Construction of Optimal Designs to Increase the Power of the Multiresponse Lack of Fit Test.

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This paper introduces two design criteria to improve the power of the multivariate lack of fit test for a linear multiresponse model. An algorithm is presented for the generation of optimal designs on the basis of these criteria.
CONSTRUCTION OF OPTIMAL DESIGNS TO INCREASE THE POWER
OF THE MULTIRESPONSE LACK OF FIT TEST

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Abstract: Two design criteria are introduced to improve the power of the
multivariate lack of fit test for a linear multiresponse model. These
criteria are extensions of the $A_1$ and $A_2$-optimality criteria discussed by
Jones and Mitchell (1978) for the single-response case. A procedure is
presented for the generation of an optimal design based on the $A_2$-
criterion.

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Multivariate lack of fit test.

1. Introduction

Detection of model inadequacy is an important consideration in the
modeling of a multiresponse function. Khuri (1985) developed a multivariate
test for lack of fit for a linear multiresponse model. The test provides a
comprehensive assessment of the adequacy of all the single-response functions associated with the multiresponse model. He also gave a procedure for determining which responses are responsible for lack of fit when the lack of fit test is significant.

In Section 2 we introduce some notation and briefly discuss Khuri's (1985) lack of fit test. In Section 3 we develop two design criteria, $A_1$ and $A_2$-optimality, to increase the power of this test. In Section 4 an iterative procedure developed by Silvey (1980) is used to obtain $A_2$-optimal designs. Numerical examples are presented in Section 5.

2. The Multiresponse Lack of Fit Test

2.1 Notation

Let $N$ be the total number of experimental runs and $r$ be the number of responses. We assume that each response depends on all or some of $k$ controllable variables denoted by $x_1, x_2, \ldots, x_k$. The fitted $i$th response model is represented as

$$E(Y_i) = X_i \beta_i, \quad i = 1, 2, \ldots, r,$$

(1)

where $Y_i$ is an $N \times 1$ vector of observations on the $i$th response, $E(Y_i)$ denotes the expected value of $Y_i$ under the fitted model, $X_i$ is an $N \times p_i$ matrix of rank $p_i$ of known functions of the settings of the controllable variables, and $\beta_i$ is a $p_i \times 1$ vector of unknown parameters ($i = 1, 2, \ldots, r$).

We suppose that the model for the true $i$th response mean ($i = 1, 2, \ldots, r$) is of the form

$$E_t(Y_i) = X_i \beta_i + Z_i \gamma_i, \quad i = 1, 2, \ldots, r,$$

(2)

where $E_t(Y_i)$ denotes the expected value of $Y_i$ under the true model, $Z_i$ is an $N \times q_i$ matrix of known functions of the settings of the controllable variables,
and $\chi_1$ is a vector of unknown parameters. If the fitted model (1) is correct, then $\chi_1$ will be equal to the zero vector.

The models given in (1) and (2) can be expressed as

$$E_a(\chi) = X_0 \beta$$

$$E_\varepsilon(\chi) = X_0 \beta + \varepsilon,$$

where $\chi = [\chi_1: \chi_2: \ldots: \chi_r]$, $X = [X_1: X_2: \ldots: X_r]$, $\varepsilon = [\varepsilon_1: \varepsilon_2: \ldots: \varepsilon_r]$, $\beta = \text{diag}(\beta_1, \beta_2, \ldots, \beta_r)$, and $\Gamma = \text{diag}(\chi_1, \chi_2, \ldots, \chi_r)$. The matrices $\chi, X, \varepsilon, \beta,$ and $\Gamma$ are of orders $N \times r, N \times p, N \times q, p \times r,$ and $q \times r,$ respectively, where $r = \sum_1^r p_i, q = \sum_1^r q_i,$ and $\chi$ is of rank $\rho (< p)$. The rows of $\chi$ are independent observations from multivariate normal populations with a common nonsingular variance-covariance matrix $\Sigma$ of order $r \times r$. Under the true model, $\chi$ has a mean given by (4) and a variance-covariance matrix $I_N \otimes \Sigma$.

For the development of the lack of fit test we assume that replicated observations are available on all $r$ responses at some points in the experimental region. Without loss of generality, it will be assumed that such replicated observations are obtained at each of the first $n$ design points, where $1 < n < N$. The number of repeated observations at the $i$th design point is denoted by $v_i$ ($v_i > 2, i = 1, 2, \ldots, n$) and the total number of repeated observations is $v = \sum_1^n v_i$.

2.2 Khuri's (1985) Lack of Fit Test

Let $X_0$ denote the matrix which consists of the columns of $X$ that correspond to all distinct terms in the $r$ fitted models given in (1). The columns of $X_0$ span the column space of $X$. We, therefore, consider that $X_0$ is of full column rank equal to $\rho$, the rank of $X$. Khuri (1985) developed a multivariate lack of fit test for the multiresponse model (3) using
where
\[
\mathbf{Q}_1 = \mathbf{Y}'\left[\mathbf{I}_N - \mathbf{X}_0'\left(\mathbf{X}_0\mathbf{X}_0'\right)^{-1}\mathbf{X}_0\right]^{-1}\mathbf{Y}
\]

(5)

\[
\mathbf{Q}_2 = \mathbf{Y}'\mathbf{Y}.
\]

In the above equations, \( \mathbf{X} = \text{diag}(\mathbf{K}_1, \mathbf{K}_2, \ldots, \mathbf{K}_n, \mathbf{0}) \) is of order \( N \times N \) with \( \mathbf{0} \) being a zero matrix of order \((N-v) \times (N-v)\) and \( \mathbf{K}_i = \mathbf{I}_{v_i} - \left(1/v_i\right)\mathbf{Z}_{v_i} \), where \( \mathbf{I}_{v_i} \) is the identity matrix of order \( v_i \times v_i \) and \( \mathbf{Z}_{v_i} \) is the matrix of ones of order \( v_i \times v_i \) \((i=1,2,\ldots,n)\). Three other test statistics can also be employed to test lack of fit; they are: (1) Wilks's likelihood ratio, \( |\mathbf{Q}_2|/|\mathbf{Q}_1 + \mathbf{Q}_2| \); (2) Pillai's trace, \( \text{tr} [\mathbf{Q}_1 (\mathbf{Q}_1 + \mathbf{Q}_2)^{-1}] \); and (3) Hotelling-Lawley's trace, \( \text{tr} (\mathbf{Q}_1 \mathbf{Q}_2^{-1}) \), where \( | | \) and \( \text{tr} \) denote the determinant and the trace of a matrix, respectively.

3. Development of Design Criteria

It is known that \( \mathbf{Q}_2 \) has the central Wishart distribution with
\[ n \varepsilon_{\text{PE}} = \sum_{i=1}^{n} (v_i - 1) \] degrees of freedom; \( \mathbf{Q}_1 \) is independent of \( \mathbf{Q}_2 \) and has the noncentral Wishart distribution with \( n \varepsilon_{\text{LF}} = (N-v - n \varepsilon_{\text{PE}}) \) degrees of freedom and a noncentrality parameter matrix given by

\[
\Omega = \mathbf{Z}^{-1}\mathbf{Y}'\mathbf{Y}\left[\mathbf{I}_N - \mathbf{X}_0'\left(\mathbf{X}_0\mathbf{X}_0'\right)^{-1}\mathbf{X}_0\right]^{-1}\mathbf{Z}\mathbf{Z}'.
\]

(6)

The power of the lack of fit test, based upon any of the four multivariate test statistics mentioned earlier, is a monotone increasing function of the eigenvalues of \( \Omega \) (see Roy et al. 1971, p. 68). Therefore, the power of this test can be increased by increasing the trace of \( \Omega \). However, the choice of the design which maximizes the trace of \( \Omega \) depends on the matrices \( \mathbf{Z} \) and \( \mathbf{Y} \) which are unknown. Thus, we are faced with the problem of finding an
expression independent of \( \mathcal{X} \) and \( \mathcal{Y} \) which, when maximized, results in an increase in the trace of \( \Omega \). This expression is found as follows: It is easy to show that

\[
\text{tr}(\Omega) > e_{\text{min}}(\mathcal{X}^{-1}) \text{tr}[\mathcal{X}' \mathcal{Z}'(I_N - \mathcal{X}_0 \mathcal{X}_0^{-1} \mathcal{X}_0') \mathcal{X}_0],
\]

(7)

where \( e_{\text{min}} \) denotes the smallest eigenvalue of the matrix inside parentheses. Inequality (7) can be rewritten as (see the Appendix)

\[
\text{tr}(\Omega) > e_{\text{min}}(\mathcal{X}^{-1}) \mathcal{Y}'(I_r \otimes \mathbf{A}) \mathcal{Y},
\]

(8)

where

\[
\mathcal{Y} = [\mathcal{Y}_1; \mathcal{Y}_2; \ldots; \mathcal{Y}_r],
\]

(9)

\[
\mathcal{A} = \mathcal{Z}_0'[I_N - \mathcal{X}_0 \mathcal{X}_0^{-1} \mathcal{X}_0'] \mathcal{Z}_0,'
\]

(10)

\[
\mathcal{L} = \text{diag}(\mathcal{H}_1', \mathcal{H}_2', \ldots, \mathcal{H}_r').
\]

(11)

In (10), \( \mathcal{Z}_0 \) is a matrix of order \( N \times p_1 (p_1 < q) \) whose columns form a basis for the column space of \( \mathcal{Z} = [\mathcal{Z}_1; \mathcal{Z}_2; \ldots; \mathcal{Z}_r]. \) Thus,

\[
\mathcal{Z}_1 = \mathcal{Z}_0 \mathcal{H}_1, \quad i = 1, 2, \ldots, r,
\]

(12)

where \( \mathcal{H}_i \) is matrix of order \( p_1 \times q_i \).

Since \( e_{\text{min}}(\mathcal{X}^{-1}) \) is a constant, the maximization of the quantity

\[
\Lambda = \mathcal{Y}' \mathcal{L} (I_r \otimes \mathbf{A}) \mathcal{L}' \mathcal{Y}
\]

(13)

will result in an increase in the trace of \( \Omega \). Still, however, the choice of design to maximize \( \Lambda \) depends on \( \mathcal{Y} \) which is unknown. In order to overcome this problem we apply the maximin method proposed by Atkinson and Fedorov (1975) and used by Jones and Mitchell (1978) in the single-response case. The maximin method consists of choosing a design which maximizes \( \Lambda_1 \), the minimum of \( \Lambda \) with respect to \( \mathcal{Y} \) over a specified region \( \tau \) in the \( \mathcal{Y} \)-space. The specification of the region \( \tau \) depends on a quantity \( \tau \) considered as a measure
of the inadequacy of the fitted model and is defined as follows: Suppose the
uth rows of $X_i$ and $Z_i$ ($i=1,2,\ldots,r; u=1,2,\ldots,N$) in (2) can be represented as
$f_i^+(x_u)$ and $g_i^+(x_u)$, respectively, then the fitted and true response functions
associated with (1) and (2) are $f_i^+(x)Z_i$ and $f_i^+(x)Z_i + g_i^+(x)Z_i$ ($i = 1,2,\ldots,r$),
respectively. We express $\tau$ as $\tau = \chi^T T \chi$, where

$$T = \text{diag}(T_1, T_2, \ldots, T_r)$$

(14)

with $T_i = \mu_i - \frac{1}{2} \mu_i (\mu_i)^{-1} \mu_i$ and the $\mu_i$ ($k, \ell = 1,2$) are the region moment
matrices defined by $\mu_i = \int f_i^+(x)Z_i f_i^+(x)Z_i dx$, $\mu_{12} = \int f_i^+(x)Z_i g_i^+(x)Z_i dx$,
$\mu_{21} = \mu_{22} = \int g_i^+(x)Z_i f_i^+(x)Z_i dx$, and $\mu_{22} = \mu_{22} = \int g_i^+(x)Z_i g_i^+(x)Z_i dx$, where $S^{-1} = \int dx$ and $X$
denotes the experimental region. This is a multiresponse extension of the
expression for $\tau$ given by Jones and Mitchell (1978). It is a measure of the
inadequacy of the fitted models given in (1) and is positive whenever the
fitted model is inadequate, otherwise, it is equal to zero.

3.1 $A_1$-Optimality

If the fitted model is inadequate, then $\tau > \delta$ for some constant $\delta > 0$. We
define $\pi = \{Y: \chi^T \chi > \delta\}$. The first design criterion is to maximize $A_1$ where

$$A_1 = \inf_{Y \in \pi} \left\{ \chi^T L_1 (I_r \otimes A) L_1^T \chi \right\}.$$  

(15)

This is a multiresponse extension of the $A_1$-optimality criterion proposed by
Jones and Mitchell (1978). As in Jones and Mitchell (1978), $A_1$ can be
expressed as

$$A_1 = \delta e_{\min}\left[ T^{-1} L_1 (I_r \otimes A) L_1^T \right].$$

(16)

A design which maximizes $e_{\min}\left[ T^{-1} L_1 (I_r \otimes A) L_1^T \right]$ is called a $A_1$-optimal
design. Note that there are situations in which $e_{\min}\left[ T^{-1} L_1 (I_r \otimes A) L_1^T \right]$ is equal
to zero for any choice of design. This occurs, for example, when \( r(N-p) < q \), where \( p \) is the number of columns of \( X_0 \) and \( q = \sum_{i=1}^{r} q_i \) is the number of columns in \( Z \) in (4), or the number of rows of the matrix \( L \) in (11). In this case the rank of the \( q \times q \) matrix \( T^{-1}_r L(I_r \otimes A)L' \) is less than or equal to \( r(N-p) \) which is less than \( q \). This matrix is, therefore, singular. Thus, \( L_1 \)-optimal designs can only be obtained under certain conditions. This leads us to propose a second design criterion which can be applied in more general situations.

3.2 \( A_2 \)-Optimality

Our second design criterion is to maximize \( \Lambda_2 \), the average of \( \Lambda \) (instead of the minimum of \( \Lambda \)) over the contour \( \tau = \delta \), i.e., we propose to select a design which maximizes

\[
\Lambda_2 = \int_{\pi_0} \chi^T L(I_r \otimes A)L' \chi \, dG / \int_{\pi_0} dG,
\]

where \( dG \) is the differential of the area on the surface of the ellipsoid \( \pi_0 = \{ \chi: \chi^T T \chi = \delta \} \). Using an identity stated in Jones and Mitchell (1978, p. 544) we have that

\[
\Lambda_2 = q^{-1} \delta A_2', \quad \text{where} \quad A_2' = \text{tr} \{ T^{-1}_r L(I_r \otimes A)L' \}.
\]

A design which maximizes \( \Lambda_2 \), or \( A_2' \), is called a \( A_2 \)-optimal (\( A_2' \)-optimal) design. Since \( q \) and \( \delta \) are constants it is clear that \( A_2 \)-optimal designs and \( A_2' \)-optimal designs are equivalent. We note that the \( A_2 \)-optimality criterion amounts to maximizing the sum of the eigenvalues of \( T^{-1}_r L(I_r \otimes A)L' \); hence, it can be applied even when this matrix has a zero eigenvalue.

If the number of design points, \( N \), is fixed beforehand, a \( A_2 \)-optimal design can be obtained by maximizing \( A_2' \) with respect to the \( N_k \) design setting (coordinates of the \( N \) design points). However, this may lead to computational difficulties especially for large values of \( N \) or \( k \). Therefore, an iterative
procedure by which design points can be chosen one at a time would be quite desirable. In the next section we develop such a procedure by using single-response optimal design theory.

4. The Generation of $\Lambda^2_{opt}$-Optimal Designs

4.1 Design Theory

Consider the single-response model

$$E(y_{x}) = h'(x)\varnothing,$$

where $y_{x}$ denotes the response value at a point $x = (x_1, x_2, \ldots, x_k)'$, the elements of the $m \times 1$ vector $h'(x)$ are functions of $x_1, x_2, \ldots, x_k$ defined over some experimental region $\chi$, a compact subset of the $k$-dimensional Euclidean space, and $\varnothing$ is a vector of unknown parameters. We assume that $\text{Var}(y_{x}) = \sigma^2$, $\text{Cov}(y_{x_1}, y_{x_2}) = 0$ for $x_1, x_2 \in \chi, x_1 \neq x_2$. Let $\mathcal{H}$ be the set of all design measures defined on $\chi$. Then the information matrix $M(\zeta), \zeta \in \mathcal{H}$, is defined as

$$M(\zeta) = \int \frac{h(x)h'(x)\zeta(dx)}{\chi}.$$

The family of matrices, $\mathbb{M} = \{M(\zeta): \zeta \in \mathcal{H}\}$, is convex (Silvey 1980, p. 16). By Caratheodory's Theorem, for any design measure $\zeta$, the matrix $M(\zeta)$ can be represented in the form

$$M(\zeta) = \sum_{u=1}^{s} \lambda_u h(x_u)h'(x_u),$$

where $x_u \in \chi (u = 1, 2, \ldots, s), s < m^* = [m(m+1)/2] + 1$, and $0 < \lambda_u < 1$ with $\sum_{u=1}^{s} \lambda_u = 1$ (see Silvey 1980, pp. 15-16). Thus, for a given $\zeta \in \mathbb{M}$ and $\tilde{\lambda} \in U = \{\tilde{\lambda}: \tilde{\lambda} = (\lambda_1, \lambda_2, \ldots, \lambda_{m^*})' \text{ such that } 0 < \lambda_u < 1 \text{ and } \sum_{u=1}^{s} \lambda_u = 1\}$, there exists a point $y^* = (\lambda_1^*, x_1^*, x_2^*, \ldots, x_{m^*}^*)$ in $U \times \chi^{m^*}$ that is associated with $M(\zeta)$. Note that in $\tilde{\lambda}$, $\lambda_u = 0$ for $s < u < m^*$. If $\phi$ is a real-valued function bounded from above on $\mathbb{M}$, then a design measure $\zeta^*$ is said to be
\( \phi \)-optimal if

\[
\phi[M(\zeta^*)] = \sup_{\zeta \in H} \phi[M(\zeta)]. \tag{22}
\]

Silvey (1980, ch. 4) presented an iterative procedure to obtain \( \phi \)-optimal designs. The basic idea used in this procedure (Silvey 1980, p. 29) is as follows: Suppose \( D_N = \{x_1, x_2, \ldots, x_N\} \) represents an \( N \)-point discrete design and \( \zeta_N \) is the design measure obtained by attaching the mass \( \lambda_u = \frac{1}{N} \) (\( u = 1, 2, \ldots, N \)) to each design point in \( D_N \). Start with an initial \( N_0 \)-point design such that \( \phi[M(\zeta_{N_0}^* \}) > -\infty \). Once \( D_N \), hence \( \zeta_N, N > N_0 \), has been determined, choose the design point \( x_{N+1} \) such that

\[
F_\phi [M(\zeta_N), h(x_{N+1})n(x_{N+1})] = \sup_{x \in X} F_\phi [M(\zeta_N), h(x)n(x)], \tag{23}
\]

where for \( M_1, M_2 \in M \), \( F_\phi (M_1 \rightarrow M_2) \) is the Fréchet derivative of \( \phi \) at \( M_1 \) in the direction of \( M_2 \) and is defined as

\[
F_\phi (M_1 \rightarrow M_2) = \lim_{\varepsilon \to 0^+} \frac{1}{\varepsilon} [\phi[(1-\varepsilon)M_1 + \varepsilon M_2] - \phi(M_1)]. \tag{24}
\]

The procedure is stopped when \( \sup_{x \in X} F_\phi [M(\zeta_N), h(x)n(x)] \) is less than some small positive preset value for some \( N^* > N_0 \). This stopping rule is based on the following lemma (Silvey 1980, p. 22):

**Lemma 1.** Let \( \phi \) be concave on \( M \) and differentiable on \( M^* = \{M(\zeta) \in M | \zeta(\zeta) \in M \} \) and \( \phi[M(\zeta)] > -\infty \). Suppose a \( \phi \)-optimal measure exists. Then \( \zeta^* \) is \( \phi \)-optimal if and only if

\[
\sup_{x \in X} F_\phi [M(\zeta^*), h(x)n(x)] = 0. \tag{25}
\]

The sequence of design measures \( \{\zeta_N\} \) defined in the iterative procedure obeys the recursive formula

\[
\zeta_{N+1} = (1-\alpha_N)\zeta_N + \alpha_N z(x_{N+1}), \tag{26}
\]
where \( a_N = 1/(N+1) \) and \( \zeta(\chi_{N+1}) \) denotes the design measure which assigns 1 to the point \( \chi_{N+1} \). Silvey (1980, pp. 35-36) shows that for such \( \{a_N\} \) the procedure converges.

Let us now consider the multiresponse model given in (3) and the \( \Lambda^2 \)-optimality criterion defined in Section 3.2. We shall apply Silvey's (1980) procedure to construct \( \Lambda^2 \)-optimal designs. For this purpose let us consider the matrices \( X_0 \) and \( Z_0 \), which are of orders \( N \times p \) and \( N \times p_1 \) and appear in (5) and (12), respectively. We introduce a single-response model of the form given in (19) with \( h^*(\chi) = [\zeta^*(\chi) \ b^*(\chi)] \), where \( \zeta^*(\chi) \) and \( b^*(\chi) \) are vectors of dimensions \( p \) and \( p_1 \) that represent a row of \( X_0 \) and a corresponding row of \( Z_0 \), respectively, evaluated at a point \( \chi \). The corresponding information matrix for a discrete \( N \)-point design measure \( \zeta_N \) can be written as

\[
M(\zeta_N) = \begin{bmatrix}
M_{XX}(\zeta_N) & M_{XZ}(\zeta_N) \\
M_{ZX}(\zeta_N) & M_{ZZ}(\zeta_N)
\end{bmatrix},
\]  

(27)

where \( M_{XX}(\zeta_N) = X_0^T X_0 / N \), \( M_{XZ}(\zeta_N) = X_0^T Z_0 / N \), \( M_{ZX}(\zeta_N) = Z_0^T X_0 / N \), and \( M_{ZZ}(\zeta_N) = Z_0^T Z_0 / N \). The corresponding expression for \( \Lambda^2 \) in (18) can now be written as a function of \( M(\zeta_N) \) of the form

\[
\Lambda^2[M(\zeta_N)] = \text{tr}[T^{-1} L [I_T \Theta A(\zeta_N)] L^T],
\]  

(28)

where \( A(\zeta_N) = N[M_{ZZ}(\zeta_N) - M_{XZ}(\zeta_N)M_{XX}^{-1}(\zeta_N)M_{XZ}(\zeta_N)] \). In general, if \( \zeta \) is any design measure defined on a compact subset, \( \chi \), of the \( k \)-dimensional Euclidean space, then an extension of the \( \Lambda^2 \) function in (28) when \( M_{XX}(\zeta) \) is nonsingular is

\[
\Lambda^2[M(\zeta)] = \text{tr}[T^{-1} L [I_T \Theta A(\zeta)] L^T],
\]  

(29)

where \( A(\zeta) = M_{ZZ}(\zeta) - M_{XZ}(\zeta)M_{XX}^{-1}(\zeta)M_{XZ}(\zeta) \) and \( M_{XX}(\zeta), M_{XZ}(\zeta), M_{ZZ}(\zeta) \), and \( M_{ZZ}(\zeta) \) provide a partitioning of \( M(\zeta) \) in (20) analogous to that of \( M(\zeta_N) \) in
If $H$ is the set of all design measures on $\chi$ and $M$ is the set $\{M(\xi): \xi \in H\}$, then a real-valued function $\phi$ can be defined on $M$ as

$$
\phi[M(\xi)] = \begin{cases} 
A_2^* [M(\xi)] & \text{if } M_{XX}(\xi) \text{ is nonsingular} \\
-\infty & \text{otherwise}
\end{cases}
$$

In this respect, the problem of finding a $A_2^*$-optimal design for a multiresponse model is equivalent to finding a $\phi$-optimal design for the single-response model (19) with $h'(\bar{x}) = [a'(\bar{x}) : b'(\bar{x})]$ as was seen earlier. The function $\phi$ defined in (30) can be shown to satisfy conditions (i), (ii), and (iii) described in Theorem 1. The proof of this theorem is given in Wijesinha and Khuri (1985).

Theorem 1. Let $M^* = \{M(\xi): M(\xi) \in M \text{ and } M_{XX}(\xi) \text{ is nonsingular}\}$. If $A_2^* [M(\xi)]$ is defined as in (29), then

(i) a $A_2^*$-optimal measure exists.

(ii) $A_2^*$ is concave on $M$.

(iii) $A_2^*$ is differentiable on $M^*$.

If $F_{A_2^*}$ denotes the Fréchet derivative of $A_2^*$, then from Lemma 1 and Theorem 1 we may conclude that a design measure $\xi^*$ is $A_2^*$-optimal if and only if

$$
\sup_{\xi \in X} F_{A_2^*} [M(\xi^*), h(\bar{x}) h'(\bar{x})] = 0,
$$

where $h'(\bar{x}) = [a'(\bar{x}) : b'(\bar{x})]$. This result will be used to construct a $A_2^*$-optimal design in an iterative manner, just like in Silvey's (1980) procedure described in Section 4.1. First, we need to obtain an explicit expression for $F_{A_2^*}$. This will be developed in the next theorem.
Theorem 2. If \( H \) is the set of all design measures on \( X \), then for \( \zeta \in H \) and \( x \in X \) we have

\[
F_{\Lambda_2} \left[ \mathbb{M}(\zeta), h(x) h'(x) \right] = \text{tr} \left[ Z_1^{-1} L_1 W_1 \right] \quad \text{where} \quad W_1 = L_1 \left[ h(x) - \mathbb{M}(\zeta) \right] \left[ h'(x) - \mathbb{M}(\zeta) \right] L_1^T
\]

where \( h(x) = \mathbb{M}_{XX}(\zeta) \mathbb{M}^{-1}(\zeta) M_x \) and \( h'(x) = [a'(x), b'(x)]^T \).

Proof. For simplicity we shall write \( \widetilde{M} \) and \( \tilde{h} \) instead of \( \mathbb{M}(\zeta) \) and \( h(x) \). By definition,

\[
F_{\Lambda_2} \left( \widetilde{M}, \tilde{h}, \tilde{h}' \right) = \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left[ \Lambda_2 \left[ \widetilde{M} \right] - \Lambda_2 \left[ \mathbb{M} \right] \right],
\]

where \( \widetilde{M} = (1-\epsilon)M + \epsilon \tilde{h} \). Recall that

\[
\Lambda_2 \left[ \widetilde{M} \right] = \text{tr} \left[ Z^{-1} L \left( L_1 \mathbb{M}_{XX}^{-1} L_1^T \right) L_1^T \right].
\]

Therefore,

\[
F_{\Lambda_2} \left( \widetilde{M}, \tilde{h}, \tilde{h}' \right) = \lim_{\epsilon \to 0} \frac{\text{tr} \left[ Z^{-1} L \left( L_1 \mathbb{M}_{XX}^{-1} L_1^T \right) L_1^T \right]}{\epsilon},
\]

where

\[
\mathbb{E} = \left( \frac{1}{\epsilon} \right) \left\{ \mathbb{M}_{ZZ} - \mathbb{M}_{XX} \mathbb{M}_{XX}^{-1} \mathbb{M}_{ZZ} - \mathbb{M}_{XX} \mathbb{M}_{XX}^{-1} \mathbb{M}_{XX} \right\},
\]

and

\[
\widetilde{\mathbb{M}} = \begin{bmatrix}
\mathbb{M}_{XX} & \mathbb{M}_{XZ} \\
\tilde{M}_{ZX} & \tilde{M}_{ZZ}
\end{bmatrix}.
\]

But from Dykstra (1971), for a nonsingular matrix \( \Lambda \) we have the following identity:

\[
(\Lambda + x_0 x_0^{-1} \Lambda) = \Lambda - \frac{\Lambda^{-1} x_0 x_0^{-1} \Lambda^{-1}}{1 + x_0 \Lambda^{-1} x_0^{-1}}.
\]

Thus, if we let \( \Lambda = (1-\epsilon)\mathbb{M}_{XX} \) and \( x_0 = \epsilon \frac{1}{2} \), we get

\[
\mathbb{M}_{XX}^{-1} = \left( (1-\epsilon)\mathbb{M}_{XX} + \epsilon \mathbb{M}_{XX}^{-1} \right)^{-1}
\]
\[ = (1-\epsilon)^{-1} (c_c/c) \left[ \epsilon c'(1-\epsilon)^2 \right] M_{XX}^{-1} \alpha a^{-1} M_{XX}, \]

where \( c^{-1} = 1 + [\epsilon/(1-\epsilon)] \alpha a^{-1} M_{XX} \alpha. \) It follows that

\[ M_{XX}^{-1} = (1-\epsilon)^{-1} M_{XX}^{-1} \left\{ \frac{\epsilon}{\epsilon + (1-\epsilon)} \right\}, \]

where \( \epsilon = 1 - \epsilon + c a^{-1} M_{XX} a \) and \( P = M_{XX} a^{-1} M_{XX}. \)

From (33) we obtain

\[ E = M_{ZZ} - M_{ZXX} - M_{ZXX}^{-1} M_{ZXX} a a^{-1} - \frac{a^2}{(1-c)^t} \mu M_{ZXX}^{-1} a a^{-1} M_{ZXX} \]

\[ + \frac{\epsilon}{\epsilon + (1-\epsilon)} M_{ZXX} a a^{-1} M_{ZXX} + \left\{ \frac{\epsilon^2}{\epsilon + (1-\epsilon)} \right\} M_{ZXX} a a^{-1} M_{ZXX}. \]

From (32) and (34) we conclude that

\[ F_{A_2} \left[ M(\xi), h(x) h'(x) \right] \]

\[ = \text{tr} \left[ T^{-1} \left[ L \Theta \left( h(x) - \bar{y}(x, \xi) \right) \left[ \bar{y}(x) - \bar{y}(x, \xi) \right] \right] L \right] - A_2 \left[ M(\xi) \right], \]

where \( \bar{y}(x, \xi) = M_{ZXX}^{-1}(\xi) a(x) \).

### 4.2 An Iterative Procedure to Obtain a \( A_2 \)-Optimal Design

Let \( h(x) = \left[ a'(x): b'(x) \right] \) and let \( M(\xi_N), N > 1 \), be defined as in (27).

The main steps of the iterative procedure for constructing a \( A_2 \)-optimal design are:

1. Start with an initial design \( D_{N_0} \) (consisting of \( N_0 \) points) for which \( M_{XX}(\xi_N) \) is nonsingular.

2. Obtain the design point \( x_{N_0+1} \) at which \( \sup_{x_{N_0}} F_{A_2} \left[ M(\xi_N), h(x) h'(x) \right] \) is attained.

3. Obtain \( D_{N_0+1} \) (hence \( \xi_{N_0+1} \)) by augmenting \( D_{N_0} \) with \( x_{N_0+1} \). Recall that \( \xi_{N_0+1} \) is the design measure obtained by assigning probability \( 1/(N_0+1) \) to each design point in \( D_{N_0+1} \).
4. Continue this process to find $x_{N_0+2}, x_{N_0+3}, \ldots$, until

$$\sup_{x \in \mathbb{R}} F_{A_2} \{ M(x_N), h(x)h'(x) \} < \varepsilon,$$  \hspace{1cm} (35)

for some $N > N_0$ and $\varepsilon$, where $\varepsilon$ is a small positive number chosen a priori.

5. **Numerical Examples**

   **Example 1.** One of the main concerns in industry is the determination of conditions on the controllable variables which lead to better yields and lower costs. In a paper by Lind et al. (1960), the authors discussed a case study of such a problem. They applied response surface techniques to a typical chemical processing operation. Three controllable variables were considered; they were $x_1, x_2,$ and $x_3$ which represent, respectively, the proportions of two complexing agents, and the extraction pH level. The response variables were $y_1 = \text{percentage yield}, y_2 = \text{cost of materials (dollars per one kilogram of product)}$. The controllable variables were coded so that $-1 \leq x_i \leq 1$ (i=1,2,3). The fitted models are given below

$$E_o(y_i) = \beta_{10} + \sum_{j=1}^{3} \beta_{ij} x_j + \beta_{112} x_1 x_2 + \beta_{113} x_1 x_3 + \beta_{123} x_2 x_3, \quad i = 1, 2.$$  

If these models are inadequate, then it is necessary that the design be chosen so that the experimenter can quickly and efficiently detect the presence of lack of fit. In this case the design can be augmented with additional points to allow the fitting of models with higher-order terms. If, however, no significant lack of fit is detected, then the models can be used to determine conditions on $x_1, x_2, \text{and } x_3$ that lead to high yield-response values and low cost-response values. Let us consider that the true model for each response is of the second degree with all pure quadratic terms, i.e., $x_1^2, x_2^2, \text{and } x_3^2$ (this model was reported to be adequate according to the study by Lind et al., 1960).
The iterative procedure described in Section 4.2 was carried out using two initial designs given in Tables 1 and 2. The augmented design points, the \( F_{A_2} \) values, and the \( \Lambda_{A_2} \) values are given in Tables 3 and 4. The figures indicate that the procedure has been successful in reducing the \( F_{A_2} \) values to a level very close to zero. A steady increase in the values of \( \Lambda_{A_2} \) is also seen. It is quite clear from these results that the choice of the initial design has a significant effect on the location of the new design points as well as on the rate of convergence of the procedure.

**Example 2.** In this example we consider a multiresponse experiment with three responses, \( y_1, y_2, y_3 \), and three controllable variables, \( x_1, x_2, x_3 \), coded so that \(-1 < x_i < 1 \) (i=1,2,3). The fitted models are

\[
E_a(y_1) = \beta_{10} + \beta_{11}x_1 + \beta_{13}x_3 + \beta_{113}x_1x_3
\]

\[
E_a(y_2) = \beta_{20} + \frac{3}{j=1} \beta_{2j}x_j + \beta_{213}x_1x_3 + \beta_{211}x_1^2 + \beta_{233}x_3^2
\]

\[
E_a(y_3) = \beta_{30} + \frac{3}{j=1} \beta_{3j}x_j.
\]

The true models are considered to be

\[
E_t(y_1) = \beta_{10} + \beta_{11}x_1 + \beta_{13}x_3 + \beta_{113}x_1x_3 + \beta_{111}x_1^2 + \beta_{133}x_3^2
\]

\[
E_t(y_2) = \beta_{20} + \frac{3}{j=1} \beta_{2j}x_j + \beta_{213}x_1x_3 + \beta_{211}x_1^2 + \beta_{233}x_3^2 + \beta_{212}x_1x_2 + \beta_{223}x_2x_3 + \beta_{222}x_2^2
\]

\[
E_t(y_3) = \beta_{30} + \frac{3}{j=1} \beta_{3j}x_j + \beta_{312}x_1x_2 + \beta_{313}x_1^2 + \beta_{323}x_2x_3 + \beta_{311}x_1^2 + \beta_{322}x_2^2 + \beta_{333}x_3^2
\]

The initial design for this example is given in Table 5 and the augmented design points are given in Table 6. As in Example 1, we can clearly see that the proposed procedure has been effective in reducing the value of \( \sup_{x \in \mathcal{X}} F_{A_2}(M(\xi_{N-1}), h(x)h'(x)) \) to a level arbitrarily close to zero.
Appendix

In this appendix we prove the inequality
\[ \text{tr}(\Omega) > e_{\min}(\Xi^{-1}) \gamma^{-1/2} (I_r \otimes A) \gamma^{-1/2}, \]
where
\[ \gamma = [\gamma_1^2; \gamma_2^2; \ldots; \gamma_r^2], \quad A = \Xi^{-1} \{ I_N - \Sigma_0 (\Sigma_0^{-1} \Sigma_0)^{-1} \Sigma_0 \} \Xi_0, \quad \text{and} \]
\[ \Xi = \text{diag}(H_1^2, H_2^2, \ldots, H_r^2). \]

Proof
\[
\text{tr}[\gamma^T \Xi^{-1} \{ I_N - \Sigma_0 (\Sigma_0^{-1} \Sigma_0)^{-1} \Sigma_0 \} \Xi_0]
\]
\[ = \sum_{i=1}^r \gamma_i^2 \Xi^{-1} \{ I_N - \Sigma_0 (\Sigma_0^{-1} \Sigma_0)^{-1} \Sigma_0 \} \Xi_0,
\]
\[ = [\gamma_1^2; \gamma_2^2; \ldots; \gamma_r^2] (I_r \otimes A) [\gamma_1^2; \gamma_2^2; \ldots; \gamma_r^2]^T,
\]
\[ = \gamma^T (I_r \otimes A) \gamma. \]

Inequality (A.1) follows from the above equality and inequality (7).

Acknowledgements

The author would like to thank the Editor and two referees for their helpful suggestions which improved the presentation of this paper. This research was partially supported by the Office of Naval Research under Grant No. N00014-86-K-0059.
Table 1. Initial Design 1 (Example 1).

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Table 3. The Augmented Design Points using Initial Design 1 (Example 1).

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<th>$A_2^* [M(\zeta_{N-1})]$</th>
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Table 4. The Augmented Design Points Using Initial Design 2 (Example 1).

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<th>$A_2^- [M(x_{N-1})]$</th>
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<td>(-1.000, -1.000, -1.000)</td>
<td>1.0772</td>
</tr>
<tr>
<td>42</td>
<td>(1.000, -1.000, -1.000)</td>
<td>0.1425</td>
</tr>
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References


END

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