\hat{\underset{\sim}{Y}}(\underset{\sim}{x}) = [\hat{y}_1(\underset{\sim}{x}), \hat{y}_2(\underset{\sim}{x}), \ldots, \hat{y}_r(\underset{\sim}{x})]'$, can be expressed as

$$\hat{\underset{\sim}{Y}}(\underset{\sim}{x}) = \underset{\sim}{\phi}'(\underset{\sim}{x})\hat{\underset{\sim}{\beta}}, \tag{7}$$

where $\underset{\sim}{\phi}'(\underset{\sim}{x})$ is the block-diagonal matrix diag$(\underset{\sim}{f}_1'(\underset{\sim}{x}), \underset{\sim}{f}_2'(\underset{\sim}{x}), \ldots, \underset{\sim}{f}_r'(\underset{\sim}{x}))$. The variance-covariance matrix of $\hat{\underset{\sim}{Y}}(\underset{\sim}{x})$ is then of the form

$$\text{var}[\hat{\underset{\sim}{Y}}(\underset{\sim}{x})] = \underset{\sim}{\phi}'(\underset{\sim}{x})[\underset{\sim}{F}_{D_N}'(\underset{\sim}{\Sigma}^{-1} \otimes \underset{\sim}{I}_N)\underset{\sim}{F}_{D_N}]^{-1}\underset{\sim}{\phi}(\underset{\sim}{x}). \tag{8}$$

2. DESIGN THEORY

The concept of a design measure as defined below is important to the theory of optimal designs.

Definition 1

A design measure defined on an experimental region χ is a probability measure $\zeta(\underset{\sim}{x})$ which satisfies $\zeta(\underset{\sim}{x}) \geq 0$ and $\int_{\chi} d\zeta(\underset{\sim}{x}) = 1$,

$\underset{\sim}{x} \in \chi$ (see Wynn, 1970; Fedorov, 1972). Given a design measure $\zeta(\underset{\sim}{x})$ on χ, the set of points $\underset{\sim}{x} \in \chi$ at which $\zeta(\underset{\sim}{x}) > 0$ is called the support or spectrum of $\zeta(\underset{\sim}{x})$. For example, for $x_1, x_2, \ldots, x_s \in \chi$, $\zeta(\underset{\sim}{x})$ may be defined as

$$\zeta(\underset{\sim}{x}) = \begin{cases} 0 & \underset{\sim}{x} \neq \underset{\sim}{x}_u \quad u = 1,2,\ldots,s \\ \lambda_u & \underset{\sim}{x} = \underset{\sim}{x}_u \quad u = 1,2,\ldots,s \end{cases}$$

such that $\sum_{i=1}^{s} \lambda_u = 1$ with $0 < \lambda_u < 1$. This measure is discrete if λ_u is a rational number for $u = 1,2,\ldots,s$, otherwise, if at least one λ_u is an irrational number, then $\zeta(\underset{\sim}{x})$ is a continuous measure. In particular, we define the discrete measure $\zeta_{D_N}(\underset{\sim}{x})$ by

$$\zeta_{D_N}(\underset{\sim}{x}) = \begin{cases} 0 & \underset{\sim}{x} \neq \underset{\sim}{x}_u, \quad u = 1,2,\ldots,s \\ \frac{n_u}{N} & \underset{\sim}{x} = \underset{\sim}{x}_u, \quad u = 1,2,\ldots,s, \end{cases} \tag{9}$$

where n_u is the number of replications at the point $\underset{\sim}{x}_u$ and $\sum_{u=1}^{s} n_u = N$. For a given design measure $\zeta(\underset{\sim}{x})$ and a given variance-covariance matrix $\underset{\sim}{\Sigma}$, we define the moment matrix $\underset{\sim}{M}(\zeta,\underset{\sim}{\Sigma})$ as

$$\underset{\sim}{M}(\zeta,\underset{\sim}{\Sigma}) = \int_{\chi} \underset{\sim}{\phi}(\underset{\sim}{x})\underset{\sim}{\Sigma}^{-1}\underset{\sim}{\phi}'(\underset{\sim}{x})d\zeta(\underset{\sim}{x}), \tag{10}$$

where $\underset{\sim}{\phi}(\underset{\sim}{x})$ is the block -diagonal matrix in (7). In particular, for the discrete design measure $\zeta_{D_N}(\underset{\sim}{x})$ described earlier,

$$\underset{\sim}{M}(\zeta_{D_N},\underset{\sim}{\Sigma}) = \frac{1}{N} \sum_{u=1}^{s} n_u \underset{\sim}{\phi}(\underset{\sim}{x}_u)\ \underset{\sim}{\Sigma}^{-1}\underset{\sim}{\phi}'(\underset{\sim}{x}_u), \tag{11}$$

or equivalently,

$$\underset{\sim}{M}(\zeta_{D_N},\underset{\sim}{\Sigma}) = [\underset{\sim}{F}'_{D_N}(\underset{\sim}{\Sigma}^{-1} \otimes \underset{\sim}{I}_N)\underset{\sim}{F}_{D_N}]/N, \tag{12}$$

where $\underset{\sim}{F}_{D_N}$ is the block-diagonal matrix in (4).

2.1 D-Optimality

Under the assumption of normality of errors and linearity of the fitted models, a confidence ellipsoid for $\underset{\sim}{\beta}$ of a given confidence coefficient is of the form

$$\{\underset{\sim}{\beta}:(\underset{\sim}{\beta}-\hat{\underset{\sim}{\beta}})'\underset{\sim}{M}(\zeta,\underset{\sim}{\Sigma})(\underset{\sim}{\beta}-\hat{\underset{\sim}{\beta}}) < \text{constant}\}, \tag{13}$$

where $\underset{\sim}{M}(\zeta,\underset{\sim}{\Sigma})$ is as defined in (10) and $\hat{\underset{\sim}{\beta}}$ is the weighted least squares estimator of $\underset{\sim}{\beta}$ given in (5) (see Silvey, 1980, p. 10 for the single response case). A more precise estimate for $\underset{\sim}{\beta}$ is thus obtained by making the volume of this ellipsoid as small as possible. Since this volume is proportional to $|\underset{\sim}{M}(\zeta,\underset{\sim}{\Sigma})|^{-1/2}$, where $|\cdot|$ denotes the determinant of a matrix, we can achieve this objective by choosing a design measure which maximizes $|\underset{\sim}{M}(\zeta,\underset{\sim}{\Sigma})|$. Such a design measure is said to be D-optimal. More formally, if $\mathcal{H}$ is the class of all design measures on χ, then $\zeta^* \in \mathcal{H}$ is D-optimal with respect to $\underset{\sim}{\Sigma}$ if

$$|\underset{\sim}{M}(\zeta^*,\underset{\sim}{\Sigma})| = \sup_{\zeta\in\mathcal{H}} |\underset{\sim}{M}(\zeta,\underset{\sim}{\Sigma})|. \tag{14}$$

In addition to improving the precision of $\hat{\underset{\sim}{\beta}}$, continuous D-optimal design measures have the desirable property of minimizing the maximum of the variance of the predicted response over the experimental region χ. This latter property is the G-optimality criterion. The equivalence of the D-optimality and G-optimality criteria was first proved by Kiefer and Wolfowitz (1960) for the single-response case. An extension of their theorem to the multi-response case was proved by Fedorov (1972, p. 212).

3. THE CONSTRUCTION OF D-OPTIMAL DESIGNS WHEN $\underset{\sim}{\Sigma}$ IS NOT KNOWN

In the multiresponse extension of the Kiefer and Wolfowitz (1960) Equivalence Theorem as given by Fedorov (1972, p. 212), the following assertions are equivalent:

(i) The design measure ζ^* is D-optimal.

(ii) The design measure ζ^* is G-optimal, that is, it minimizes $\max_{\underset{\sim}{x} \in \chi} \operatorname{tr}[\underset{\sim}{\Sigma}^{-1} \underset{\sim}{V}(\underset{\sim}{x}, \zeta, \underset{\sim}{\Sigma})]$, $\zeta \in \mathbf{H}$.

(iii) $\max_{\underset{\sim}{x} \in \chi} \operatorname{tr}[\underset{\sim}{\Sigma}^{-1} \underset{\sim}{V}(\underset{\sim}{x}, \zeta^*, \underset{\sim}{\Sigma})] = p$

where

$$\underset{\sim}{V}(\underset{\sim}{x}, \zeta, \underset{\sim}{\Sigma}) = \underset{\sim}{\phi}'(\underset{\sim}{x}) \underset{\sim}{M}^{-1}(\zeta, \underset{\sim}{\Sigma}) \underset{\sim}{\phi}(\underset{\sim}{x}), \quad \underset{\sim}{x} \in \chi, \ \zeta \in \mathbf{H}, \tag{15}$$

and where $\underset{\sim}{\phi}(\underset{\sim}{x})$ and $\underset{\sim}{M}(\zeta, \underset{\sim}{\Sigma})$ are the same matrices as in (10), and p is the total number of parameters in the multiresponse model. It is to be noted that if $\hat{\underset{\sim}{Y}}(\underset{\sim}{x})$ is the vector of predicted responses given in (7), and if the design measure is discrete, then the matrix $\underset{\sim}{V}(\underset{\sim}{x}, \zeta, \underset{\sim}{\Sigma})$ is related to $\operatorname{var}[\hat{\underset{\sim}{Y}}(\underset{\sim}{x})]$ according to the expression

$$\underset{\sim}{V}(\underset{\sim}{x}, \zeta_{D_N}, \underset{\sim}{\Sigma}) = N \operatorname{var}[\hat{\underset{\sim}{Y}}(\underset{\sim}{x})].$$

We, therefore, refer to $\underset{\sim}{V}(\underset{\sim}{x}, \zeta, \underset{\sim}{\Sigma})$ as the prediction variance matrix. On the basis of this equivalence theorem, Fedorov (1972, Ch.5) developed an iterative procedure to construct a multireponse D-optimal design provided that $\underset{\sim}{\Sigma}$ is known. The main steps of his procedure are as follows (for convenience, throughout the remainder of this paper, we shall write ζ_N instead of ζ_{D_N} to denote a discrete design measure as in (9)):

(i) An initial nondegenerate design D_{N_0}, that is, a design for which $\underset{\sim}{M}(\zeta_{N_0}, \underset{\sim}{\Sigma})$ is nonsingular, is chosen. The design measure ζ_{N_0} is defined by assigning the weight $1/N_0$ to each point in D_{N_0}.

(ii) A design D_{N_0+N} is constructed from $D_{N_0+N-1} (N \geq 1)$ by augmenting it with the point $\underset{\sim}{x}_{N_0+N}$ which satisfies

$$\mathrm{tr}[\underset{\sim}{\Sigma}^{-1}\underset{\sim}{V}(\underset{\sim}{x}_{N_0+N},\zeta_{N_0+N-1},\underset{\sim}{\Sigma})] = \max_{\underset{\sim}{x}\in\chi} \mathrm{tr}[\underset{\sim}{\Sigma}^{-1}\underset{\sim}{V}(\underset{\sim}{x},\zeta_{N_0+N-1},\underset{\sim}{\Sigma})],$$

where $\underset{\sim}{V}$ is the matrix defined in (15), and the design measure ζ_{N_0+N} is defined by assigning the weight $1/(N_0+N)$ to each point in $D_{N_0+N}(N\geq 1)$.

The stopping point for this procedure is reached when an integer $N'\geq 1$ satisfying

$$\max_{\underset{\sim}{x}\in\chi} \mathrm{tr}[\underset{\sim}{\Sigma}^{-1}\underset{\sim}{V}(\underset{\sim}{x},\zeta_{N_0+N'-1},\underset{\sim}{\Sigma})] - p < \delta$$

is found, where δ is a small positive number chosen a priori. In other words, the procedure stops when $\max_{\underset{\sim}{x}\in\chi} \mathrm{tr}[\underset{\sim}{\Sigma}^{-1}\underset{\sim}{V}(\underset{\sim}{x},\zeta_{N_0+N-1},\underset{\sim}{\Sigma})]$ is sufficiently close to p. This is based on Assertion (iii) of the Equivalence Theorem by Fedorov (1972) and noting that by Assertion (ii), p is the minimum value of $\max_{\underset{\sim}{x}\in\chi} \mathrm{tr}[\underset{\sim}{\Sigma}^{-1}\underset{\sim}{V}(\underset{\sim}{x},\zeta,\underset{\sim}{\Sigma})]$ which is attained when the design measure is D-optimal.

The above procedure, however, requires knowledge of $\underset{\sim}{\Sigma}$. If $\underset{\sim}{\Sigma}$ is not known, a consistent estimator of $\underset{\sim}{\Sigma}$ can be used to construct a sequence of design measures which converges in probability to a D-optimal design measure with respect to $\underset{\sim}{\Sigma}$. A consistent estimator of $\underset{\sim}{\Sigma}$ was proposed by Zellner (1962) and is given by $\hat{\underset{\sim}{\Sigma}}_N = (\hat{\sigma}^N_{ij})$, where

$$N\hat{\sigma}^N_{ij} = (\underset{\sim}{Y}_i - \underset{\sim}{F}_i\hat{\underset{\sim}{\beta}}_i)'(\underset{\sim}{Y}_j - \underset{\sim}{F}_j\hat{\underset{\sim}{\beta}}_j), \quad i,j = 1,2,\ldots,r, \tag{16}$$

where $\underset{\sim}{F}_i$ is the $N\times p_i$ matrix in (2), and $\hat{\underset{\sim}{\beta}}_i$ is the ordinary least squares estimator $(\underset{\sim}{F}_i'\underset{\sim}{F}_i)^{-1}\underset{\sim}{F}_i'\underset{\sim}{Y}_i$ $(i = 1,2,\ldots,r)$ based on the ith individual response model in (2). We now define the matrix $\underset{\sim}{A}$ as

$$\underset{\sim}{A} = [\mathrm{diag}(\underset{\sim}{\Sigma}^{-1})]^{-1/2}\underset{\sim}{\Sigma}^{-1}[\mathrm{diag}(\underset{\sim}{\Sigma}^{-1})]^{-1/2}. \tag{17}$$

The following theorem (Wijesinha, 1984, Appendix D) implies that a

D-optimal design measure with respect to Σ is equivalent to a D-optimal design measure with respect to A^{-1}:

Theorem 1. If $M(\zeta,\Sigma)$ is the moment matrix in (10), then

$$|M(\zeta,\Sigma)| = \prod_{i=1}^{r} (\sigma^{ii})^{p_i} |M(\zeta,A^{-1})|, \ \zeta \in H, \ \Sigma^{-1} = (\sigma^{ij}),$$

where H is the class of all design measures defined on the region χ. It can be seen from the expression on the right-hand side that only $|M(\zeta,A^{-1})|$ depends on the design measure ζ. Hence, a design measure maximizes $|M(\zeta,A^{-1})|$ if and only if it maximizes $|M(\zeta,\Sigma)|$. It follows that Fedorov's (1972) sequential procedure to obtain a D-optimal design measure can be applied with Σ replaced by A^{-1}.

When Σ, and hence A, is unknown, we can modify Fedorov's procedure so that A is replaced by the estimate

$$\hat{A}_N = [\mathrm{diag}(\hat{\Sigma}_N^{-1})]^{-1/2} \ \hat{\Sigma}_N^{-1} \ [\mathrm{diag}(\hat{\Sigma}_N^{-1})]^{-1/2} \qquad (18)$$

where $\hat{\Sigma}_N$ is Zellner's (1962) estimate of Σ as given in (16). A sequential procedure is introduced in Section 3.1 for the construction of a D-optimal design in this case whereby $\hat{A}_N$ is reevaluated at each stage of the procedure. In Appendix E in Wijesinha (1984) it is shown that $\hat{A}_N$ is a consistent estimator of A.

The construction of a D-optimal design with respect to A^{-1} (instead of Σ) is more desirable for two reasons

(i) Since the elements of A lie between -1 and 1, it is expected that $\hat{A}_N$ reaches stability much faster than $\hat{\Sigma}_N^{-1}$ thereby giving rise to a rapidly convergent D-optimal design measure in the sequential procedure.

(ii) Since the diagonal elements of A are equal to unity, the number of elements of A to be estimated is reduced by r.

3.1 The Sequential Procedure When Σ Is Not Known

(i) Start with an initial design D_{N_0} such that $M(\zeta_{N_0}, I_r)$

is nonsingular, where $\underset{\sim}{I}_r$ is the identity matrix of order $r \times r$.

(ii) Once D_{N_0+N-1}, $N \geq 1$, is obtained,

(a) compute $\hat{\underset{\sim}{\Sigma}}_{N_0+N-1}$ and $\hat{\underset{\sim}{A}}_{N_0+N-1}$ on the basis of the observations on all r responses measured at the points of D_{N_0+N-1} using (16) and (18),

(b) construct the design measure ζ_{N_0+N-1} by assigning the weight $1/(N_0+N-1)$ to each point in D_{N_0+N-1}.

(iii) Construct D_{N_0+N} by augmenting D_{N_0+N-1} with the point $\underset{\sim}{x}_{N_0+N}$ which satisfies

$$\mathrm{tr}[\hat{\underset{\sim}{A}}_{N_0+N-1}\underset{\sim}{V}(\underset{\sim}{x}_{N_0+N},\ \zeta_{N_0+N-1},\ \hat{\underset{\sim}{A}}^{-1}_{N_0+N-1})]$$

$$= \max_{\underset{\sim}{x} \in \chi} \mathrm{tr}[\hat{\underset{\sim}{A}}_{N_0+N-1}\underset{\sim}{V}(\underset{\sim}{x},\ \zeta_{N_0+N-1},\ \hat{\underset{\sim}{A}}^{-1}_{N_0+N-1})],$$

where $\underset{\sim}{V}$ is the prediction variance matrix in (15).

(iv) Continue this procedure until an integer $N'(\geq 1)$ is reached such that

$$\max_{\underset{\sim}{x} \in \chi} \mathrm{tr}[\hat{\underset{\sim}{A}}_{N_0+N'-1}\underset{\sim}{V}(\underset{\sim}{x},\ \zeta_{N_0+N'-1},\ \hat{\underset{\sim}{A}}^{-1}_{N_0+N'-1})] - p < \delta$$

where δ is a small positive number chosen a priori, and p is the total number of parameters in the multiresponse model.

In Wijesinha (1984) it is shown that the above sequential procedure converges to a D-optimal design. More specifically, let $\mathcal{A}$ be the set of all $r \times r$ symmetric matrices $\underset{\sim}{A} = (a_{ij})$ such that $a_{ii} = 1$, $i = 1,2,\ldots,r$, and $-1 \leq a_{ij} \leq 1$, $1 \leq i < j \leq r$. Define $\underset{\sim}{b}(\underset{\sim}{A}) = (b_1, b_2, \ldots, b_{r'})'$, where $r' = r(r-1)/2$. This vector consists of the elements of $\underset{\sim}{A}$ above its diagonal taken in order from left to right for each row starting with the first. We call $\underset{\sim}{b}(\underset{\sim}{A})$ the r'-dimensional vector associated with $\underset{\sim}{A}$. Note that since $\underset{\sim}{A} \in \mathcal{A}$ is symmetric and all its diagonal elements are equal to 1, $\underset{\sim}{A}$

can be completely described by the r' elements a_{ij}, $1 \le i < j \le r'$. It is clear that $\underset{\sim}{A}$ and $\hat{\underset{\sim}{A}}_N$ defined in (17) and (18), respectively, belong to $\mathcal{A}$. Since $\hat{\underset{\sim}{A}}_N$ is a consistent estimator of $\underset{\sim}{A}$ (Wijesinha, 1984, Appendix E), then $\hat{e}_N$ converges in probability to 0, where $\hat{e}_N$ is the Euclidean distance between $\underset{\sim}{b}(\hat{\underset{\sim}{A}}_N)$ and $\underset{\sim}{b}(\underset{\sim}{A})$.

It is conjectured that the convergence in probability to 0 of $\hat{e}_N$ is sufficient for the above sequential procedure to converge. However, we were only able to prove convergence by assuming a stronger condition, namely that $\sum_{u=1}^{N} \hat{e}_u$ converges in probability to some random variable e. This can be formally stated as follows:

<u>Theorem 2</u>. Suppose that $\sum_{u=1}^{N} \hat{e}_u$ converges in probability to some random variable e. Then for a given $\delta > 0$, there exists an integer $N > 0$ such that

$$\max_{\underset{\sim}{x} \in \chi} \operatorname{tr}\left[\hat{\underset{\sim}{A}}_N \underset{\sim}{V}(\underset{\sim}{x}, \zeta_N, \hat{\underset{\sim}{A}}_N^{-1})\right] - p < \delta$$

with probability 1. The proof of this theorem is given in Wijesinha (1984). It is fairly long and will not be included in this paper.

4. <u>EXAMPLES</u>

In this section we present some examples to illustrate the procedure described in Section 3.1. In each example $\underset{\sim}{\Sigma}$ is predetermined and the error vector (assumed to be normally distributed with a zero mean vector an a variance-covariance matrix given by the direct product of $\underset{\sim}{\Sigma}$ with the identity matrix of a proper order) is computer generated. At the Nth $(N \geq 1)$ stage, the (i,j)th element of the matrix $\hat{\underset{\sim}{\Sigma}}_{N_0+N-1}$ described in (16) is calculated using the formula

$$(N_0+N-1)\,\hat{\sigma}_{ij}^{N_0+N-1} = \underset{\sim}{\varepsilon}_i'(\underset{\sim}{I}-\underset{\sim}{R}_i)'(\underset{\sim}{I}-\underset{\sim}{R}_j)\underset{\sim}{\varepsilon}_j, \quad 1 \le i,\ j \le r, \tag{19}$$

where $\underset{\sim}{R}_i = \underset{\sim}{F}_i(\underset{\sim}{F}_i'\underset{\sim}{F}_i)^{-1}\underset{\sim}{F}_i$ and $\underset{\sim}{F}_i$ is of order $(N_0+N-1) \times p_i$ $(i = 1,2,\ldots,r)$. The (i,j)th element of the corresponding $\hat{\underset{\sim}{A}}_{N_0+N-1}$ matrix is determined from (18) after substituting $\hat{\underset{\sim}{\Sigma}}_{N_0+N-1}$ for $\hat{\underset{\sim}{\Sigma}}_N$. It should be noted that although the matrix $\underset{\sim}{\Sigma}$ is used to generate the error vector $\underset{\sim}{\varepsilon}$, it is not used in the sequential generation of the D-optimal design. In an actual experimental situation, observed response values would be available, hence, $\hat{\sigma}_{ij}^{N_0+N-1}$ should be calculated using (16) instead of (19).

In all the examples we have considered, the final value of $\max_{\underset{\sim}{x}\in\chi} \operatorname{tr}[\hat{\underset{\sim}{A}}_{N_0+N-1}\underset{\sim}{V}(\underset{\sim}{x}, \zeta_{N_0+N-1}, \hat{\underset{\sim}{A}}^{-1}_{N_0+N-1})]$ met the stopping rule described in Theorem 2 for a value of δ determined a priori.

<u>Example 1</u>. *Consider an experiment involving three responses and three controllable variables.* The experimental region $\chi = \{\underset{\sim}{x} = (x_1,x_2,x_3): |x_i| \le 1,\ i = 1,2,3\}$ and the fitted models are

$$\begin{aligned} y_1 &= \beta_{10} + \beta_{11}x_1 + \beta_{12}x_2 + \varepsilon_1 \\ y_2 &= \beta_{20} + \beta_{21}x_1 + \beta_{22}x_2 + \beta_{23}x_3 + \varepsilon_2 \\ y_3 &= \beta_{30} + \beta_{31}x_1 + \beta_{32}x_2 + \varepsilon_3. \end{aligned} \tag{20}$$

When all the models are linear, $\operatorname{tr}[\underset{\sim}{A}^{-1}\underset{\sim}{V}(\underset{\sim}{x},\zeta,\underset{\sim}{A}^{-1})]$ for $\underset{\sim}{x} \in \chi$, $\zeta \in \mathbf{H}$, and $\underset{\sim}{A} \in \mathbf{A}$ is a convex function in χ, and since χ is a convex set, $\max_{\underset{\sim}{x}\in\chi} \operatorname{tr}[\underset{\sim}{A}^{-1}\underset{\sim}{V}(\underset{\sim}{x},\zeta,\underset{\sim}{A}^{-1})]$ will occur on one of the extremal points of χ. Therefore, the search for additional support points of the D-optimal design was restricted to the vertices of χ. Also, all the points of the initial design were chosen to be extremal points (see Table 1). For this example $\underset{\sim}{\Sigma}$ was chosen as

$$\underset{\sim}{\Sigma} = \begin{bmatrix} 3.000 & .030 & 1.600 \\ .030 & .600 & .800 \\ 1.600 & .800 & 3.300 \end{bmatrix}.$$

Therefore,

$$\underset{\sim}{\Sigma}^{-1} = \begin{bmatrix} .524 & .462 & -.366 \\ .462 & 2.870 & -.920 \\ -.366 & -.920 & .703 \end{bmatrix} \text{ and } \underset{\sim}{A} = \begin{bmatrix} 1 & .376 & -.602 \\ .376 & 1 & -.647 \\ -.602 & -.647 & 1 \end{bmatrix}.$$

TABLE 1

THE INITIAL DESIGN (EXAMPLE 1)

x_1	x_2	x_3
1	1	1
1	1	-1
1	-1	1
-1	1	1
-1	-1	1

TABLE 2

THE AUGMENTED DESIGN POINTS FOR A D-OPTIMAL DESIGN (EXAMPLE 1)

N_0+N	$\max_{\underset{\sim}{x}\in X} \operatorname{tr}[\hat{\underset{\sim}{A}}_{N_0+N-1}\underset{\sim}{V}(\underset{\sim}{x}, \zeta_{N_0+N-1}, \hat{\underset{\sim}{A}}^{-1}_{N_0+N-1})]$	x_1	x_2	x_3
6	22.1429	-1	-1	-1
7	14.0000	-1	1	-1
8	15.4000	1	-1	-1

Table 2 displays the augmented support points and corresponding max trace values. Using the design consisting of the five initial design points in Table 1 and the three augmented design points in Table 2, it was found that $\max_{\underset{\sim}{x} \in \chi} \mathrm{tr}[\hat{\underset{\sim}{A}}_8^{-1} \underset{\sim}{V}(\underset{\sim}{x}, \zeta_8, \hat{\underset{\sim}{A}}_8^{-1})]$ was equal to 10. The fast drop in the max trace function to its anticipated value of p=10 in this example is quite noteworthy.

In the following examples the maximization with respect to $\underset{\sim}{x}$ of the trace function at every iteration was carried out using a computer program based on the controlled random search procedure introduced by Price (1977). The procedure uses a random search to locate an optimal point from among a collection of points, the number of which is determined by the user.

Example 2. In this example we have two responses and two controllable variables. The experimental region is $\chi = \{\underset{\sim}{x} = (x_1, x_2): x_1^2 + x_2^2 \le 2\}$, and the fitted models are

$$\begin{aligned} y_1 &= \beta_{10} + \beta_{11}x_1 + \beta_{12}x_2 + \beta_{112}x_1x_2 + \varepsilon_1 \\ y_2 &= \beta_{20} + \beta_{21}x_1 + \beta_{22}x_2 + \beta_{212}x_1x_2 + \beta_{211}x_1^2 + \beta_{222}x_2^2 + \varepsilon_2. \end{aligned} \tag{21}$$

Thus p = 10. The points for the initial design were arbitrarily chosen and are given in Table 3. The matrix $\underset{\sim}{\Sigma}$ is given the value

$$\underset{\sim}{\Sigma} = \begin{bmatrix} .800 & .500 \\ .500 & 3.000 \end{bmatrix}$$

Hence,

$$\underset{\sim}{\Sigma}^{-1} = \begin{bmatrix} 1.395 & -.233 \\ -.233 & .372 \end{bmatrix} \quad \text{and} \quad \underset{\sim}{A} = \begin{bmatrix} 1 & -.323 \\ -.323 & 1 \end{bmatrix}.$$

TABLE 3

THE INITIAL DESIGN (EXAMPLE 2)

x_1	x_2
1.0	1.0
1.0	-1.0
-1.0	1.0
-1.0	-1.0
0.0	0.5
0.5	0.0
0.0	0.0

TABLE 4

THE AUGMENTED DESIGN FOR A D-OPTIMAL DESIGN (EXAMPLE 2)

N_0+N	$\max_{\underset{\sim}{x} \in \chi} tr[\hat{\underset{\sim}{A}}_{N_0+N-1} \underset{\sim}{V}(\underset{\sim}{x}, \zeta_{N_0+N-1}, \hat{\underset{\sim}{A}}^{-1}_{N_0+N-1})]$	x_1	x_2	$x_1^2 + x_2^2$
8	257.7074	0.0137	-1.414	1.999
9	28.3742	-1.414	-0.095	2.000
10	20.9817	1.409	-0.122	2.000
11	20.0266	-0.025	1.414	2.000
12	13.9047	1.029	0.969	2.000
13	14.4880	-1.009	0.991	2.000
14	14.8490	-1.002	-0.997	1.999
15	15.0983	0.939	-1.057	2.000
16	11.1210	-1.127	0.847	1.987
17	11.8267	0.746	1.201	2.000
18	12.2723	-0.911	-1.081	2.000
19	12.6633	1.391	-0.252	1.999
20	12.5054	0.475	-1.332	2.000
21	11.1222	-1.376	-0.327	2.000
22	11.3869	-0.793	1.170	1.999
23	11.5757	0.968	1.030	2.000
24	11.0369	1.136	-0.837	1.991
25	10.0579	-0.033	-0.033	0.002

As shown in Table 4, $\max_{\underset{\sim}{x} \in \chi} tr[\hat{\underset{\sim}{A}}_{24} \underset{\sim}{V}(\underset{\sim}{x}, \zeta_{24}, \hat{\underset{\sim}{A}}_{24}^{-1})]$ satisfies the stopping rule in Theorem 2 with $\delta = .06$. We conclude that the design points in Table 4 together with the initial design points form a nearly D-optimal design. In Table 5 we can see the change in the values of the elements of the $\hat{\underset{\sim}{\Sigma}}$, $\hat{\underset{\sim}{\Sigma}}^{-1}$, and $\hat{\underset{\sim}{A}}$ matrices.

TABLE 5

THE ESTIMATES FOR $\underset{\sim}{\Sigma}$, $\underset{\sim}{\Sigma}^{-1}$, and $\underset{\sim}{A}$ (EXAMPLE 2)

N_0+N-1	$\hat{\sigma}_{11}$	$\hat{\sigma}_{12}$	$\hat{\sigma}_{22}$	$\hat{\sigma}^{11}$	$-\hat{\sigma}^{12}$	$\hat{\sigma}^{22}$	$-\hat{a}_{12}$
7	.258	.030	.078	4.061	1.551	13.477	.210
8	.275	.080	.385	3.872	0.807	2.767	.247
9	.266	.131	.418	4.447	1.396	2.832	.393
10	.519	-.052	.532	1.945	-0.189	1.899	.098
11	.577	.162	1.213	1.801	0.240	0.857	.193
12	.772	-.024	1.215	1.296	-0.026	0.823	.025
13	.713	-.028	1.197	1.404	-0.032	0.836	.030
14	.669	.125	2.352	1.510	0.081	0.430	.100
15	.622	.091	2.305	1.617	0.064	0.436	.076
16	.757	.125	2.164	1.333	0.077	0.467	.097
17	.710	.128	2.096	1.425	0.087	0.482	.105
18	.828	.494	2.903	1.338	0.223	0.382	.312
19	.831	.720	3.514	1.462	0.299	0.346	.421
20	.816	.660	3.343	1.459	0.288	0.356	.400
21	.525	.414	3.005	2.137	0.295	0.374	.330
22	.753	.515	3.270	1.489	0.235	0.343	.328
23	.808	.485	3.368	1.353	0.195	0.325	.280
24	.760	.459	3.210	1.440	0.206	0.341	.294

Example 3. Here the responses and the controllable variables are the same as in Example 2. The experimental region is $\chi = \{\underset{\sim}{x}=(x_1,x_2) : -\sqrt{2} \leq x_1,x_2 \leq \sqrt{2}\}$ and

$$\underset{\sim}{\Sigma} = \begin{bmatrix} 1.000 & .900 \\ .900 & 3.000 \end{bmatrix}.$$

Thus,

$$\underset{\sim}{\Sigma}^{-1} = \begin{bmatrix} 1.370 & -0.411 \\ -0.411 & .457 \end{bmatrix} \text{ and } \underset{\sim}{A} = \begin{bmatrix} 1 & -.520 \\ -.520 & 1 \end{bmatrix}.$$

The fitted models are

$$\begin{aligned} y_1 &= \beta_{10} + \beta_{11}x_1 + \beta_{12}x_2 + \beta_{112}x_1x_2 + \varepsilon_1 \\ y_2 &= \beta_{20} + \beta_{21}x_1 + \beta_{22}x_2 + \beta_{212}x_1x_2 + \beta_{211}x_1^2 + \beta_{222}x_2^2 + \varepsilon_2. \end{aligned} \tag{22}$$

The initial design for this example was chosen arbitrarily and is given in Table 6.

TABLE 6

THE INITIAL DESIGN (EXAMPLE 3)

x_1	x_2
1	1
1	-1
-1	1
-1	-1
0	-1.414
1.414	0
0	0

A nearly D-optimal design for this example consists of the augmented design points given in Table 7 and the initial design points given in Table 6. At the 15th iteration ($N_0 + N = 22$ in Table 7) the stopping rule is satisfied with $\delta = .07$. The elements of $\hat{\underset{\sim}{\Sigma}}$, $\hat{\underset{\sim}{\Sigma}}^{-1}$, and $\hat{\underset{\sim}{A}}$ at these iterations are given in Table 8.

TABLE 7

THE AUGMENTED DESIGN POINTS FOR A D-OPTIMAL DESIGN (EXAMPLE 3)

N_0+N	$\max_{x \in X} tr[\hat{A}_{N_0+N-1} V(x, \zeta_{N_0+N-1}, \hat{A}_{N_0+N-1})]$	x_1	x_2
8	39.0014	-1.414	1.414
9	45.5963	-1.414	-1.414
10	41.6899	1.414	-1.414
11	33.3881	1.414	1.414
12	15.1616	-1.414	-1.414
13	15.9091	1.414	-1.414
14	17.1823	-1.414	1.414
15	14.8294	0.059	-1.414
16	17.6392	1.414	1.414
17	14.1912	-1.414	0.002
18	12.4739	-1.414	-1.414
19	13.0994	-1.414	1.414
20	13.7740	1.414	1.414
21	14.3783	1.414	-1.414
22	10.0685	-1.405	1.384

TABLE 8

THE ESTIMATES FOR Σ, Σ^{-1}, AND A (EXAMPLE 3)

N_0+N-1	$\hat{\sigma}_{11}$	$\hat{\sigma}_{12}$	$\hat{\sigma}_{22}$	$\hat{\sigma}^{11}$	$-\hat{\sigma}^{12}$	$\hat{\sigma}^{22}$	$-\hat{a}_{12}$
7	.347	.821	2.390	15.457	5.311	2.243	.902
8	.314	.745	2.111	19.429	6.857	2.893	.914
9	.366	.656	1.888	7.218	2.507	1.400	.789
10	.743	.373	1.863	1.496	0.300	0.597	.317
11	.694	.405	1.753	1.666	0.385	0.659	.367
12	.701	.277	1.705	1.525	0.248	0.627	.254
13	.643	.280	1.577	1.685	0.299	0.687	.278
14	.671	.563	2.884	1.781	0.347	0.414	.404
15	.634	.553	2.716	1.917	0.390	0.448	.421
16	.738	.506	2.526	1.571	0.314	0.459	.370
17	.977	.856	3.166	1.342	0.363	0.414	.487
18	.815	.855	3.607	1.634	0.387	0.369	.499
19	.816	.950	3.906	1.708	0.415	0.357	.532
20	.791	.880	3.714	1.717	0.407	0.366	.513
21	.759	.823	3.546	1.762	0.409	0.377	.502

4.1 Choice of the Initial Design.

It is interesting to note that in the above examples, most of the augmented support points of the D-optimal designs are boundary points of the experimental region. This suggests that the boundary of the experimental region may be an optimal location for the support points of a D-optimal design. Therefore, boundary points of χ can be appropriately chosen as initial design points. In order to investigate this possibility, Example 3 was again considered with an initial design consisting of boundary points of χ. The results given in Example 4 below indicate that the use of the new initial designs can reduce the number of iterations required for the convergence of the procedure.

Example 4. The models, the experimental region, and the value of $\underset{\sim}{\Sigma}$ for this example are as in Example 3. The initial design is given in Table 9.

TABLE 9

THE INITIAL DESIGN (EXAMPLE 4)

x_1	x_2
1.414	1.414
1.414	-1.414
-1.414	1.414
-1.414	-1.414
0.000	1.414
1.414	0.000
0.000	-1.414

This example shows that the use of an initial design consisting of boundary points of χ reduces the number of iterations required to stop the procedure. The stopping rule was first satisfied with $\delta = .02$ at the 2nd iteration ($N_0 + N=9$ in Table 10). However, the value of the max trace function at this iteration was not stable enough as can be seen from Table 10. This is also reflected by the lack of stability in the values of the elements of $\hat{\underset{\sim}{\Sigma}}$,$\hat{\underset{\sim}{\Sigma}}^{-1}$, and $\hat{\underset{\sim}{A}}$ (see Table 11). The sequential procedure was, therefore, continued until the 11th iteration ($N_0+N = 18$ in Table 10) at which the stopping rule was satisfied with $\delta = .06$.

TABLE 10

THE AUGMENTED DESIGN FOR A D-OPTIMAL DESIGN (EXAMPLE 4)

N_0+N	$\max_{\underset{\sim}{x} \in X} tr[\hat{\underset{\sim}{A}}_{N_0+N-1} \underset{\sim}{V}(\underset{\sim}{x}, \zeta_{N_0+N-1}, \hat{\underset{\sim}{A}}^{-1}_{N_0+N-1})]$	x_1	x_2
8	16.8823	-1.414	0.000
9	10.0199	0.000	-0.001
10	13.5012	-1.414	1.414
11	14.8885	1.414	-1.414
12	16.2449	1.414	1.414
13	17.5928	-1.414	-1.414
14	10.9800	-1.414	1.414
15	11.8062	1.414	-1.414
16	12.6181	1.414	1.414
17	13.4383	-1.414	-1.414
18	10.0505	1.414	1.414

TABLE 11

THE ESTIMATES FOR $\underset{\sim}{\Sigma}$, $\underset{\sim}{\Sigma}^{-1}$, AND $\underset{\sim}{A}$ (EXAMPLE 4)

N_0+N-1	$\hat{\sigma}_{11}$	$\hat{\sigma}_{12}$	$\hat{\sigma}_{22}$	$\hat{\sigma}^{11}$	$-\hat{\sigma}^{12}$	$\hat{\sigma}^{22}$	$-\hat{a}_{12}$
7	0.309	0.137	0.304	4.039	1.821	4.111	.447
8	0.294	0.399	0.752	12.255	6.506	4.784	.848
9	0.257	0.478	1.26	13.020	4.913	2.644	.837
10	0.454	0.199	1.522	2.334	0.306	0.697	.239
11	0.419	0.210	1.651	2.552	0.325	0.647	.252
12	1.067	0.777	2.508	1.210	0.375	0.515	.475
13	1.751	0.861	2.090	0.716	0.295	0.600	.450
14	1.499	1.081	3.105	0.890	0.310	0.430	.501
15	1.919	1.249	3.065	0.709	0.289	0.444	.515
16	1.577	1.032	2.781	0.838	0.311	0.475	.493
17	1.569	1.000	2.653	0.838	0.316	0.496	.490

5. CONCLUDING REMARKS

The main advantage of the sequential procedure we have proposed is that Σ (the variance-covariance matrix of the responses) is not required to be known. The basic idea used in the sequential procedure is to choose the point $\underset{\sim}{x}_{N_0+N}$ which maximizes the trace function, that is,

$$\mathrm{tr}[\hat{\underset{\sim}{A}}_{N_0+N-1}\underset{\sim}{V}(\underset{\sim}{x}_{N_0+N},\ \zeta_{N_0+N-1},\ \hat{\underset{\sim}{A}}^{-1}_{N_0+N-1})] =$$

$$\max_{\underset{\sim}{x}\in\chi} \mathrm{tr}[\hat{\underset{\sim}{A}}_{N_0+N-1}\underset{\sim}{V}(\underset{\sim}{x},\ \zeta_{N_0+N-1},\ \hat{\underset{\sim}{A}}^{-1}_{N_0+N-1})]$$

where N_0 is the number of points in the initial design. The procedure is continued until $\max_{\underset{\sim}{x}\in\chi} \mathrm{tr}[\hat{\underset{\sim}{A}}_{N_0+N-1}\underset{\sim}{V}(\underset{\sim}{x},\ \zeta_{N_0+N-1},$ $\hat{\underset{\sim}{A}}^{-1}_{N_0+N-1})]$ is sufficiently close to p.

The examples described earlier show that our procedure has a fast rate of convergence in that the quantity

$$\max_{\underset{\sim}{x}\in\chi} \mathrm{tr}[\hat{\underset{\sim}{A}}_{N_0+N-1}\underset{\sim}{V}(\underset{\sim}{x},\ \zeta_{N_0+N-1},\ \hat{\underset{\sim}{A}}^{-1}_{N_0+N-1})]$$

reduces to its anticipated limit, namely p quite rapidly. In addition, a comparison of the estimated values of $\hat{\underset{\sim}{\Sigma}}^{-1}_{N_0+N-1}$ and $\hat{\underset{\sim}{A}}_{N_0+N-1}$ demonstrate that $\hat{\underset{\sim}{A}}_{N_0+N-1}$ stabilizes much faster. This supports the idea of using $\hat{\underset{\sim}{A}}^{-1}_{N_0+N-1}$ in the procedure in place of $\hat{\underset{\sim}{\Sigma}}_{N_0+N-1}$.

The examples also indicate that the use of initial designs consisting of boundary points of χ does reduce the number of iterations required to meet the stopping rule. Therefore, the boundary of the experimental region can be an appropriate choice for the selection of the initial design points. It should be noted, however, that this is a conjecture based only on the above examples and has no theoretical justification. We feel that this is a topic which should be investigated in future research.

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