Design admissibility,invariance and optimality in multiresponse linear models

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Contents

1. Introduction

Motivation:

- The considerations on admissibility and invariance of designs are key to reduction of complicated design problems.
- These concepts are addressed in detail and applied successfully for finding optimal designs in single-response models

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$$y_i = \eta(x_i, \theta) + \varepsilon, \quad i = 1, 2, ..., n.$$

- For example,
    - Kiefer (1959),
    - Gaffke (1987),
    - Heiligers (1992),
    - Pukelsheim (1993),
    - Yang and Stufken (2009),
    - Yang (2010),
    - Dette and Melas (2011),
    - Yang and Stufken (2012),
    - Dette and Schorning (2013),
    - ......

Purpose of the present study:

To extend the considerations on admissibility and invariance to multiresponse designs.

Multiresponse experiments:

- In a multiresponse situation, several responses are considered simultaneously, which are usually correlated.
- Data on more than one response variable is recorded from the same experimental unit through application of same treatment.
- They occur in, e.g., engineering, pharmaceutical, biomedical, environmental research.

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2. Multiresponse model

Suppose that we have a system of r response variables,

$$y_1, y_2, \cdots, y_r$$

each of which depends on the same set of q input variables denoted by

$$x_1, x_2, \cdots, x_q$$

with an experimental region $\mathcal{X} \subset \mathbb{R}^q$.

Multiresponse linear model:

$$Y(x) = F(x)\theta + \varepsilon \qquad (2.1)$$

- $Y(x) = (y_1(x), ..., y_r(x))^T$
- $x = (x_1, \cdots, x_q) \in \mathcal{X} \subset \mathbb{R}^q$
- $F(x) = (f_1(x), \cdots, f_r(x))^T \in \mathbb{R}^{r \times p}$
- θ : a vector of unknown parameters in $\mathbb{R}^p$
- ε : an r-dim vector of random errors

$$E(\varepsilon) = 0, \quad Cov(\varepsilon) = \Sigma = (\sigma_{ij})_{r\times r} > 0$$

Design and Information matrix:

- An approximate design ξ: a probability measure with finite supports on $\mathcal{X}$

$$\xi = \begin{Bmatrix} x_1 & \cdots & x_n \\ w_1 & \cdots & w_n \end{Bmatrix}, \ w_i \geq 0, \ \sum_{i=1}^{n} w_i = 1.$$

Ξ: the set of all approximate designs.

- The information matrix of ξ on $\mathcal{X}$:

$$M(\xi) = \int_{\mathcal{X}} F^T(x)\Sigma^{-1}F(x)\, d\xi(x).$$

$\mathcal{M}(\Xi)$: the set of all information matrices on Ξ.

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Reformulation for (2.1) :

- Let $g(x) = (g_1(x), \cdots, g_k(x))^T$ be the k-dimensional vector consisting of all different elements in $F(x)$.
- $f_i(x)$ in (2.1) can be expressed as

$$f_i(x) = V_i^T U_i g(x),$$

U_i, V_i are full row-rank matrices satisfying

$$f_i^T(x)\theta = g^T(x) U_i^T V_i \theta, \quad i = 1, 2, \cdots, r.$$

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$$f_i^T(x)\theta = g^T(x) U_i^T V_i \theta, \quad i = 1, 2, \cdots, r.$$

- $F(x)$ in (2.1) can be rewritten as

$$\begin{aligned} F(x) &= (f_1(x), \cdots, f_r(x))^T \\ &= \begin{pmatrix} g^T(x) & 0 & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & g^T(x) \end{pmatrix} \begin{pmatrix} U_1^T V_1 \\ \vdots \\ U_r^T V_r \end{pmatrix} \\ &= [I_r \otimes g^T(x)] L_{UV} \end{aligned} \quad (2.2)$$

- Model (2.1) can be rewritten as

$$\begin{aligned} & Y(x) = [I_r \otimes g^T(x)] L_{UV} \theta + \varepsilon, \\ & E(\varepsilon) = 0, \quad Cov(\varepsilon) = \Sigma. \end{aligned} \quad (2.3)$$

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- The information matrix of ξ is expressed by

$$M(\xi) = L_{UV}^T[\Sigma^{-1} \otimes M_g(\xi)]L_{UV}, \quad (2.4)$$

where

$$M_g(\xi) = \int_{\mathcal{X}} g(x)g^T(x)d\xi(x) \quad (2.5)$$

is the information matrix of ξ under the following single-response linear model with homoscedastic errors

$$\begin{aligned} y(x) &= g^T(x)\beta + e, \\ E(e) &= 0, \quad Cov(e) = \sigma^2. \end{aligned} \quad (2.6)$$

Example 1. Linear and Quadratic reg.

Krafft and Schaefer (1992)

$$\begin{cases} y_1 = \theta_{10} + \theta_{11}x + \varepsilon_1 \\ y_2 = \theta_{20} + \theta_{21}x + \theta_{22}x^2 + \varepsilon_2 \end{cases} \quad (2.7)$$

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix} \quad (2.8)$$

where $x \in \mathcal{X} = [-1,1]$, $|\rho| < 1$.

$$\begin{aligned} f_1(x) &= (1,x,0,0,0)^T \\ f_2(x) &= (0,0,1,x,x^2)^T \\ \theta &= (\theta_{10},\theta_{11},\theta_{20},\theta_{21},\theta_{22})^T \end{aligned}$$

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Reformulation: $g(x) = (1, x, x^2)^T$

$$U_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},\ U_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$V_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix},$$

$$V_2 = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Example 2. Berman's model on an arc

Berman (1983)

$$\begin{cases} y_1(t) = \theta_1 + \theta_3 \cos t - \theta_4 \sin t + \varepsilon_1, \\ y_2(t) = \theta_2 + \theta_3 \sin t + \theta_4 \cos t + \varepsilon_2, \end{cases} \quad (2.9)$$

$$\Sigma = \sigma^2 I_2,$$

$$t \in \mathcal{X} = [-\alpha/2, \alpha/2], \quad \alpha \in [0, 2\pi]$$

$$\begin{aligned} f_1(t) &= (1, 0, \cos t, -\sin t)^T \\ f_2(t) &= (0, 1, \sin t, \cos t)^T \\ \theta &= (\theta_1, \theta_2, \theta_3, \theta_4)^T \end{aligned}$$

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Reformulation: $g(t) = (1, \cos t, \sin t)^T,$

$$U_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad U_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

$$V_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad V_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Example 3. Parallel linear model

Huang, Chen, Lin and Wong (2006)

$$\begin{cases} y_1(x) = \theta_{01} + \theta_1 x_1 + \varepsilon_1, \\ y_2(x) = \theta_{02} + \theta_1 x_2 + \varepsilon_2, \end{cases} \quad \Sigma = \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \tag{2.10}$$

where $x = (x_1, x_2) \in \mathcal{X} = [-1,1] \times [-1,1]$.

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3. Admissibility of designs

Definition of Admissibility

Pukelsheim (1993)

- An information matrix $M \in \mathcal{M}(\Xi)$ is called admissible in $\mathcal{M}(\Xi)$ when every competing information matrix $A \in \mathcal{M}(\Xi)$ with $A \geq M$ is actually equal to M.
- A design ξ is called admissible in Ξ when its information matrix $M(\xi)$ is admissible in $\mathcal{M}(\Xi)$.

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Definition of an optimality criterion:

A criterion is a nonnegative function

$$\phi : \mathrm{NND}(s) \to \mathbb{R}$$

that is isotonic relative to the Loewner ordering, positively homogeneous and superadditive.

- Isotonic relative to the Loewner ordering:

$$A \geq B > 0 \quad \to \quad \phi(A) \geq \phi(B).$$

- Positive homogeneity:

$$\phi(\delta A) = \delta\phi(A) \quad \forall\delta > 0, \forall A \in \mathrm{NND}(s).$$

- Superadditivity:

$$\phi(A+B) \geq \phi(A) + \phi(B) \quad \forall A, B \in \mathrm{NND}(s).$$

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The Elfving set:

- The Elfving set is defined by

$$\mathcal{R}_g = \text{conv}\left(\{g(x)|x \in \mathcal{X}\} \cup \{-g(x)|x \in \mathcal{X}\}\right) \tag{3.1}$$

  where conv(P) denotes the convex hull of the set P of points in $\mathbb{R}^k$.

- $\mathcal{R}_g$ is a symmetric compact convex subset of $\mathbb{R}^k$ that contains the origin in its relative interior.

- In order to find optimal support points, we need only to search the "extreme points" of the set $\mathcal{R}_g$.

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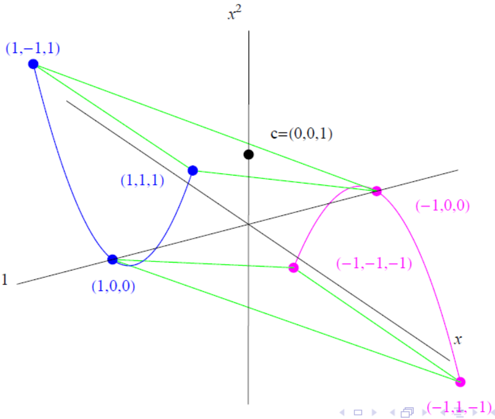
Elfving set corresponding to model (2.7):

$$g(x) = (1, x, x^2)^T, \quad \mathcal{X} = [-1, 1]$$

$$\mathcal{R}_1 = \text{conv}\left(\{g(x) \mid x \in \mathcal{X}\} \cup \{-g(x) \mid x \in \mathcal{X}\}\right)$$



Location of the support points of admissible designs:

Theorem 1. Let $\widetilde{\mathcal{R}}_g$ be the set consisting of extreme points of the Elfving set $\mathcal{R}_g$, which do not lie on a straight line connecting any other two distinct points of the Elfving set $\mathcal{R}_g$. Then for any $\eta \in \Xi$ with support not included in $\widetilde{\mathcal{R}}_g$, there exists a design $\xi \in \Xi$ with support included in $\widetilde{\mathcal{R}}_g$ such that

$$M(\xi) \underset{\neq}{\geq} M(\eta).$$

Bound for the support size:

Theorem 2. Let ϕ be an optimality criterion. If there is a ϕ-optimal information matrix M_g for the k-dimensional parameter vector β in the single-response model (2.6), then there exists a ϕ-optimal design ξ for θ in the multiresponse model (2.1) such that its support size, $\sharp\,\mathrm{supp}(\xi)$, is bounded according to

$$p/r \leq \sharp\,\mathrm{supp}(\xi) \leq \min\left(\frac{k(k+1)}{2}, \frac{p(p+1)}{2}\right)$$

Admissible designs:

Theorem 3. Suppose $k \leq p$. If the p-dim unit vectors

$$e_{sk+1}, \cdots, e_{(s+1)k} \in \text{Range}(L_{UV})$$

for some $s \geq 0$, then:

ξ is admissible for the multiresponse (2.1)

$\Leftrightarrow$ ξ is admissible for the single-response (2.6).

Linear and Quadratic model (2.7):

- The Elfving set: $\mathcal{R}_1$
- Need to consider designs supported on the "extreme points" of $\mathcal{R}_1$ only.
- The support size is not more than 6 (Th2).
- Note that $e_{sk+1}, \cdots, e_{(s+1)k} \in \text{Range}(L_{UV})$ for $s = 1$ $(k = 3)$.

Corollary 1. A design $\xi \in \Xi$ is admissible in model (2.7) on $[-1, 1]$ $\Leftrightarrow$ ξ has at most one support in the open interval $(-1, 1)$.

4. Invariance of designs

Definition of $\mathcal{Q}$-invariant:

The design problem for θ in $\mathcal{M}(\Xi)$ is said to be $\mathcal{Q}$-invariant when $\mathcal{Q}$ is a subgroup of the general linear group of order p, GL(p), and all transformations $Q \in \mathcal{Q}$ fulfill

$$Q\mathcal{M}(\Xi)Q^T = \mathcal{M}(\Xi). \tag{4.1}$$

GL(p) is the set of $p \times p$ invertible matrices, together with the operation of ordinary matrix multiplication.

Definition of $\mathcal{H}$-invariant:

An optimality criterion ϕ on NND(p) is called $\mathcal{H}$-invariant when $\mathcal{H}$ is a subgroup of GL(p) and all transformations $H \in \mathcal{H}$ fulfill

$$\phi(C) = \phi(HCH^T) \quad \forall\, C \in \text{NND}(p). \quad (4.2)$$

Definition of Equivariance:

Let L: NND$(s) \to$ Sym(p) be the mapping $L(B) = L^T BL$, where L has full column rank p. Assume $\mathcal{Q}$ to be a subgroup of GL(s) and there exists a group homomorphism H from $\mathcal{Q}$ into GL(p) so that

$$L(QBQ^T) = H(Q)L(B)H(Q)^T, \quad \forall B \in \text{NND}(s),\ Q \in \mathcal{Q}$$

holds for the matrix $H(Q)$ in the image group $\mathcal{H}_{\mathcal{Q}} = \{H(Q)|Q \in \mathcal{Q}\}$. Then the mapping L is said to be $\mathcal{Q} - \mathcal{H}_{\mathcal{Q}}$-equivariant.

Lemma 1. Let

$$L_T : \text{NND}(k) \to \text{Sym}(p)$$
$$L_T(A) = L^T(T \otimes A)L$$

for a given $rk \times p$ matrix L with $\text{rank}(L) = p$, and a positive definite matrix T of order r. Assume $\mathcal{Q}$ to be a subgroup of $\text{GL}(k)$. Define $N_Q = I_r \otimes Q$ and

$$\mathcal{N}_{\mathcal{Q}} = \{N_Q \mid Q \in \mathcal{Q}\}.$$

We then have the following claims:

a. (Equivariance) There exists a group homomorphism $H : \mathcal{Q} \to \mathrm{GL}(k)$ such that L_T is equivariant under H,

$$L_T(QAQ^T) = H(Q)L_T(A)H(Q)^T, \quad \forall A \in \mathrm{NND}(k),\ Q \in \mathcal{Q},$$

if and only if the range of L is invariant under each transformation $N_Q \in \mathcal{N}_\mathcal{Q}$,

$$\mathrm{Range}(N_Q^T L) = \mathrm{Range}(L), \quad \forall N_Q \in \mathcal{N}_\mathcal{Q}.$$

b. (Uniqueness) Suppose L_T is equivariant under the group homomorphism $H : \mathcal{Q} \to \text{GL}(p)$. Then $H(Q)$ or $-H(Q)$ is the unique nonsingular $p \times p$ matrix H that satisfies $N_Q^T L = LH$ for all $N_Q \in \mathcal{N}_\mathcal{Q}$.

c. (Orthogonal transformation) Suppose L_T is equivariant under the group homomorphism $H : \mathcal{Q} \to \text{GL}(p)$. If matrix L fulfills $L^T L = I_p$ and $Q \in \mathcal{Q}$ is an orthogonal matrix of order k, then $H(Q) = \pm L^T N_Q^T L$ is an orthogonal matrix of order p.

The set

$$\mathcal{H}_{\mathcal{Q}} = \Big\{ H \in \mathsf{GL}(p) \mid N_Q^T L = LH \quad \text{for some } N_Q \in \mathcal{N}_{\mathcal{Q}} \Big\}$$

is called the *equivariance group* that is induced by the $\mathcal{N}_{\mathcal{Q}}$-invariance of the design problem for θ in $\mathcal{M}(\Xi)$.

Theorem 4. Let $\mathcal{Q}$ be a subgroup of $\mathrm{GL}(k)$ and $\mathcal{N}_{\mathcal{Q}}$ the set $\{N_Q = I_r \otimes Q \mid Q \in \mathcal{Q}\}$. If all $Q \in \mathcal{Q}$ fulfill

$$Q\mathcal{M}_g(\Xi)Q^T = \mathcal{M}_g(\Xi)$$

and

$$\mathrm{Range}(N_Q^T L_{UV}) = \mathrm{Range}(L_{UV}), \quad \forall\, N_Q \in \mathcal{N}_{\mathcal{Q}},$$

then the design problem for the multiresponse model (2.1) in $\mathcal{M}(\Xi)$ is $\mathcal{H}_{\mathcal{Q}}$-invariant.

Linear and Quadratic model (2.7):

$$\begin{cases} y_1 = \theta_{10} + \theta_{11}x + \varepsilon_1, \\ y_2 = \theta_{20} + \theta_{21}x + \theta_{22}x^2 + \varepsilon_2, \end{cases} \quad \Sigma = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix},$$

where $x \in \mathcal{X} = [-1, 1]$, $|\rho| < 1$.

Consider the reflection transformation acting on $\mathcal{X}$: $R(x) = -x$.

$$g(-x) = (1, -x, x^2)^T = Q_R\, g(x),$$

$$Q_R = \text{diag}(1, -1, 1).$$

Then $R(x) = -x$ together with the identity transformation induce a group of order 2:

$$\mathcal{Q} = \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\} \subset \text{GL}(3).$$

Since

$$L_{UV} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad (I_2 \otimes Q_R)L_{UV} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

this implies that L_{UV} and $(I_2 \otimes Q_R)L_{UV}$ have the same range. By Th4, this means that the design problem for model (2.7) is $\mathcal{H}_{\mathcal{Q}}$-invariant.

Here the equivariance group $\mathcal{H}_{\mathcal{Q}}$ is of order 2 as is $\mathcal{Q}$, containing the identity I_5 as well as H=diag $(1, -1, 1, -1, 1)$.

Together with Corollary 1, we obtain a complete class Ξ_{com} with minimum support size for model (2.7), which is composed of the following designs:

$$\xi = \begin{Bmatrix} -1 & 0 & 1 \\ w & 1-2w & w \end{Bmatrix}, \quad w \in \left[0, \frac{1}{2}\right]. \quad (4.3)$$

5. Elfving's theorem for D-optimality

Elfving set:

Elfving set for multiresponse (2.1) is

$$\mathcal{R}_p = \text{conv}\left\{F^T(x)\Sigma^{-1/2}K \middle| x \in \mathcal{X}, K \in \mathbb{R}^{r\times p}, \|K\| = 1\right\} \subseteq \mathbb{R}^{p\times p},$$

where conv(B) denotes the convex hull of matrices $B \subseteq \mathbb{R}^{p\times p}$, and $\|K\|$ is the Frobenius norm of the matrix K, i.e.,

$$\|K\|^2 = \text{tr}(K^T K).$$

Theorem 5. A design

$$\xi = \left\{ \begin{array}{cccc} x_1 & x_2 & \cdots & x_s \\ w_1 & w_2 & \cdots & w_s \end{array} \right\}$$

is D-optimal for the multiresponse model (2.1) if and only if $(pM(\xi))^{-1/2} \in \mathbb{R}^{p\times p}$ is a supporting hyperplane of the Elfving set $\mathcal{R}_p$ with supports

$$F^T(x_i)\Sigma^{-1/2}K_i, \quad i = 1, \cdots, s$$

where $\quad K_i = (p\Sigma)^{-1/2}F(x_i)M^{-1/2}(\xi).$

D-optimal design for model (2.10):

$$\begin{cases} y_1(x) = \theta_{01} + \theta_1 x_1 + \varepsilon_1, \\ y_2(x) = \theta_{02} + \theta_1 x_2 + \varepsilon_2, \end{cases} \qquad \Sigma = \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}$$

where $x = (x_1, x_2) \in \mathcal{X} = [-1, 1] \times [-1, 1]$.

$$\xi^* = \left\{ \begin{matrix} (-1, 1) & (1, -1) \\ 1/2 & 1/2 \end{matrix} \right\} \quad \text{if } \rho > 0,$$

and

$$\xi^* = \left\{ \begin{matrix} (-1, -1) & (1, 1) \\ 1/2 & 1/2 \end{matrix} \right\} \quad \text{if } \rho < 0,$$

which can be verified by Theorem 5.

6. Concluding remarks

- We obtained the necessary and sufficient conditions for a design to be admissible and invariant for multiresponse linear models.
- We established an Elfving's theorem for D-optimality which can be used for the characterization of D-optimal designs.
- A further study: Liu X., Yue R.-X. and Wong W.-K. (2018). D-optimal design for the heteroscedastic Berman's model on an arc. Submitted to *J. Multi. Anal.*, revised.

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