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Optimality of some experimental designs under mixed effects linear model*

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SUMMARY

A design which is universally optimal for estimating a given set of parameters under the fixed effects model is also universally optimal for estimating a reduced set of parameters under the related mixed effects model. The aim of the paper is to study conditions under which a design universally optimal in the model without random effects (i.e. a model in which variances of random effects are zero) is also universally optimal in the mixed effects model. Using the Kiefer ordering some sufficient conditions are established.

KEY WORDS: mixed effects model, Schur complement, G-majorization, Kiefer ordering, Kiefer optimality, optimal experimental designs, row-column designs, repeated measurements designs.

1. Introduction and preliminaries

Consider the linear model associated with the design $d \in \mathcal{D}$

$$\mathbf{y} = \mathbf{X}_{1,d}\boldsymbol{\vartheta}_1 + \mathbf{X}_{2,d}\boldsymbol{\vartheta}_2 + \mathbf{X}_{3,d}\boldsymbol{\vartheta}_3 + \boldsymbol{\varepsilon} \ , \tag{1}$$

where $\mathbf{X}_{i,d} \in \mathbf{R}^{n\times r_i}$, $i = 1,2,3$, are known, $\boldsymbol{\varepsilon}$ is a random error with $E(\boldsymbol{\varepsilon}) = \mathbf{0}$, $Cov(\boldsymbol{\varepsilon}) = \mathbf{I}_n$ and $\boldsymbol{\vartheta}_i$ are parameters vectors. Further, let $\mathbf{C}_{d,q}$, $q \in \{0, \infty, V\}$ denote information matrices of d for estimating $\boldsymbol{\vartheta}_1$ in a model $\mathcal{M}_q$ under normality, where

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the underlying model is

$\mathcal{M}_0$	model (1) without $\boldsymbol{\vartheta}_2$ (i.e., $\boldsymbol{\vartheta}_2 = \mathbf{0}$),
$\mathcal{M}_\infty$	model (1) with fixed, non-random $\boldsymbol{\vartheta}_2$,
$\mathcal{M}_V$	model (1) with random effects $\boldsymbol{\vartheta}_2$ uncorrelated with $\boldsymbol{\varepsilon}$. $E(\boldsymbol{\vartheta}_2) = \mathbf{0}$, and $Cov(\boldsymbol{\vartheta}_2) = \mathbf{V}$, (known).

Following Kunert (1983) models $\mathcal{M}_0, \mathcal{M}_\infty$, and $\mathcal{M}_V$ can be called the simpler model, the finer fixed model, and the finer mixed model, respectively.

The information matrices $\mathbf{C}_{d,q}$ can be expressed as the Schur complement of $\mathbf{T}_{d,q}$ in $\mathbf{M}_{d,q}$, i.e.

$$\mathbf{C}_{d,q} = [\mathbf{M}_{d,q}/\mathbf{T}_{d,q}], \; q \in \{0, \infty, V\}, \tag{2}$$

where

$$\begin{aligned}
\mathbf{M}_{d,0} &= \left(\mathbf{X}'_{i,d}\mathbf{X}_{j,d}\right)_{i,j\in\{1,3\}},\\
\mathbf{M}_{d,\infty} &= \left(\mathbf{X}'_{i,d}\mathbf{X}_{j,d}\right)_{1\le i,j\le 3},\\
\mathbf{M}_{d,V} &= \left(\mathbf{X}'_{i,d}(\mathbf{I}_n + \mathbf{X}_{2,d}\mathbf{V}\mathbf{X}'_{2,d})^{-1}\mathbf{X}_{j,d}\right)_{i,j\in\{1,3\}},\\
\mathbf{T}_{d,0} &= \mathbf{X}'_{3,d}\mathbf{X}_{3,d},\\
\mathbf{T}_{d,\infty} &= \left(\mathbf{X}'_{i,d}\mathbf{X}_{j,d}\right)_{2\le i,j\le 3},\\
\mathbf{T}_{d,V} &= \mathbf{X}'_{3,d}(\mathbf{I}_n + \mathbf{X}_{2,d}\mathbf{V}\mathbf{X}'_{2,d})^{-1}\mathbf{X}_{3,d},
\end{aligned}$$

see e.g. Pukelsheim (1993, Chapter 3). Recall that for a given nonnegative-definite $k \times k$ matrix $\mathbf{A} = (\mathbf{A}_{i,j})_{1\le i,j\le 2}$ the Schur complement of $\mathbf{A}_{22}$ in $\mathbf{A}$ is

$$[\mathbf{A}/\mathbf{A}_{22}] = \mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-}\mathbf{A}_{21}, \tag{3}$$

where $\mathbf{A}_{22}^{-}$ is a g-inverse of $\mathbf{A}_{22}$.

In the sequel the symbols NND(n) and Ort(n) will denote the set of all $n \times n$ nonnegative-definite matrices and the set of all $n \times n$ orthogonal matrices, respectively. Let $\mathcal{H}$ be a subgroup of Ort(k) and let $\mathbf{\Phi}(\mathcal{H})$ be a class of all functionals φ on NND(k) satisfying the following conditions:

(a) φ is concave,

(b) φ is isotonic (increasing) with respect to the Loewner partial ordering,

(c) φ is $\mathcal{H}$-invariant, i.e. $\varphi(\mathbf{A}) = \varphi(\mathbf{HAH}')$ for every $\mathbf{A} \in$NND(k) and $\mathbf{H} \in \mathcal{H}$.

A design d^* will be termed *universally optimal* w.r.t. $\mathbf{\Phi}(\mathcal{H})$ over the class $\mathcal{D}$ of designs under consideration if d^* maximizes $\varphi(\mathbf{C}_d)$ for every functional $\varphi \in \mathbf{\Phi}(\mathcal{H})$; see e.g. Kiefer (1975), Giovagnoli et al. (1987) and Pukelsheim (1993).

In Section 2 we investigate conditions under which a design universally optimal for estimating $\boldsymbol{\vartheta}_1$ in $\mathcal{M}_0$ preserves its optimality in $\mathcal{M}_V$. These conditions are imposed on the information matrix

$$\mathbf{W}_d = \left[\mathbf{M}_{d,\infty}/\mathbf{X}'_{3,d}\mathbf{X}_{3,d}\right] \tag{4}$$

for estimating simultaneously ϑ_1 and ϑ_2 in the fixed effects model $\mathcal{M}_\infty$. It is based on the functional relationships between information matrices $\mathbf{C}_{d,q}$ and $\mathbf{W}_d$. In particular $\mathbf{C}_{d,V}$ can be expressed as

$$\mathbf{C}_{d,V} = \left[\mathbf{W}_{d,V}/(\mathbf{V}^{1/2}\mathbf{X}'_{2,d}\mathbf{Q}_{X_{3,d}}\mathbf{X}_{2,d}\mathbf{V}^{1/2} + \mathbf{I}_{r_2})\right], \tag{5}$$

where

$$\mathbf{W}_{d,V} = \mathbf{\Lambda}\mathbf{W}_d\mathbf{\Lambda} + \mathrm{diag}(\mathbf{0}, \mathbf{I}_{r_2}) \tag{6}$$

with $\mathbf{\Lambda} = \mathrm{diag}(\mathbf{I}_{r_1}, \mathbf{V}^{1/2})$, while $\mathbf{Q}_L = \mathbf{I}_m - \mathbf{L}(\mathbf{L}'\mathbf{L})^-\mathbf{L}'$ denotes the orthogonal projectors on the orthocomplement of $\mathrm{Im}(\mathbf{L})$, the range of a given $m \times n$ matrix $\mathbf{L}$. For more details see Markiewicz (1997, Theorem 1).

2. Optimality results

First we recall a notion of the Kiefer ordering and the Kiefer optimality; cf. Pukelsheim (1993). Given two symmetric matrices $\mathbf{A}$ and $\mathbf{B} \in \mathrm{Sym}(k)$ and the group $\mathcal{H} \subseteq \mathrm{Ort}(k)$, we say that $\mathbf{A}$ is below $\mathbf{B}$ w.r.t. the *Kiefer ordering* relative to $\mathcal{H}$ ($\mathbf{B}$ is *more informative than* $\mathbf{A}$) and we write $\mathbf{A} \ll_{\mathrm{H}} \mathbf{B}$ when $\mathbf{B}$ is better in the Loewner ordering than some matrix $\mathbf{D}$ which is H-majorized by $\mathbf{A}$, i.e.

$$\mathbf{A} \ll_{\mathrm{H}} \mathbf{B} \iff \mathbf{D} \preceq_L \mathbf{B} \text{ for some } \mathbf{D} \in Sym(k) \text{ such that } \mathbf{D} \prec_{\mathrm{H}} \mathbf{A},$$

where $\mathbf{D} \prec_{\mathrm{H}} \mathbf{A}$ means that $\mathbf{D} \in conv\{\mathbf{HAH}' : \mathbf{H} \in \mathcal{H}\}$ while $\mathbf{D} \preceq_L \mathbf{B}$ means that $\mathbf{B} - \mathbf{D} \in \mathrm{NND}(k)$. A sufficient condition of maximality of a matrix $\mathbf{A}_0$ in $\mathcal{A}$ w.r.t. the Kiefer ordering related to $\mathcal{H}$ is its $\mathcal{H}$-symmetry, i.e. $\mathbf{A}_0 = \mathbf{HA}_0\mathbf{H}'$ for all $\mathbf{H} \in \mathcal{H}$, and its maximality w.r.t. the Loewner ordering over the set of $\mathcal{H}$-centers: $\{\bar{\mathbf{A}},\ \mathbf{A} \in \mathcal{A}\}$, where the $\mathcal{H}$-center $\bar{\mathbf{A}}$ of $\mathbf{A}$ is the average of $\mathbf{HAH}'$ over $\mathbf{H} \in \mathcal{H}$; cf. Pukelsheim (1993, Ch. 14).

A design d^* will be termed *Kiefer optimal* w.r.t. the group $\mathcal{H}$ over the class $\mathcal{D}$ of designs under consideration if $\mathbf{C}_d \ll_{\mathrm{H}} \mathbf{C}_{d^*}$ for all $d \in \mathcal{D}$. Evidently the Kiefer optimality w.r.t. $\mathcal{H}$ implies the universal optimality w.r.t. $\mathbf{\Phi}(\mathcal{H})$.

In the context of estimation of ϑ_1 and ϑ_2 simultaneously we will consider a relabelling group $\mathcal{G} = \mathcal{G}_1 \oplus \mathcal{G}_2$, a direct sum of $\mathcal{G}_1$ and $\mathcal{G}_2$, compact subgroups of $\mathrm{Ort}(r_1)$ and $\mathrm{Ort}(r_2)$, respectively. The subset of $\mathrm{NND}(k)$ consisting of all matrices symmetric with respect to the group $\mathcal{H}$, i.e. matrices $\mathbf{A} \in \mathrm{NND}(k)$ such that $\mathbf{HAH}' = \mathbf{A}$ for all $\mathbf{H} \in \mathcal{H}$, will be denoted by $\mathrm{NND}(k, \mathcal{H})$. The following proposition will be useful in the sequel; see Markiewicz (1997, Corollary 2).

PROPOSITION. *If a design $d^* \in \mathcal{D}$ is Kiefer optimal w.r.t. $\mathcal{G} = \mathcal{G}_1 \oplus \mathcal{G}_2$ for estimating ϑ_1 and ϑ_2 simultaneously over $\mathcal{D}$ in $\mathcal{M}_\infty$ then d^* is Kiefer optimal w.r.t. $\mathcal{G}_1$ for estimating ϑ_1 in models $\mathcal{M}_0, \mathcal{M}_\infty$ and in $\mathcal{M}_V$ provided $\mathbf{V} \in \mathrm{NND}(r_2, \mathcal{G}_2)$.*

Let $\mathcal{D}$ denote the set of designs under consideration and let $\mathcal{D}^* \subseteq \mathcal{D}$ denote the set of all $d \in \mathcal{D}$ which are Kiefer optimal w.r.t. $\mathcal{G}_1$ for estimating ϑ_1 over $\mathcal{D}$ in $\mathcal{M}_0$. We seek a design $d^* \in \mathcal{D}^*$ which is universally optimal w.r.t. $\mathbf{\Phi}(\mathcal{G}_1)$ in $\mathcal{M}_V$. We will consider two special cases corresponding to Strategy 1 and 2 in Kunert (1983).

CASE 1. Assume that there is a $d^* \in \mathcal{D}^*$ fulfilling the adjusted orthogonality condition

$$\mathbf{X}'_{1,d}\mathbf{Q}_{X_{3,d}}\mathbf{X}_{2,d} = \mathbf{0}, \tag{7}$$

i.e. $\mathbf{W}_{d^*}$ is a block-diagonal matrix with left upper block equal to $\mathbf{C}_{d^*,0}$. Then from (4), (5), (6), and (7) it follows that $\mathbf{C}_{d^*,0} = \mathbf{C}_{d^*,\infty} = \mathbf{C}_{d^*,V}$ and

$$\mathbf{C}_{d,\infty} \ll_{G1} \mathbf{C}_{d^*,0}, \quad \mathbf{C}_{d,V} \ll_{G1} \mathbf{C}_{d^*,0} \quad \text{for all } d \in D \quad \text{and arbitrary } \mathbf{V} \in \mathrm{NND}(r_2).$$

It means that d^* is universally optimal w.r.t. $\mathbf{\Phi}(\mathcal{G}_1)$ over $\mathcal{D}$ in $\mathcal{M}_\infty$ as well as in $\mathcal{M}_V$ for arbitrary $\mathbf{V} \in \mathrm{NND}(r_2)$.

If no design $d \in \mathcal{D}^*$ fulfils its adjusted orthogonality condition (7) we will proceed in the following way.

CASE 2. Find a $d^* \in D^*$ such that

$$\mathbf{W}_d \ll_G \mathbf{W}_{d^*} \quad \text{for all } d \in \tilde{\mathcal{D}} \subseteq \mathcal{D}.$$

Then d^* is Kiefer optimal w.r.t. $\mathcal{G}$ for estimating ϑ_1 and ϑ_2 simultaneously over $\tilde{\mathcal{D}}$ in $\mathcal{M}_\infty$. According to Proposition d^* is also universally optimal w.r.t. $\mathbf{\Phi}(\mathcal{G}_1)$ for estimating ϑ_1 over $\tilde{\mathcal{D}}$ in $\mathcal{M}_\infty$ as well as in $\mathcal{M}_V$ for any $\mathbf{V} \in \mathrm{NND}(r_2, \mathcal{G}_2)$.

3. Examples

3.1. Row-column designs for comparing treatments with a control

Consider the set $\mathcal{D}$ of row-column designs for comparing t test treatments with a control treatment, say 0, in which ab experimental units are arranged in the form of an $a \times b$ array of entries from the set $\{0, 1, 2, ..., t\}$, with $r_0/a = k_0$ and $(b - k_0)/t$ integers, where r_0 is a fixed number of replications of the 0 treatment. Now, in model (1) notation $\vartheta_1, \vartheta_2, \vartheta_3$ are vectors of treatments effects, rows effects, and columns effects, respectively. Let $\mathcal{D}^*$ be the set of BTB (BTIB) designs on columns, i.e. designs which are Kiefer optimal w.r.t. $\mathcal{G}_1 = \{1\} \oplus \mathcal{P}_t$, for estimating ϑ_1 over $\mathcal{D}$ in $\mathcal{M}_0$, where $\mathcal{P}_t$ denotes the set of all $t \times t$ permutation matrices; see e.g. Bechhofer and Tamhane

(1981). Further, let $\mathbf{N}_{1,d} \in \mathbb{R}^{t+1 \times a}$ and $\mathbf{N}_{2,d} \in \mathbb{R}^{t+1 \times b}$ be the incidence matrices of treatments vs. rows and treatments vs. columns, respectively. In this case, the matrix $\mathbf{W}_d$ can be written as

$$\mathbf{W}_d = \begin{pmatrix} \mathbf{r}_d^{\delta} - 1/a(t+1)\mathbf{N}_{2,d}\mathbf{N}_{2,d}' & \mathbf{N}_{1,d} - 1/a\mathbf{N}_{2,d}\mathbf{J}_{ba} \\ \mathbf{N}_{1,d}' - 1/a\mathbf{J}_{ab}\mathbf{N}_{2,d}' & bt\mathbf{I}_a - (t+1)/a\mathbf{J}_{aa} \end{pmatrix},$$

where $\mathbf{r}_d = \mathbf{N}_{1,d}\mathbf{1}_a = \mathbf{N}_{2,d}\mathbf{1}_b$ is a vector of replications and $\mathbf{r}_d^{\delta} = \operatorname{diag}(r_{0d}, r_{1d}, ..., r_{td})$. For a design $d^* \in \mathcal{D}^*$ which has treatments equally replicated, and the total number of replications for each treatment, test or control, divided equally among the a rows, the adjusted orthogonality condition (7) holds, i.e. $\mathbf{N}_{1,d} - (1/a)\mathbf{N}_{2,d}\mathbf{J}_{ba} = \mathbf{0}$. Then, according to CASE 1, d^* is universally optimal w.r.t. $\mathbf{\Phi}(\{1\} \oplus \mathcal{P}_t)$ for estimating treatment effects in the models $\mathcal{M}_\infty$ (see e.g. Hedayat et al., 1988; Giovagnoli and Verdinelli, 1988, p. 484) and $\mathcal{M}_V$ with $\mathbf{V} \in \mathrm{NND}(a)$.

3.2. Repeated measurements designs

Consider the set $\mathcal{D} = \Lambda_{t,n,p}$ of all non-circular repeated measurements designs, abbreviated as RMD(t,n,p), in which no treatment is allowed to be preceded by itself. A model for RMD(t,n,p) is usually written as

$$\mathbf{Y}_d = \mathbf{G}_d\boldsymbol{\tau} + \mathbf{F}_d\boldsymbol{\rho} + \mathbf{P}\boldsymbol{\alpha} + \mathbf{U}\boldsymbol{\beta} + \mathbf{e},$$

where $\boldsymbol{\tau}$ is the vector of direct treatment effects, $\boldsymbol{\rho}$ the vector of residual effects, $\boldsymbol{\alpha}$ the vector of period effects, and $\boldsymbol{\beta}$ the vector of effects of units; see e.g. Cheng and Wu (1980), and Kunert (1983). In model (1) notation,

$$\mathbf{X}_{1,d} = \mathbf{G}_d,\ \mathbf{X}_{2,d} = (\mathbf{F}_d \,\vdots\, \mathbf{P}),\ \mathbf{X}_{3,d} = \mathbf{U},$$

while

$$\boldsymbol{\vartheta}_1 = \boldsymbol{\tau},\ \boldsymbol{\vartheta}_2 = (\boldsymbol{\rho}', \boldsymbol{\alpha}')',\ \boldsymbol{\vartheta}_3 = \boldsymbol{\beta}.$$

Let $\mathcal{D}^*$ be the set of all balanced block designs on the units, i.e. designs which are universally optimal (and Kiefer optimal w.r.t. $\mathcal{P}_t$) for estimating $\boldsymbol{\tau}$ over $\mathcal{D}$ in $\mathcal{M}_0$. Suppose that for every $d \in \mathcal{D}$ the adjusted orthogonality condition (7) does not hold. Further, Suppose that in $\mathcal{D}^*$ there is a balanced uniform design d^*. From Proposition 2 in Markiewicz (1997) it follows that d^* is Kiefer optimal w.r.t. $\mathcal{G} = (\mathbf{I}_2 \otimes \mathcal{P}_t) \oplus \{\mathbf{I}_p\}$ for estimating $\boldsymbol{\tau}, \boldsymbol{\rho}$, and $\boldsymbol{\alpha}$ simultaneously over $\tilde{\mathcal{D}} \subseteq \Lambda_{t,n,p}$, the set of designs which are uniform on units and the last period, in M_∞. Then, according to CASE 2, d^* is universally optimal (w.r.t. $\mathbf{\Phi}(\mathcal{P}_t)$) for estimating $\boldsymbol{\tau}$ over $\Lambda_{t,n,p}$ in $\mathcal{M}_\infty$ and in $\mathcal{M}_V$ with $\mathbf{V} \in \mathrm{NND}(t+p, P_t \oplus \{\mathbf{I}_p\})$.

References

Bechhofer, R.E. and Tamhane, A.C. (1981). Incomplete block designs for comparing treatments with a control: General theory. *Technometrics* **23**, 45-57.

Cheng, C.S. and Wu, C.F. (1980). Balanced repeated measurements designs. *Ann. Statist.* **8**, 1272-1283. Corrigenda: *Ann. Statist.* **11**, 349.

Giovagnoli, A., Pukelsheim, F. and Wynn, H.P. (1987). Group invariant orderings and experimental designs. *J. Statist. Plann. Inference* **17**, 159-171.

Giovagnoli, A. and Verdinelli, I. (1988). Comment to: Optimum designs for comparing test treatments with controls by A.S. Hedayat, M. Jacroux and D. Majumdar. *Statistical Science* **3**, 482-484.

Hedayat, A.S., Jacroux, M. and Majumdar, D. (1988). Optimum designs for comparing test treatments with controls. *Statistical Science* **3**, 462-476.

Jones, B., Kunert, J. and Wynn, H.P. (1992). Information matrices for mixed effects models with applications to the optimality of repeated measurements designs. *J. Statist. Plann. Inference* **33**, 261-274.

Kiefer, J. (1975). Construction and optimality of generalized Youden designs. In: J.N. Srivastava, Ed., *A Survey of Statistical Designs and Linear Models.* North-Holland, Amsterdam.

Kunert, J. (1983). Optimal design and refinement of the linear model with applications to repeated measurements designs. *Ann. Statist.* **11**, 247-257.

Markiewicz, A. (1997). Properties of information matrices for linear models and universal optimality of experimental designs. *J. Statist. Plann. Inference* **59**, 127-137.

Pukelsheim, F. (1993). *Optimal Designs of Experiments.* Wiley, New York.

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Optymalność pewnych układów doświadczalnych w mieszanym modelu liniowym

Streszczenie

Układ, który jest uniwersalnie optymalny dla estymacji danego zbioru parametrów w modelu stałym jest również uniwersalnie optymalny dla estymacji zredukowanego zbioru parametrów w odpowiednim modelu mieszanym. Celem pracy jest zbadanie warunków, przy których układ uniwersalnie optymalny w modelu bez efektów losowych (tzn. w modelu, w którym wariancje efektów losowych są równe zero) jest również uniwersalnie optymalny w modelu mieszanym. Wyprowadzono pewne warunki dostateczne z wykorzystaniem porządku Kiefera.

Słowa kluczowe: model mieszany, uzupełnienie Schura, majoryzacja grupowa, porządek Kiefera, optymalne układy eksperymentalne, układy wierszowo-kolumnowe, układy z powtarzanymi pomiarami.