Contributions to Statistics

S. Ejaz Ahmed
Francisco Carvalho
Simo Puntanen *Editors*

Matrices, Statistics and Big Data

Selected Contributions from IWMS 2016

Springer

Contributions to Statistics

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Editors

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To Ingram Olkin

Preface

The 25th International Workshop on Matrices and Statistics (IWMS-2016) was held in the city of Funchal on the beautiful Madeira Island, the Pearl of the Atlantic, on 6–9 June 2016.

The purpose of this workshop was to bring together researchers sharing an interest in a variety of aspects of statistics and its applications as well as matrix analysis and its applications to statistics and to offer them a possibility to discuss current developments in these subjects. The workshop contributed to bridge the gap among statisticians, computer scientists, and mathematicians in understanding each other's tools.

The Local Organizing Committee was chaired by Francisco Carvalho (Tomar, Portugal) and the International Organizing Committee by Simo Puntanen (Tampere, Finland), while George P. H. Styan (Montréal, Québec, Canada) was the Honorary Chair.

IWMS-2016 was organized by the Instituto Politécnico de Tomar and Universidade da Madeira and was supported by the CMA (Centro de Matemática e Aplicações) (FCT, UNL), CIMA (Centro de Investigação em Matemática e Aplicações) (UE), PSE (Produtos e Serviços de Estatística), INE (Instituto Nacional de Estatística), FLAD (Fundação Luso-Americana para o Desenvolvimento), Delta Cafés, and Associação de Promoção da Madeira.

The workshop comprised invited talks, contributed talks, and special sessions; for the details, see the conference report on IWMS-2016 in IMAGE, The Bulletin of the International Linear Algebra Society, Issue Number 57, pp. 18–19. The final program and the *Book of Abstracts*, edited by Daniel Klein and Francisco Carvalho, are online on the IWMS-2016 website.

For previous IWMS workshops, see the IWMS-website, from where, for example, "a short history of the International Workshop on Matrices and Statistics" can be downloaded: online pdf. The 26th International Workshop on Matrices and Statistics was held in Montréal, Québec, Canada, in 2018, and the 27th International Workshop on Matrices and Statistics will be held in Shanghai, China, in 2019.

This volume, *Matrices, Statistics, and Big Data*, in the series Contributions to Statistics published by Springer, comprises selected refereed papers presented at the IWMS-2016.

We would like to thank all the authors for their valuable contributions to this volume. Our special thanks go to all the reviewers for their diligent reviews.

St. Catharines, ON, Canada — S. Ejaz Ahmed
Tomar, Portugal — Francisco Carvalho
Tampere, Finland — Simo Puntanen
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Further Properties of the Linear Sufficiency in the Partitioned Linear Model

Augustyn Markiewicz and Simo Puntanen

Abstract A linear statistic $\mathbf{Fy}$, where $\mathbf{F}$ is an $f \times n$ matrix, is called linearly sufficient for estimable parametric function $\mathbf{K}\boldsymbol{\beta}$ under the model $\mathscr{M} = \{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{V}\}$, if there exists a matrix $\mathbf{A}$ such that $\mathbf{AFy}$ is the BLUE for $\mathbf{K}\boldsymbol{\beta}$. In this paper we consider some particular aspects of the linear sufficiency in the partitioned linear model where $\mathbf{X} = (\mathbf{X}_1 : \mathbf{X}_2)$ with $\boldsymbol{\beta}$ being partitioned accordingly. We provide new results and new insightful proofs for some known facts, using the properties of relevant covariance matrices and their expressions via certain orthogonal projectors. Particular attention will be paid to the situation under which adding new regressors (in $\mathbf{X}_2$) does not affect the linear sufficiency of $\mathbf{Fy}$.

Keywords Best linear unbiased estimator · Generalized inverse · Linear model · Linear sufficiency · Orthogonal projector · Löwner ordering · Transformed linear model

1 Introduction

In this paper we consider the partitioned linear model $\mathbf{y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2 + \boldsymbol{\varepsilon}$, or shortly denoted

$$\mathscr{M}_{12} = \{\mathbf{y},\ \mathbf{X}\boldsymbol{\beta},\ \mathbf{V}\} = \{\mathbf{y},\ \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2,\ \mathbf{V}\}\,, \tag{1}$$

where we may drop off the subscripts from $\mathscr{M}_{12}$ if the partitioning is not essential in the context. In (1), $\mathbf{y}$ is an n-dimensional observable response variable, and $\boldsymbol{\varepsilon}$ is an

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unobservable random error with a known covariance matrix $\mathrm{cov}(\boldsymbol{\varepsilon}) = \mathbf{V} = \mathrm{cov}(\mathbf{y})$ and expectation $\mathrm{E}(\boldsymbol{\varepsilon}) = \mathbf{0}$. The matrix $\mathbf{X}$ is a known $n \times p$ matrix, i.e., $\mathbf{X} \in \mathbb{R}^{n\times p}$, partitioned columnwise as $\mathbf{X} = (\mathbf{X}_1 : \mathbf{X}_2)$, $\mathbf{X}_i \in \mathbb{R}^{n\times p_i}$, $i = 1, 2$. Vector $\boldsymbol{\beta} = (\boldsymbol{\beta}_1', \boldsymbol{\beta}_2')' \in \mathbb{R}^p$ is a vector of fixed (but unknown) parameters; here, symbol $'$ stands for the transpose. Sometimes we will denote $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$, $\boldsymbol{\mu}_i = \mathbf{X}_i\boldsymbol{\beta}_i$, $i = 1, 2$.

As for notations, the symbols $\mathrm{r}(\mathbf{A})$, $\mathbf{A}^-$, $\mathbf{A}^+$, $\mathscr{C}(\mathbf{A})$, and $\mathscr{C}(\mathbf{A})^\perp$ denote, respectively, the rank, a generalized inverse, the Moore–Penrose inverse, the column space, and the orthogonal complement of the column space of the matrix $\mathbf{A}$. By $\mathbf{A}^\perp$ we denote any matrix satisfying $\mathscr{C}(\mathbf{A}^\perp) = \mathscr{C}(\mathbf{A})^\perp$. Furthermore, we will write $\mathbf{P}_\mathbf{A} = \mathbf{P}_{\mathscr{C}(\mathbf{A})} = \mathbf{A}\mathbf{A}^+ = \mathbf{A}(\mathbf{A}'\mathbf{A})^-\mathbf{A}'$ to denote the orthogonal projector (with respect to the standard inner product) onto $\mathscr{C}(\mathbf{A})$. In particular, we denote $\mathbf{M} = \mathbf{I}_n - \mathbf{P}_\mathbf{X}$, $\mathbf{M}_i = \mathbf{I}_n - \mathbf{P}_{\mathbf{X}_i}$, $i = 1, 2$.

In addition to the *full* model $\mathscr{M}_{12}$, we will consider the *small* models $\mathscr{M}_i = \{\mathbf{y},\ \mathbf{X}_i\boldsymbol{\beta}_i,\ \mathbf{V}\}$, $i = 1, 2$, and the *reduced* model

$$\mathscr{M}_{12\cdot 2} = \{\mathbf{M}_2\mathbf{y},\ \mathbf{M}_2\mathbf{X}_1\boldsymbol{\beta}_1,\ \mathbf{M}_2\mathbf{V}\mathbf{M}_2\}\,, \tag{2}$$

which is obtained by premultiplying the model $\mathscr{M}_{12}$ by $\mathbf{M}_2 = \mathbf{I}_n - \mathbf{P}_{\mathbf{X}_2}$. There is one further model that takes lot of our attention, it is the *transformed* model

$$\mathscr{M}_t = \{\mathbf{F}\mathbf{y},\ \mathbf{F}\mathbf{X}\boldsymbol{\beta},\ \mathbf{F}\mathbf{V}\mathbf{F}'\} = \{\mathbf{F}\mathbf{y},\ \mathbf{F}\mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{F}\mathbf{X}_2\boldsymbol{\beta}_2,\ \mathbf{F}\mathbf{V}\mathbf{F}'\}\,, \tag{3}$$

which is obtained be premultiplying $\mathscr{M}_{12}$ by matrix $\mathbf{F} \in \mathbb{R}^{f\times n}$.

We assume that the models under consideration are consistent which in the case of $\mathscr{M}$ means that the observed value of the response variable satisfies

$$\mathbf{y} \in \mathscr{C}(\mathbf{X} : \mathbf{V}) = \mathscr{C}(\mathbf{X} : \mathbf{V}\mathbf{X}^\perp) = \mathscr{C}(\mathbf{X}) \oplus \mathscr{C}(\mathbf{V}\mathbf{X}^\perp)\,, \tag{4}$$

where "$\oplus$" refers to the direct sum of column spaces.

Under the model $\mathscr{M}$, the statistic $\mathbf{G}\mathbf{y}$, where $\mathbf{G}$ is an $n \times n$ matrix, is the best linear unbiased estimator, BLUE, of $\mathbf{X}\boldsymbol{\beta}$ if $\mathbf{G}\mathbf{y}$ is unbiased, i.e., $\mathbf{G}\mathbf{X} = \mathbf{X}$, and it has the smallest covariance matrix in the Löwner sense among all unbiased linear estimators of $\mathbf{X}\boldsymbol{\beta}$; shortly denoted

$$\mathrm{cov}(\mathbf{G}\mathbf{y}) \le_\mathrm{L} \mathrm{cov}(\mathbf{C}\mathbf{y}) \quad \text{for all } \mathbf{C} \in \mathbb{R}^{n\times n} :\ \mathbf{C}\mathbf{X} = \mathbf{X}\,. \tag{5}$$

The BLUE of an estimable parametric function $\mathbf{K}\boldsymbol{\beta}$, where $\mathbf{K} \in \mathbb{R}^{k\times p}$, is defined in the corresponding way. Recall that $\mathbf{K}\boldsymbol{\beta}$ is said to be estimable if it has a linear unbiased estimator which happens if and only if $\mathscr{C}(\mathbf{K}') \subset \mathscr{C}(\mathbf{X}')$, i.e.,

$$\mathbf{K}\boldsymbol{\beta} \text{ is estimable under } \mathscr{M} \iff \mathscr{C}(\mathbf{K}') \subset \mathscr{C}(\mathbf{X}')\,. \tag{6}$$

The structure of our paper is as follows. In Sect. 2 we provide some preliminary results that are not only needed later on but they also have some matrix-algebraic interest in themselves. In Sects. 3 and 4 we consider the estimation of $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$ and

$\boldsymbol{\mu}_1 = \mathbf{X}_1\boldsymbol{\beta}_1$, respectively. In Sect. 5 we study the linear sufficiency under $\mathscr{M}_1$ vs. $\mathscr{M}_{12}$. We characterize the linearly sufficient statistic $\mathbf{Fy}$ by using the covariance matrices of the BLUEs under $\mathscr{M}_{12}$ and under its transformed version $\mathscr{M}_t$. In particular, certain orthogonal projectors appear useful in our considerations. From a different angle, the linear sufficiency in a partitioned linear model has been treated, e.g., in Isotalo and Puntanen [10, 11], Markiewicz and Puntanen [16], and Kala and Pordzik [13]. Baksalary [1, 2, §3.3, §5] considered linear sufficiency under $\mathscr{M}_{12}$ and $\mathscr{M}_1$ assuming that $\mathbf{V} = \mathbf{I}_n$. Dong et al. [6] study interesting connections between the BLUEs under two transformed models using the so-called matrix-rank method.

2 Some Preliminary Results

For the proof of the following fundamental lemma, see, e.g., Rao [22, p. 282].

Lemma 1 *Consider the general linear model* $\mathscr{M} = \{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{V}\}$. *Then the statistic* $\mathbf{Gy}$ *is the* BLUE *for* $\mathbf{X}\boldsymbol{\beta}$ *if and only if* $\mathbf{G}$ *satisfies the equation*

$$\mathbf{G}(\mathbf{X} : \mathbf{V}\mathbf{X}^\perp) = (\mathbf{X} : \mathbf{0})\,, \tag{7}$$

in which case we denote $\mathbf{G} \in \{\mathbf{P}_{\mathbf{X}|\mathbf{V}\mathbf{X}^\perp}\}$. *The corresponding condition for* $\mathbf{By}$ *to be the* BLUE *of an estimable parametric function* $\mathbf{K}\boldsymbol{\beta}$ *is*

$$\mathbf{B}(\mathbf{X} : \mathbf{V}\mathbf{X}^\perp) = (\mathbf{K} : \mathbf{0})\,. \tag{8}$$

Two estimators $\mathbf{G}_1\mathbf{y}$ and $\mathbf{G}_2\mathbf{y}$ are said to be equal (with probability 1) whenever $\mathbf{G}_1\mathbf{y} = \mathbf{G}_2\mathbf{y}$ for all $\mathbf{y} \in \mathscr{C}(\mathbf{X} : \mathbf{V}) = \mathscr{C}(\mathbf{X} : \mathbf{V}\mathbf{X}^\perp)$. When talking about the equality of estimators we sometimes may drop the phrase "with probability 1". Thus for any $\mathbf{G}_1, \mathbf{G}_2 \in \{\mathbf{P}_{\mathbf{X}|\mathbf{V}\mathbf{X}^\perp}\}$ we have $\mathbf{G}_1(\mathbf{X} : \mathbf{V}\mathbf{X}^\perp) = \mathbf{G}_2(\mathbf{X} : \mathbf{V}\mathbf{X}^\perp)$, and thereby $\mathbf{G}_1\mathbf{y} = \mathbf{G}_2\mathbf{y}$ with probability 1.

One well-known solution for $\mathbf{G}$ in (7) (which is always solvable) is

$$\mathbf{P}_{\mathbf{X};\mathbf{W}^-} := \mathbf{X}(\mathbf{X}'\mathbf{W}^-\mathbf{X})^-\mathbf{X}'\mathbf{W}^-, \tag{9}$$

where $\mathbf{W}$ is a matrix belonging to the set of nonnegative definite matrices defined as

$$\mathscr{W} = \left\{\mathbf{W} \in \mathbb{R}^{n\times n} : \mathbf{W} = \mathbf{V} + \mathbf{X}\mathbf{U}\mathbf{U}'\mathbf{X}',\ \mathscr{C}(\mathbf{W}) = \mathscr{C}(\mathbf{X} : \mathbf{V})\right\}. \tag{10}$$

For clarity, we may use the notation $\mathscr{W}_{\mathscr{A}}$ to indicate which model is under consideration. Similarly, $\mathbf{W}_{\mathscr{A}}$ may denote a member of class $\mathscr{W}_{\mathscr{A}}$. We will also use the phrase "$\mathbf{W}_{\mathscr{A}}$ is a $\mathbf{W}$-matrix under the model $\mathscr{A}$".

For the partitioned linear model $\mathscr{M}_{12}$ we will say that $\mathbf{W} \in \mathscr{W}$ if the following properties hold:

$$\begin{aligned}\mathbf{W} &= \mathbf{V} + \mathbf{X}\mathbf{U}\mathbf{U}'\mathbf{X}' = \mathbf{V} + (\mathbf{X}_1 : \mathbf{X}_2)\begin{pmatrix}\mathbf{U}_1\mathbf{U}_1' & \mathbf{0}\\ \mathbf{0} & \mathbf{U}_2\mathbf{U}_2'\end{pmatrix}\begin{pmatrix}\mathbf{X}_1'\\ \mathbf{X}_2'\end{pmatrix}\\ &= \mathbf{V} + \mathbf{X}_1\mathbf{U}_1\mathbf{U}_1'\mathbf{X}_1' + \mathbf{X}_2\mathbf{U}_2\mathbf{U}_2'\mathbf{X}_2', \qquad (11a)\\ \mathbf{W}_i &= \mathbf{V} + \mathbf{X}_i\mathbf{U}_i\mathbf{U}_i'\mathbf{X}_i', \quad i = 1, 2, \qquad (11b)\\ \mathscr{C}(\mathbf{W}) &= \mathscr{C}(\mathbf{X} : \mathbf{V}), \quad \mathscr{C}(\mathbf{W}_i) = \mathscr{C}(\mathbf{X}_i : \mathbf{V}), \quad i = 1, 2. \qquad (11c)\end{aligned}$$

For example, the following statements concerning $\mathbf{W} \in \mathscr{W}$ are equivalent:

$$\mathscr{C}(\mathbf{X} : \mathbf{V}) = \mathscr{C}(\mathbf{W}), \quad \mathscr{C}(\mathbf{X}) \subset \mathscr{C}(\mathbf{W}), \quad \mathscr{C}(\mathbf{X}'\mathbf{W}^{-}\mathbf{X}) = \mathscr{C}(\mathbf{X}'). \qquad (12)$$

Instead of $\mathscr{W}$, several corresponding properties also hold in the extended set

$$\mathscr{W}_* = \left\{\mathbf{W} \in \mathbb{R}^{n\times n} : \mathbf{W} = \mathbf{V} + \mathbf{X}\mathbf{N}\mathbf{X}', \ \mathscr{C}(\mathbf{W}) = \mathscr{C}(\mathbf{X} : \mathbf{V})\right\}, \qquad (13)$$

where $\mathbf{N} \in \mathbb{R}^{p\times p}$ can be any (not necessarily nonnegative definite) matrix satisfying $\mathscr{C}(\mathbf{W}) = \mathscr{C}(\mathbf{X} : \mathbf{V})$. However, in this paper we consider merely the set $\mathscr{W}$. For further properties of $\mathscr{W}_*$, see, e.g., Puntanen et al. [21, §12.3] and Kala et al. [15].

Using (9), the BLUEs of $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$ and of estimable $\mathbf{K}\boldsymbol{\beta}$, respectively, can be expressed as

$$\mathrm{BLUE}(\mathbf{X}\boldsymbol{\beta} \mid \mathscr{M}) = \tilde{\boldsymbol{\mu}}(\mathscr{M}) = \mathbf{X}(\mathbf{X}'\mathbf{W}^{-}\mathbf{X})^{-}\mathbf{X}'\mathbf{W}^{-}\mathbf{y}, \qquad (14a)$$

$$\mathrm{BLUE}(\mathbf{K}\boldsymbol{\beta} \mid \mathscr{M}) = \mathbf{K}(\mathbf{X}'\mathbf{W}^{-}\mathbf{X})^{-}\mathbf{X}'\mathbf{W}^{-}\mathbf{y}, \qquad (14b)$$

where $\mathbf{W}$ belongs to the class $\mathscr{W}$. The representations (14a)–(14b) are invariant with respect to the choice of generalized inverses involved; this can be shown using (12) and the fact that for any nonnull $\mathbf{A}$ and $\mathbf{C}$ the following holds [Rao and Mitra [23, Lemma 2.2.4]]:

$$\mathbf{A}\mathbf{B}^{-}\mathbf{C} = \mathbf{A}\mathbf{B}^{+}\mathbf{C} \text{ for all } \mathbf{B}^{-} \iff \mathscr{C}(\mathbf{C}) \subset \mathscr{C}(\mathbf{B}) \text{ and } \mathscr{C}(\mathbf{A}') \subset \mathscr{C}(\mathbf{B}'). \qquad (15)$$

Notice that part $\mathbf{X}(\mathbf{X}'\mathbf{W}^{-}\mathbf{X})^{-}\mathbf{X}'$ of $\mathbf{P}_{\mathbf{X};\mathbf{W}^{-}}$ in (9) is invariant with respect to the choice of generalized inverses involved but

$$\mathbf{P}_{\mathbf{X};\mathbf{W}^{+}} = \mathbf{X}(\mathbf{X}'\mathbf{W}^{+}\mathbf{X})^{+}\mathbf{X}'\mathbf{W}^{+} = \mathbf{X}(\mathbf{X}'\mathbf{W}^{-}\mathbf{X})^{-}\mathbf{X}'\mathbf{W}^{+} \qquad (16)$$

for any choice of $\mathbf{W}^{-}$ and $(\mathbf{X}'\mathbf{W}^{-}\mathbf{X})^{-}$.

The concept of linear sufficiency was introduced by Baksalary and Kala [3] and Drygas [7] who considered linear statistics, which are "sufficient" for $\mathbf{X}\boldsymbol{\beta}$ under $\mathscr{M}$, or in other words, "linear transformations preserving best linear unbiased estimators". A linear statistic $\mathbf{F}\mathbf{y}$, where $\mathbf{F} \in \mathbb{R}^{f\times n}$, is called linearly sufficient for

$\mathbf{X}\boldsymbol{\beta}$ under the model $\mathscr{M}$ if there exists a matrix $\mathbf{A} \in \mathbb{R}^{n\times f}$ such that $\mathbf{AFy}$ is the BLUE for $\mathbf{X}\boldsymbol{\beta}$. Correspondingly, $\mathbf{Fy}$ is linearly sufficient for estimable $\mathbf{K}\boldsymbol{\beta}$, where $\mathbf{K} \in \mathbb{R}^{k\times p}$, if there exists a matrix $\mathbf{A} \in \mathbb{R}^{k\times f}$ such that $\mathbf{AFy}$ is the BLUE for $\mathbf{K}\boldsymbol{\beta}$.

Sometimes we will denote shortly $\mathbf{Fy} \in \mathrm{S}(\mathbf{X}\boldsymbol{\beta})$ or $\mathbf{Fy} \in \mathrm{S}(\mathbf{X}\boldsymbol{\beta} \mid \mathscr{M})$, to indicate that $\mathbf{Fy}$ is linearly sufficient for $\mathbf{X}\boldsymbol{\beta}$ under the model $\mathscr{M}$ (if the model is not obvious from the context).

Drygas [7] introduced the concept of linear minimal sufficiency and defined it as follows: $\mathbf{Fy}$ is linearly minimal sufficient if for any other linearly sufficient statistics $\mathbf{Sy}$, there exists a matrix $\mathbf{A}$ such that $\mathbf{Fy} = \mathbf{ASy}$ almost surely.

In view of Lemma 1, $\mathbf{Fy}$ is linearly sufficient for $\mathbf{X}\boldsymbol{\beta}$ if and only if the equation

$$\mathbf{AF}(\mathbf{X} : \mathbf{VM}) = (\mathbf{X} : \mathbf{0}) \tag{17}$$

has a solution for $\mathbf{A}$. Baksalary and Kala [3] and Drygas [7] proved part (a) and Baksalary and Kala [4] part (b) of the following:

Lemma 2 *Consider the model* $\mathscr{M} = \{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{V}\}$ *and let* $\mathbf{K}\boldsymbol{\beta}$ *be estimable. Then:*

(a) *The statistic* $\mathbf{Fy}$ *is linearly sufficient for* $\mathbf{X}\boldsymbol{\beta}$ *if and only if*

$$\mathscr{C}(\mathbf{X}) \subset \mathscr{C}(\mathbf{WF}'), \quad \text{where } \mathbf{W} \in \mathscr{W}. \tag{18}$$

Moreover, $\mathbf{Fy}$ *is linearly minimal sufficient for* $\mathbf{X}\boldsymbol{\beta}$ *if and only if* $\mathscr{C}(\mathbf{X}) = \mathscr{C}(\mathbf{WF}')$.

(b) *The statistic* $\mathbf{Fy}$ *is linearly sufficient for* $\mathbf{K}\boldsymbol{\beta}$ *if and only if*

$$\mathscr{C}[\mathbf{X}(\mathbf{X}'\mathbf{W}^{-}\mathbf{X})^{-}\mathbf{K}'] \subset \mathscr{C}(\mathbf{WF}'), \quad \text{where } \mathbf{W} \in \mathscr{W}. \tag{19}$$

Moreover, $\mathbf{Fy}$ *is linearly minimal sufficient for* $\mathbf{K}\boldsymbol{\beta}$ *if and only if equality holds in* (19).

Actually, Kala et al. [15] showed that in Lemma 2 the class $\mathscr{W}$ can be replaced with the more general class $\mathscr{W}_*$ defined in (13). For further related references, see Baksalary and Mathew [5] and Müller [19].

Supposing that $\mathbf{Fy}$ is linearly sufficient for $\mathbf{X}\boldsymbol{\beta}$, one could expect that both $\mathscr{M}$ and its transformed version $\mathscr{M}_t = \{\mathbf{Fy}, \mathbf{FX}\boldsymbol{\beta}, \mathbf{FVF}'\}$ provide the same basis for obtaining the BLUE of $\mathbf{X}\boldsymbol{\beta}$. This connection was proved by Baksalary and Kala [3, 4]. Moreover, Tian and Puntanen [24, Th. 2.8] and Kala et al. [14, Th. 2] showed the following:

Lemma 3 *Consider the model* $\mathscr{M} = \{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{V}\}$ *and* $\mathscr{M}_t = \{\mathbf{Fy}, \mathbf{FX}\boldsymbol{\beta}, \mathbf{FVF}'\}$, *and let* $\mathbf{K}\boldsymbol{\beta}$ *be estimable under* $\mathscr{M}_{12}$ *and* $\mathscr{M}_t$. *Then the following statements are equivalent:*

(a) $\mathbf{Fy}$ *is linearly sufficient for* $\mathbf{K}\boldsymbol{\beta}$.

(b) $\mathrm{BLUE}(\mathbf{K}\boldsymbol{\beta} \mid \mathscr{M}) = \mathrm{BLUE}(\mathbf{K}\boldsymbol{\beta} \mid \mathscr{M}_t)$ *with probability* 1.

(c) *There exists at least one representation of* BLUE *of* $\mathbf{K}\boldsymbol{\beta}$ *under* $\mathscr{M}$ *which is the* BLUE *also under the transformed model* $\mathscr{M}_t$.

Later we will need the following Lemma 4. The proofs are parallel to those in Puntanen et al. [21, §5.13] and Markiewicz and Puntanen [17, Th. 5.2]. In this lemma the notation $\mathbf{A}^{1/2}$ stands for the nonnegative definite square root of a nonnegative definite matrix $\mathbf{A}$. Similarly $\mathbf{A}^{+1/2}$ denotes the Moore–Penrose inverse of $\mathbf{A}^{1/2}$. Notice that in particular $\mathbf{P}_{\mathbf{A}} = \mathbf{A}^{1/2}\mathbf{A}^{+1/2} = \mathbf{A}^{+1/2}\mathbf{A}^{1/2}$.

Lemma 4 *Let* $\mathbf{W}$, $\mathbf{W}_1$ *and* $\mathbf{W}_2$ *be defined as in* (11a)–(11c)*. Then:*

(a) $\mathscr{C}(\mathbf{VM})^{\perp} = \mathscr{C}(\mathbf{WM})^{\perp} = \mathscr{C}(\mathbf{W}^{+}\mathbf{X} : \mathbf{Q}_{\mathbf{W}})$, *where* $\mathbf{Q}_{\mathbf{W}} = \mathbf{I}_n - \mathbf{P}_{\mathbf{W}}$,
(b) $\mathscr{C}(\mathbf{W}^{1/2}\mathbf{M})^{\perp} = \mathscr{C}(\mathbf{W}^{+1/2}\mathbf{X} : \mathbf{Q}_{\mathbf{W}})$,
(c) $\mathscr{C}(\mathbf{W}^{1/2}\mathbf{M}) = \mathscr{C}(\mathbf{W}^{+1/2}\mathbf{X} : \mathbf{Q}_{\mathbf{W}})^{\perp} = \mathscr{C}(\mathbf{W}^{+1/2}\mathbf{X})^{\perp} \cap \mathscr{C}(\mathbf{W})$,
(d) $\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{M}} = \mathbf{P}_{\mathbf{W}} - \mathbf{P}_{\mathbf{W}^{+1/2}\mathbf{X}} = \mathbf{P}_{\mathscr{C}(\mathbf{W})\cap\mathscr{C}(\mathbf{W}^{+1/2}\mathbf{X})^{\perp}}$.

Moreover, in (a)–(d) *the matrices* $\mathbf{X}$, $\mathbf{M}$ *and* $\mathbf{W}$ *can be replaced with* $\mathbf{X}_i$, $\mathbf{M}_i$ *and* $\mathbf{W}_i$, $i = 1, 2$, *respectively, so that, for example,* (a) *becomes*

(e) $\mathscr{C}(\mathbf{VM}_i)^{\perp} = \mathscr{C}(\mathbf{W}_i\mathbf{M}_i)^{\perp} = \mathscr{C}(\mathbf{W}_i^{+}\mathbf{X}_i : \mathbf{Q}_{\mathbf{W}_i}), \quad i = 1, 2.$

Similarly, reversing the roles of $\mathbf{X}$ *and* $\mathbf{M}$*, the following, for example, holds:*

(f) $\mathscr{C}(\mathbf{W}^{+}\mathbf{X})^{\perp} = \mathscr{C}(\mathbf{WM} : \mathbf{Q}_{\mathbf{W}})$ *and* $\mathscr{C}(\mathbf{W}^{+}\mathbf{X}) = \mathscr{C}(\mathbf{VM})^{\perp} \cap \mathscr{C}(\mathbf{W})$.

Also the following lemma appears to be useful for our considerations.

Lemma 5 *Consider the partitioned linear model* $\mathscr{M}_{12}$ *and suppose that* $\mathbf{F}$ *is an* $f \times n$ *matrix and* $\mathbf{W} \in \mathscr{W}$*. Then*

(a) $\mathscr{C}(\mathbf{F}'\mathbf{Q}_{\mathbf{FX}_2}) = \mathscr{C}(\mathbf{F}') \cap \mathscr{C}(\mathbf{M}_2)$, *where* $\mathbf{Q}_{\mathbf{FX}_2} = \mathbf{I}_f - \mathbf{P}_{\mathbf{FX}_2}$,
(b) $\mathscr{C}(\mathbf{WF}'\mathbf{Q}_{\mathbf{FX}_2}) = \mathscr{C}(\mathbf{WF}') \cap \mathscr{C}(\mathbf{WM}_2)$,
(c) $\mathscr{C}(\mathbf{W}^{1/2}\mathbf{F}'\mathbf{Q}_{\mathbf{FX}_2}) = \mathscr{C}(\mathbf{W}^{1/2}\mathbf{F}') \cap \mathscr{C}(\mathbf{W}^{1/2}\mathbf{M}_2)$,
(d) $\mathbf{F}'\mathbf{Q}_{\mathbf{FX}_2} = \mathbf{M}_2\mathbf{F}'\mathbf{Q}_{\mathbf{FX}_2}$.

Proof In light of Rao and Mitra [23, Complement 7, p. 118], we get

$$\mathscr{C}(\mathbf{F}') \cap \mathscr{C}(\mathbf{M}_2) = \mathscr{C}[\mathbf{F}'(\mathbf{FM}_2^{\perp})^{\perp}] = \mathscr{C}(\mathbf{F}'\mathbf{Q}_{\mathbf{FX}_2}), \tag{20}$$

and so (a) is proved. In view of Lemma 4, we have $\mathscr{C}(\mathbf{W}^{1/2}\mathbf{M}_2)^{\perp} = \mathscr{C}(\mathbf{W}^{+1/2}\mathbf{X}_2 : \mathbf{Q}_{\mathbf{W}})$, and hence

$$\begin{aligned}\mathscr{C}(\mathbf{W}^{1/2}\mathbf{F}') \cap \mathscr{C}(\mathbf{W}^{1/2}\mathbf{M}_2) &= \mathscr{C}\{\mathbf{W}^{1/2}\mathbf{F}'[\mathbf{FW}^{1/2}(\mathbf{W}^{1/2}\mathbf{M}_2)^{\perp}]^{\perp}\} \\ &= \mathscr{C}\{\mathbf{W}^{1/2}\mathbf{F}'[\mathbf{FW}^{1/2}(\mathbf{W}^{+1/2}\mathbf{X}_2 : \mathbf{Q}_{\mathbf{W}})]^{\perp}\} \\ &= \mathscr{C}[\mathbf{W}^{1/2}\mathbf{F}'(\mathbf{FX}_2)^{\perp}] = \mathscr{C}(\mathbf{W}^{1/2}\mathbf{F}'\mathbf{Q}_{\mathbf{FX}_2}). \end{aligned} \tag{21}$$

Obviously in (21) $\mathbf{W}^{1/2}$ can be replaced with $\mathbf{W}$. The statement (d) follows immediately from the inclusion $\mathscr{C}(\mathbf{F}'\mathbf{Q}_{\mathbf{FX}_2}) \subset \mathscr{C}(\mathbf{M}_2)$. □

Next we present an important lemma characterizing the estimability under $\mathscr{M}_{12}$ and $\mathscr{M}_t$.

Lemma 6 *Consider the models $\mathscr{M}_{12}$ and its transformed version $\mathscr{M}_t$ and let* $\mathbf{F}$ *be an* $f \times n$ *matrix. Then the followings statements hold:*

(a) $\mathbf{X}\boldsymbol{\beta}$ *is estimable under* $\mathscr{M}_t$ *if and only if*

$$\mathscr{C}(\mathbf{X}') = \mathscr{C}(\mathbf{X}'\mathbf{F}'), \quad \textit{i.e.,} \quad \mathscr{C}(\mathbf{X}) \cap \mathscr{C}(\mathbf{F}')^{\perp} = \{\mathbf{0}\}\,. \tag{22}$$

(b) $\mathbf{X}_1\boldsymbol{\beta}_1$ *is estimable under* $\mathscr{M}_{12}$ *if and only if*

$$\mathscr{C}(\mathbf{X}_1') = \mathscr{C}(\mathbf{X}_1'\mathbf{M}_2)\,, \quad \textit{i.e.,} \quad \mathscr{C}(\mathbf{X}_1) \cap \mathscr{C}(\mathbf{X}_2) = \{\mathbf{0}\}\,. \tag{23}$$

(c) $\mathbf{X}_1\boldsymbol{\beta}_1$ *is estimable under* $\mathscr{M}_t$ *if and only if*

$$\mathscr{C}(\mathbf{X}_1') = \mathscr{C}(\mathbf{X}_1'\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2})\,, \tag{24}$$

or, equivalently, if and only if

$$\mathscr{C}(\mathbf{X}_1') = \mathscr{C}(\mathbf{X}_1'\mathbf{F}') \quad \textit{and} \quad \mathscr{C}(\mathbf{F}\mathbf{X}_1) \cap \mathscr{C}(\mathbf{F}\mathbf{X}_2) = \{\mathbf{0}\}\,. \tag{25}$$

(d) $\boldsymbol{\beta}$ *is estimable under* $\mathscr{M}_{12}$ *if and only if* $\mathrm{r}(\mathbf{X}) = p$.
(e) $\boldsymbol{\beta}_1$ *is estimable under* $\mathscr{M}_{12}$ *if and only if* $\mathrm{r}(\mathbf{X}_1'\mathbf{M}_2) = p_1$.
(f) $\boldsymbol{\beta}_1$ *is estimable under* $\mathscr{M}_t$ *if and only if* $\mathrm{r}(\mathbf{X}_1'\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}) = \mathrm{r}(\mathbf{X}_1) = p_1$.

Proof In view of (6), $\mathbf{X}\boldsymbol{\beta}$ is estimable under $\mathscr{M}_t$ if and only if $\mathscr{C}(\mathbf{X}') \subset \mathscr{C}(\mathbf{X}'\mathbf{F}')$, i.e., $\mathscr{C}(\mathbf{X}') = \mathscr{C}(\mathbf{X}'\mathbf{F}')$. The alternative claim in (a) follows from

$$\mathrm{r}(\mathbf{F}\mathbf{X}) = \mathrm{r}(\mathbf{X}) - \mathscr{C}(\mathbf{X}) \cap \mathscr{C}(\mathbf{F}')^{\perp}, \tag{26}$$

where we have used the rank rule of Marsaglia and Styan [18, Cor. 6.2] for the matrix product. For the claim (b), see, e.g., Puntanen et al. [21, §16.1]. To prove (c), we observe that $\mathbf{X}_1\boldsymbol{\beta}_1 = (\mathbf{X}_1 : \mathbf{0})\boldsymbol{\beta}$ is estimable under $\mathscr{M}_t$ if and only if

$$\mathscr{C}\begin{pmatrix}\mathbf{X}_1'\\ \mathbf{0}\end{pmatrix} \subset \mathscr{C}\begin{pmatrix}\mathbf{X}_1'\mathbf{F}'\\ \mathbf{X}_2'\mathbf{F}'\end{pmatrix}, \text{ i.e., } \mathbf{X}_1' = \mathbf{X}_1'\mathbf{F}'\mathbf{A} \text{ and } \mathbf{0} = \mathbf{X}_2'\mathbf{F}'\mathbf{A}\,, \tag{27}$$

for some $\mathbf{A}$. The equality $\mathbf{0} = \mathbf{X}_2'\mathbf{F}'\mathbf{A}$ means that $\mathbf{A} = \mathbf{Q}_{\mathbf{F}\mathbf{X}_2}\mathbf{B}$ for some $\mathbf{B}$, and thereby $\mathbf{X}_1' = \mathbf{X}_1'\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}\mathbf{B}$ which holds if and only if $\mathscr{C}(\mathbf{X}_1') = \mathscr{C}(\mathbf{X}_1'\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2})$. Thus we have proved condition (24). Notice that (24) is equivalent to

$$\begin{aligned}\mathrm{r}(\mathbf{X}_1') &= \mathrm{r}(\mathbf{X}_1'\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}) = \mathrm{r}(\mathbf{X}_1'\mathbf{F}') - \dim \mathscr{C}(\mathbf{F}\mathbf{X}_1) \cap \mathscr{C}(\mathbf{F}\mathbf{X}_2)\\ &= \mathrm{r}(\mathbf{X}_1) - \dim \mathscr{C}(\mathbf{X}_1) \cap \mathscr{C}(\mathbf{F}')^{\perp} - \dim \mathscr{C}(\mathbf{F}\mathbf{X}_1) \cap \mathscr{C}(\mathbf{F}\mathbf{X}_2)\,,\end{aligned} \tag{28}$$

which confirms (25). The proofs of (d)–(f) are obvious. □

For the proof Lemma 7, see, e.g., Puntanen et al. [21, p. 152].

Lemma 7 *The following three statements are equivalent:*

$$\mathbf{P_A} - \mathbf{P_B} \text{ is an orthogonal projector}, \quad \mathbf{P_A} - \mathbf{P_B} \geq_{\mathrm{L}} \mathbf{0}, \quad \mathscr{C}(\mathbf{B}) \subset \mathscr{C}(\mathbf{A}). \tag{29}$$

If any of the above conditions holds, then $\mathbf{P_A} - \mathbf{P_B} = \mathbf{P}_{\mathscr{C}(\mathbf{A}) \cap \mathscr{C}(\mathbf{B})^\perp} = \mathbf{P}_{(\mathbf{I}-\mathbf{P_B})\mathbf{A}}$.

3 Linearly Sufficient Statistic for $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$ in $\mathscr{M}_{12}$

Let us consider a partitioned linear model $\mathscr{M}_{12} = \{\mathbf{y}, \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2, \mathbf{V}\}$, and its transformed version $\mathscr{M}_t = \{\mathbf{Fy}, \mathbf{FX}_1\boldsymbol{\beta}_1 + \mathbf{FX}_2\boldsymbol{\beta}_2, \mathbf{FVF}'\}$. Choosing $\mathbf{W} = \mathbf{V} + \mathbf{XUU}'\mathbf{X}' \in \mathscr{W}$, we have, for example, the following representations for the covariance matrix of the BLUE for $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$:

$$\begin{aligned}
\operatorname{cov}(\tilde{\boldsymbol{\mu}} \mid \mathscr{M}_{12}) &= \mathbf{V} - \mathbf{VM}(\mathbf{MVM})^-\mathbf{MV} = \mathbf{W} - \mathbf{WM}(\mathbf{MWM})^-\mathbf{MW} - \mathbf{T} \\
&= \mathbf{W}^{1/2}(\mathbf{I}_n - \mathbf{P}_{\mathbf{W}^{1/2}\mathbf{M}})\mathbf{W}^{1/2} - \mathbf{T} = \mathbf{W}^{1/2}\mathbf{P}_{\mathbf{W}^{+1/2}\mathbf{X}}\mathbf{W}^{1/2} - \mathbf{T} \\
&= \mathbf{X}(\mathbf{X}'\mathbf{W}^{+}\mathbf{X})^-\mathbf{X}' - \mathbf{T} = \mathbf{X}(\mathbf{X}'\mathbf{W}^{+1/2}\mathbf{W}^{+1/2}\mathbf{X})^-\mathbf{X}' - \mathbf{T}\,,
\end{aligned} \tag{30}$$

where $\mathbf{T} = \mathbf{XUU}'\mathbf{X}'$. Above we have used Lemma 4d which gives

$$\mathbf{I}_n - \mathbf{P}_{\mathbf{W}^{1/2}\mathbf{M}} = \mathbf{Q}_{\mathbf{W}} + \mathbf{P}_{\mathbf{W}^{+1/2}\mathbf{X}}\,. \tag{31}$$

Consider then the transformed model $\mathscr{M}_t$ and assume that $\mathbf{X}\boldsymbol{\beta}$ is estimable under $\mathscr{M}_t$, i.e., (22) holds. Under $\mathscr{M}_t$ we can choose the $\mathbf{W}$-matrix as

$$\mathbf{W}_{\mathscr{M}_t} = \mathbf{FVF}' + \mathbf{FXUU}'\mathbf{X}'\mathbf{F}' = \mathbf{FWF}' \in \mathscr{W}_{\mathscr{M}_t}\,, \tag{32}$$

and so, denoting $\mathbf{T} = \mathbf{XUU}'\mathbf{X}$, we have

$$\begin{aligned}
\tilde{\boldsymbol{\mu}}(\mathscr{M}_t) &= \mathrm{BLUE}(\mathbf{X}\boldsymbol{\beta} \mid \mathscr{M}_t) =: \mathbf{G}_t\mathbf{y} \\
&= \mathbf{X}[\mathbf{X}'\mathbf{F}'(\mathbf{FWF}')^-\mathbf{FX}]^-\mathbf{X}'\mathbf{F}'(\mathbf{FWF}')^-\mathbf{Fy}\,, \qquad (33) \\
\operatorname{cov}(\tilde{\boldsymbol{\mu}} \mid \mathscr{M}_t) &= \mathbf{X}[\mathbf{X}'\mathbf{F}'(\mathbf{FWF}')^-\mathbf{FX}]^-\mathbf{X}' - \mathbf{T} \\
&= \mathbf{X}(\mathbf{X}'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{F}'}\mathbf{W}^{+1/2}\mathbf{X})^-\mathbf{X}' - \mathbf{T}\,. \qquad (34)
\end{aligned}$$

Of course, by the definition of the BLUE, we always have the Löwner ordering

$$\operatorname{cov}(\tilde{\boldsymbol{\mu}} \mid \mathscr{M}_{12}) \leq_{\mathrm{L}} \operatorname{cov}(\tilde{\boldsymbol{\mu}} \mid \mathscr{M}_t)\,. \tag{35}$$

However, it is of interest to confirm (35) algebraically. To do this we see at once that

$$\mathbf{X}'\mathbf{W}^{+1/2}\mathbf{W}^{+1/2}\mathbf{X} \geq_{\mathrm{L}} \mathbf{X}'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{F}'}\mathbf{W}^{+1/2}\mathbf{X}\,. \tag{36}$$

Now (36) is equivalent to

$$(\mathbf{X}'\mathbf{W}^{+1/2}\mathbf{W}^{+1/2}\mathbf{X})^{+} \leq_{\mathrm{L}} (\mathbf{X}'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{F}'}\mathbf{W}^{+1/2}\mathbf{X})^{+}. \tag{37}$$

Notice that the equivalence of (36) and (37) holds in view of the following result: Let $\mathbf{0} \leq_{\mathrm{L}} \mathbf{A} \leq_{\mathrm{L}} \mathbf{B}$. Then $\mathbf{A}^{+} \geq_{\mathrm{L}} \mathbf{B}^{+}$ if and only if $\mathrm{r}(\mathbf{A}) = \mathrm{r}(\mathbf{B})$; see Milliken and Akdeniz [20]. Now $\mathrm{r}(\mathbf{X}'\mathbf{W}^{+}\mathbf{X}) = \mathrm{r}(\mathbf{X}'\mathbf{W}) = \mathrm{r}(\mathbf{X})$, and

$$\begin{aligned}\mathrm{r}(\mathbf{X}'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{F}'}\mathbf{W}^{+1/2}\mathbf{X}) &= \mathrm{r}(\mathbf{X}'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{F}'}) \\ &= \mathrm{r}(\mathbf{X}'\mathbf{P}_{\mathbf{W}}\mathbf{F}') = \mathrm{r}(\mathbf{X}'\mathbf{F}') = \mathrm{r}(\mathbf{X})\,, \end{aligned} \tag{38}$$

where the last equality follows from the estimability condition (25). Now (37) implies

$$\mathbf{X}(\mathbf{X}'\mathbf{W}^{+1/2}\mathbf{W}^{+1/2}\mathbf{X})^{-}\mathbf{X}' \leq_{\mathrm{L}} \mathbf{X}(\mathbf{X}'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{F}'}\mathbf{W}^{+1/2}\mathbf{X})^{-}\mathbf{X}', \tag{39}$$

which is just (35).

Now $\mathrm{E}(\mathbf{G}_t\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$, and hence by Lemma 3, $\mathbf{F}\mathbf{y}$ is linearly sufficient for $\mathbf{X}\boldsymbol{\beta}$ if and only if

$$\mathrm{cov}(\tilde{\boldsymbol{\mu}} \mid \mathscr{M}_{12}) = \mathrm{cov}(\tilde{\boldsymbol{\mu}} \mid \mathscr{M}_t)\,. \tag{40}$$

Next we show directly that (40) is equivalent to (18). First we observe that (40) holds if and only if

$$\mathbf{X}(\mathbf{X}'\mathbf{W}^{+1/2}\mathbf{W}^{+1/2}\mathbf{X})^{-}\mathbf{X}' = \mathbf{X}(\mathbf{X}'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{F}'}\mathbf{W}^{+1/2}\mathbf{X})^{-}\mathbf{X}'. \tag{41}$$

Pre- and postmultiplying (41) by $\mathbf{X}^{+}$ and by $(\mathbf{X}')^{+}$, respectively, and using the fact that $\mathbf{P}_{\mathbf{X}'} = \mathbf{X}^{+}\mathbf{X}$, gives an equivalent form to (41):

$$(\mathbf{X}'\mathbf{W}^{+1/2}\mathbf{W}^{+1/2}\mathbf{X})^{+} = (\mathbf{X}'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{F}'}\mathbf{W}^{+1/2}\mathbf{X})^{+}. \tag{42}$$

Obviously (42) holds if and only if $\mathscr{C}(\mathbf{W}^{+1/2}\mathbf{X}) \subset \mathscr{C}(\mathbf{W}^{1/2}\mathbf{F}')$, which further is equivalent to

$$\mathscr{C}(\mathbf{X}) \subset \mathscr{C}(\mathbf{W}\mathbf{F}')\,, \tag{43}$$

which is precisely the condition (18) for $\mathbf{F}\mathbf{y}$ being linearly sufficient for $\mathbf{X}\boldsymbol{\beta}$. As a summary we can write the following:

Theorem 1 *Let $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$ be estimable under $\mathscr{M}_t$ and let $\mathbf{W} \in \mathscr{W}$. Then*

$$\mathrm{cov}(\tilde{\boldsymbol{\mu}} \mid \mathscr{M}_{12}) \leq_{\mathrm{L}} \mathrm{cov}(\tilde{\boldsymbol{\mu}} \mid \mathscr{M}_t)\,. \tag{44}$$

Moreover, the following statements are equivalent:

(a) $\mathrm{cov}(\tilde{\boldsymbol{\mu}} \mid \mathscr{M}_{12}) = \mathrm{cov}(\tilde{\boldsymbol{\mu}} \mid \mathscr{M}_t)$,
(b) $\mathbf{X}(\mathbf{X}'\mathbf{W}^{+}\mathbf{X})^{-}\mathbf{X}' = \mathbf{X}(\mathbf{X}'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{F}'}\mathbf{W}^{+1/2}\mathbf{X})^{-}\mathbf{X}$,
(c) $\mathbf{X}'\mathbf{W}^{+}\mathbf{X} = \mathbf{X}'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{F}'}\mathbf{W}^{+1/2}\mathbf{X}$,
(d) $\mathscr{C}(\mathbf{W}^{+1/2}\mathbf{X}) \subset \mathscr{C}(\mathbf{W}^{1/2}\mathbf{F}')$,
(e) $\mathscr{C}(\mathbf{X}) \subset \mathscr{C}(\mathbf{W}\mathbf{F}')$,
(f) $\mathbf{F}\mathbf{y}$ *is linearly sufficient for* $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$ *under* $\mathscr{M}_{12}$.

4 Linearly Sufficient Statistic for $\boldsymbol{\mu}_1 = \mathbf{X}_1\boldsymbol{\beta}_1$ in $\mathscr{M}_{12}$

Consider then the estimation of $\boldsymbol{\mu}_1 = \mathbf{X}_1\boldsymbol{\beta}_1$ under $\mathscr{M}_{12}$. We assume that (23) holds so that $\boldsymbol{\mu}_1$ is estimable under $\mathscr{M}_{12}$. Premultiplying the model $\mathscr{M}_{12}$ by $\mathbf{M}_2 = \mathbf{I}_n - \mathbf{P}_{\mathbf{X}_2}$ yields the reduced model

$$\mathscr{M}_{12\cdot 2} = \{\mathbf{M}_2\mathbf{y},\ \mathbf{M}_2\mathbf{X}_1\boldsymbol{\beta}_1,\ \mathbf{M}_2\mathbf{V}\mathbf{M}_2\}\,. \tag{45}$$

Now the well-known Frisch–Waugh–Lovell theorem, see, e.g., Groß and Puntanen [8], states that the BLUEs of $\boldsymbol{\mu}_1$ under $\mathscr{M}_{12}$ and $\mathscr{M}_{12\cdot 2}$ coincide (with probability 1):

$$\mathrm{BLUE}(\boldsymbol{\mu}_1 \mid \mathscr{M}_{12}) = \mathrm{BLUE}(\boldsymbol{\mu}_1 \mid \mathscr{M}_{12\cdot 2})\,. \tag{46}$$

Hence, we immediately see that $\mathbf{M}_2\mathbf{y}$ is linearly sufficient for $\boldsymbol{\mu}_1$.

Now any matrix of the form

$$\mathbf{M}_2\mathbf{V}\mathbf{M}_2 + \mathbf{M}_2\mathbf{X}_1\mathbf{U}_1\mathbf{U}_1'\mathbf{X}_1'\mathbf{M}_2 \tag{47}$$

satisfying $\mathscr{C}(\mathbf{M}_2\mathbf{V} : \mathbf{M}_2\mathbf{X}_1\mathbf{U}_1) = \mathscr{C}(\mathbf{M}_2\mathbf{V} : \mathbf{M}_2\mathbf{X}_1)$, is a $\mathbf{W}$-matrix in $\mathscr{M}_{12\cdot 2}$. We may denote this class as $\mathscr{W}_{\mathscr{M}_{12\cdot 2}}$, and

$$\mathbf{W}_{\mathscr{M}_{12\cdot 2}} = \mathbf{M}_2\mathbf{W}\mathbf{M}_2 = \mathbf{M}_2\mathbf{W}_1\mathbf{M}_2 \in \mathscr{W}_{\mathscr{M}_{12\cdot 2}}\,, \tag{48}$$

where $\mathbf{W}$ and $\mathbf{W}_1$ are defined as in (11a)–(11c).

It is interesting to observe that in (47) the matrix $\mathbf{U}_1$ can be chosen as a null matrix if and only if

$$\mathscr{C}(\mathbf{M}_2\mathbf{X}_1) \subset \mathscr{C}(\mathbf{M}_2\mathbf{V})\,, \tag{49}$$

which can be shown to be equivalent to

$$\mathscr{C}(\mathbf{X}_1) \subset \mathscr{C}(\mathbf{X}_2 : \mathbf{V})\,. \tag{50}$$

Namely, it is obvious that (50) implies (49) while the reverse implication follows from the following:

$$\mathscr{C}(\mathbf{X}_1) \subset \mathscr{C}(\mathbf{X}_1 : \mathbf{X}_2) = \mathscr{C}(\mathbf{X}_2 : \mathbf{M}_2\mathbf{X}_1) \subset \mathscr{C}(\mathbf{X}_2 : \mathbf{M}_2\mathbf{V}) = \mathscr{C}(\mathbf{X}_2 : \mathbf{V})\,. \tag{51}$$

This means that

$$\mathbf{M}_2\mathbf{V}\mathbf{M}_2 \in \mathscr{W}_{\mathscr{M}_{12\cdot 2}} \iff \mathscr{C}(\mathbf{X}_1) \subset \mathscr{C}(\mathbf{X}_2 : \mathbf{V})\,. \tag{52}$$

One expression for the BLUE of $\boldsymbol{\mu}_1 = \mathbf{X}_1\boldsymbol{\beta}_1$, obtainable from $\mathscr{M}_{12\cdot 2}$, is

$$\text{BLUE}(\boldsymbol{\mu}_1 \mid \mathscr{M}_{12}) = \tilde{\boldsymbol{\mu}}_1(\mathscr{M}_{12}) = \mathbf{X}_1(\mathbf{X}_1'\dot{\mathbf{M}}_{2W}\mathbf{X}_1)^{-}\mathbf{X}_1'\dot{\mathbf{M}}_{2W}\mathbf{y}\,, \tag{53}$$

where

$$\dot{\mathbf{M}}_{2W} = \mathbf{M}_2\mathbf{W}^{-}_{\mathscr{M}_{12\cdot 2}}\mathbf{M}_2 = \mathbf{M}_2(\mathbf{M}_2\mathbf{W}\mathbf{M}_2)^{-}\mathbf{M}_2\,. \tag{54}$$

In particular, if (50) holds then we can choose $\mathbf{W}_{\mathscr{M}_{12\cdot 2}} = \mathbf{M}_2\mathbf{V}\mathbf{M}_2$, and

$$\dot{\mathbf{M}}_{2W} = \mathbf{M}_2(\mathbf{M}_2\mathbf{V}\mathbf{M}_2)^{-}\mathbf{M}_2 =: \dot{\mathbf{M}}_2\,. \tag{55}$$

Notice that by Lemma 4d, we have

$$\begin{aligned}
\mathbf{P}_{\mathbf{W}}\dot{\mathbf{M}}_{2W}\mathbf{P}_{\mathbf{W}} &= \mathbf{P}_{\mathbf{W}}\mathbf{M}_2(\mathbf{M}_2\mathbf{W}\mathbf{M}_2)^{-}\mathbf{M}_2\mathbf{P}_{\mathbf{W}} \\
&= \mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{M}_2}\mathbf{W}^{+1/2} \\
&= \mathbf{W}^{+1/2}(\mathbf{P}_{\mathbf{W}} - \mathbf{P}_{\mathbf{W}^{+1/2}\mathbf{X}_2})\mathbf{W}^{+1/2} \\
&= \mathbf{W}^{+} - \mathbf{W}^{+}\mathbf{X}_2(\mathbf{X}_2'\mathbf{W}^{+}\mathbf{X}_2)^{-}\mathbf{X}_2'\mathbf{W}^{+},
\end{aligned} \tag{56}$$

and hence, for example,

$$\begin{aligned}
\mathbf{W}\dot{\mathbf{M}}_{2W}\mathbf{X}_1 &= \mathbf{W}[\mathbf{W}^{+} - \mathbf{W}^{+}\mathbf{X}_2(\mathbf{X}_2'\mathbf{W}^{+}\mathbf{X}_2)^{-}\mathbf{X}_2'\mathbf{W}^{+}]\mathbf{X}_1 \\
&= [\mathbf{I}_n - \mathbf{X}_2(\mathbf{X}_2'\mathbf{W}^{+}\mathbf{X}_2)^{-}\mathbf{X}_2'\mathbf{W}^{+}]\mathbf{X}_1\,.
\end{aligned} \tag{57}$$

Observe that in (54), (56) and (57) the matrix $\mathbf{W}$ can be replaced with $\mathbf{W}_1$. For a thorough review of the properties of $\dot{\mathbf{M}}_{2W}$, see Isotalo et al. [12].

In the next theorem we collect some interesting properties of linearly sufficient estimators of $\boldsymbol{\mu}_1$.

Theorem 2 *Let $\boldsymbol{\mu}_1 = \mathbf{X}_1\boldsymbol{\beta}_1$ be estimable under $\mathscr{M}_{12}$ and let $\mathbf{W} \in \mathscr{W}$. Then the statistic $\mathbf{F}\mathbf{y}$ is linearly sufficient for $\boldsymbol{\mu}_1$ under $\mathscr{M}_{12}$ if and only if*

$$\mathscr{C}(\mathbf{W}\dot{\mathbf{M}}_{2W}\mathbf{X}_1) \subset \mathscr{C}(\mathbf{W}\mathbf{F}')\,, \tag{58}$$

or, equivalently,

$$\mathscr{C}\{[\mathbf{I}_n - \mathbf{X}_2(\mathbf{X}_2'\mathbf{W}^+\mathbf{X}_2)^-\mathbf{X}_2'\mathbf{W}^+]\mathbf{X}_1\} \subset \mathscr{C}(\mathbf{W}\mathbf{F}')\,, \tag{59}$$

where $\dot{\mathbf{M}}_{2W} = \mathbf{M}_2(\mathbf{M}_2\mathbf{W}\mathbf{M}_2)^-\mathbf{M}_2$. *Moreover,*

(a) $\mathbf{M}_2\mathbf{y}$ *is linearly sufficient for* $\boldsymbol{\mu}_1$.
(b) $\dot{\mathbf{M}}_{2W}\mathbf{y} = \mathbf{M}_2(\mathbf{M}_2\mathbf{W}\mathbf{M}_2)^-\mathbf{M}_2\mathbf{y}$ *is linearly sufficient for* $\boldsymbol{\mu}_1$.
(c) $\mathbf{X}_1'\dot{\mathbf{M}}_{2W}\mathbf{y}$ *is linearly minimal sufficient for* $\boldsymbol{\mu}_1$.
(d) *If* $\mathscr{C}(\mathbf{X}_1) \subset \mathscr{C}(\mathbf{X}_2 : \mathbf{V})$, (58) *becomes*

$$\mathscr{C}(\mathbf{W}\dot{\mathbf{M}}_2\mathbf{X}_1) \subset \mathscr{C}(\mathbf{W}\mathbf{F}')\,, \quad \text{where } \dot{\mathbf{M}}_2 = \mathbf{M}_2(\mathbf{M}_2\mathbf{V}\mathbf{M}_2)^-\mathbf{M}_2\,. \tag{60}$$

(e) *If* $\mathbf{V}$ *is positive definite,* (58) *becomes* $\mathscr{C}(\dot{\mathbf{M}}_2\mathbf{X}_1) \subset \mathscr{C}(\mathbf{F}')$.
(f) *If* $\boldsymbol{\beta}_1$ *is estimable under* $\mathscr{M}_{12}$, *then*

$$\mathbf{F}\mathbf{y} \in \mathrm{S}(\mathbf{X}_1\boldsymbol{\beta}_1 \mid \mathscr{M}_{12}) \iff \mathbf{F}\mathbf{y} \in \mathrm{S}(\boldsymbol{\beta}_1 \mid \mathscr{M}_{12})\,. \tag{61}$$

Proof The sufficiency condition (58) was proved by Kala et al. [15, §3], and, using a different approach, by Isotalo and Puntanen [10, Th. 2]. Claims (a), (b), (c) and (e) are straightforward to confirm and (d) was considered already before the Theorem. Let us confirm part (f). If $\mathbf{F}\mathbf{y} \in \mathrm{S}(\mathbf{X}_1\boldsymbol{\beta}_1 \mid \mathscr{M}_{12})$, then there exists a matrix $\mathbf{A}$ such that

$$\mathbf{A}\mathbf{F}(\mathbf{X}_1 : \mathbf{X}_2 : \mathbf{V}\mathbf{M}) = (\mathbf{X}_1 : \mathbf{0} : \mathbf{0})\,. \tag{62}$$

Because of the estimability of $\boldsymbol{\beta}_1$, the matrix $\mathbf{X}_1$ has a full column rank. Premultiplying (62) by $(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'$ yields

$$\mathbf{B}\mathbf{F}(\mathbf{X}_1 : \mathbf{X}_2 : \mathbf{V}\mathbf{M}) = (\mathbf{I}_{p_1} : \mathbf{0} : \mathbf{0})\,, \tag{63}$$

where $\mathbf{B} = (\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{A}$, and thereby $\mathbf{F}\mathbf{y} \in \mathrm{S}(\mathbf{X}_1\boldsymbol{\beta}_1 \mid \mathscr{M}_{12})$ implies $\mathbf{F}\mathbf{y} \in \mathrm{S}(\boldsymbol{\beta}_1 \mid \mathscr{M}_{12})$. The reverse direction can be proved in the corresponding way. Thus we have confirmed that claim (e) indeed holds. □

The covariance matrix of the BLUE of $\boldsymbol{\mu}_1 = \mathbf{X}_1\boldsymbol{\beta}_1$ under $\mathscr{M}_{12}$ can be expressed as

$$\begin{aligned}
\mathrm{cov}(\tilde{\boldsymbol{\mu}}_1 \mid \mathscr{M}_{12}) &= \mathbf{X}_1(\mathbf{X}_1'\dot{\mathbf{M}}_{2W}\mathbf{X}_1)^-\mathbf{X}_1' - \mathbf{T}_1 \\
&= \mathbf{X}_1[\mathbf{X}_1'\mathbf{M}_2(\mathbf{M}_2\mathbf{W}\mathbf{M}_2)^-\mathbf{M}_2\mathbf{X}_1]^-\mathbf{X}_1' - \mathbf{T}_1 \\
&= \mathbf{X}_1[\mathbf{X}_1'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{M}_2}\mathbf{W}^{+1/2}\mathbf{X}_1]^-\mathbf{X}_1' - \mathbf{T}_1\,,
\end{aligned} \tag{64}$$

where $\mathbf{T}_1 = \mathbf{X}_1\mathbf{U}_1\mathbf{U}_1'\mathbf{X}_1'$ and $\mathbf{W}$ can be replaced with $\mathbf{W}_1$.

Remark 1 The rank of the covariance matrix of the BLUE($\boldsymbol{\beta}$), as well as that of BLUE($\mathbf{X}\boldsymbol{\beta}$), under $\mathscr{M}_{12}$ is

$$\mathrm{r}[\mathrm{cov}(\tilde{\boldsymbol{\beta}} \mid \mathscr{M}_{12})] = \dim \mathscr{C}(\mathbf{X}) \cap \mathscr{C}(\mathbf{V})\,; \tag{65}$$

see, e.g., Puntanen et al. [21, p. 137]. Hence for estimable $\boldsymbol{\beta}$,

$$\mathscr{C}(\mathbf{X}) \subset \mathscr{C}(\mathbf{V}) \iff \mathrm{cov}(\tilde{\boldsymbol{\beta}} \mid \mathscr{M}_{12}) \text{ is positive definite.} \tag{66}$$

Similarly, for estimable $\boldsymbol{\beta}_1$,

$$\begin{aligned}\mathrm{r}[\mathrm{cov}(\tilde{\boldsymbol{\beta}}_1 \mid \mathscr{M}_{12})] &= \mathrm{r}[\mathrm{cov}(\tilde{\boldsymbol{\beta}}_1 \mid \mathscr{M}_{12\cdot 2})] = \dim \mathscr{C}(\mathbf{M}_2\mathbf{X}_1) \cap \mathscr{C}(\mathbf{M}_2\mathbf{V}\mathbf{M}_2) \\ &= \dim \mathscr{C}(\mathbf{M}_2\mathbf{X}_1) \cap \mathscr{C}(\mathbf{M}_2\mathbf{V}) \le \mathrm{r}(\mathbf{M}_2\mathbf{X}_1)\,. \end{aligned} \tag{67}$$

The estimability of $\boldsymbol{\beta}_1$ means that $\mathrm{r}(\mathbf{M}_2\mathbf{X}_1) = p_1$ and thereby

$$\mathrm{r}[\mathrm{cov}(\tilde{\boldsymbol{\beta}}_1 \mid \mathscr{M}_{12})] = p_1 \iff \mathscr{C}(\mathbf{M}_2\mathbf{X}_1) \subset \mathscr{C}(\mathbf{M}_2\mathbf{V})\,. \tag{68}$$

Thus, by the equivalence of (49) and (50), for estimable $\boldsymbol{\beta}_1$ the following holds:

$$\mathscr{C}(\mathbf{X}_1) \subset \mathscr{C}(\mathbf{X}_2 : \mathbf{V}) \iff \mathrm{cov}(\tilde{\boldsymbol{\beta}}_1 \mid \mathscr{M}_{12}) \text{ is positive definite.} \quad \square \tag{69}$$

What is the covariance matrix of the BLUE of $\boldsymbol{\mu}_1 = \mathbf{X}_1\boldsymbol{\beta}_1$ under $\mathscr{M}_t$? First we need to make sure that $\mathbf{X}_1\boldsymbol{\beta}_1$ is estimable under $\mathscr{M}_t$, i.e., (24) holds.

Let us eliminate the $\mathbf{F}\mathbf{X}_2\boldsymbol{\beta}_2$-part by premultiplying $\mathscr{M}_t$ by $\mathbf{Q}_{\mathbf{F}\mathbf{X}_2} = \mathbf{I}_f - \mathbf{P}_{\mathbf{F}\mathbf{X}_2}$. Thus we obtain the reduced transformed model

$$\begin{aligned}\mathscr{M}_{t\cdot 2} &= \{\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}\mathbf{F}\mathbf{y},\ \mathbf{Q}_{\mathbf{F}\mathbf{X}_2}\mathbf{F}\mathbf{X}_1\boldsymbol{\beta}_1,\ \mathbf{Q}_{\mathbf{F}\mathbf{X}_2}\mathbf{F}\mathbf{V}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}\} \\ &= \{\mathbf{N}'\mathbf{y}, \mathbf{N}'\mathbf{X}_1\boldsymbol{\beta}_1, \mathbf{N}'\mathbf{V}\mathbf{N}\}\,, \end{aligned} \tag{70}$$

where $\mathbf{N} = \mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2} \in \mathbb{R}^{n\times f}$, and, see Lemma 5, the matrix $\mathbf{N}$ has the property

$$\mathscr{C}(\mathbf{N}) = \mathscr{C}(\mathbf{F}') \cap \mathscr{C}(\mathbf{M}_2)\,. \tag{71}$$

Notice also that in view of (71) and part (c) of Lemma 6,

$$\begin{aligned}\mathrm{r}(\mathbf{N}'\mathbf{X}_1) &= \mathrm{r}(\mathbf{X}_1) - \dim \mathscr{C}(\mathbf{X}_1) \cap \mathscr{C}(\mathbf{N})^{\perp} \\ &= \mathrm{r}(\mathbf{X}_1) - \dim \mathscr{C}(\mathbf{X}_1) \cap \mathscr{C}[(\mathbf{F}')^{\perp} : \mathbf{X}_2] = \mathrm{r}(\mathbf{X}_1)\,, \end{aligned} \tag{72}$$

so that

$$\mathrm{r}(\mathbf{X}_1'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{N}}\mathbf{W}^{+1/2}\mathbf{X}_1) = \mathrm{r}(\mathbf{X}_1'\mathbf{W}^{+1/2}\mathbf{W}^{1/2}\mathbf{N}) = \mathrm{r}(\mathbf{X}_1'\mathbf{N}) = \mathrm{r}(\mathbf{X}_1)\,. \tag{73}$$

Correspondingly, we have

$$\mathrm{r}(\mathbf{X}_1'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{M}_2}\mathbf{W}^{+1/2}\mathbf{X}_1) = \mathrm{r}(\mathbf{X}_1)\,. \tag{74}$$

The $\mathbf{W}$-matrix under $\mathscr{M}_{t\cdot 2}$ can be chosen as

$$\mathbf{W}_{\mathscr{M}_{t\cdot 2}} = \mathbf{Q}_{\mathbf{F}\mathbf{X}_2}\mathbf{F}\mathbf{W}_1\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2} = \mathbf{N}'\mathbf{W}_1\mathbf{N}\,, \tag{75}$$

where $\mathbf{W}_1$ can be replaced with $\mathbf{W}$. In view of the Frisch–Waugh–Lowell theorem, the BLUE of $\boldsymbol{\mu}_1 = \mathbf{X}_1\boldsymbol{\beta}_1$ is

$$\tilde{\boldsymbol{\mu}}_1(\mathscr{M}_t) = \tilde{\boldsymbol{\mu}}_1(\mathscr{M}_{t\cdot 2}) = \mathbf{X}_1[\mathbf{X}_1'\mathbf{N}(\mathbf{N}'\mathbf{W}\mathbf{N})^{-}\mathbf{N}'\mathbf{X}_1]^{-}\mathbf{X}_1'\mathbf{N}(\mathbf{N}'\mathbf{W}\mathbf{N})^{-}\mathbf{N}'\mathbf{y}\,, \tag{76}$$

while the corresponding covariance matrix is

$$\begin{aligned}\mathrm{cov}(\tilde{\boldsymbol{\mu}}_1 \mid \mathscr{M}_t) &= \mathbf{X}_1[\mathbf{X}_1'\mathbf{N}(\mathbf{N}'\mathbf{W}\mathbf{N})^{-}\mathbf{N}'\mathbf{X}_1]^{-}\mathbf{X}_1' - \mathbf{T}_1 \\ &= \mathbf{X}_1(\mathbf{X}_1'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{N}}\mathbf{W}^{+1/2}\mathbf{X}_1)^{-}\mathbf{X}_1' - \mathbf{T}_1\,,\end{aligned} \tag{77}$$

where $\mathbf{T}_1 = \mathbf{X}_1\mathbf{U}_1\mathbf{U}_1'\mathbf{X}_1'$ (and $\mathbf{W}$ can be replaced with $\mathbf{W}_1$).

By definition we of course have

$$\mathrm{cov}(\tilde{\boldsymbol{\mu}}_1 \mid \mathscr{M}_{12}) \le_{\mathrm{L}} \mathrm{cov}(\tilde{\boldsymbol{\mu}}_1 \mid \mathscr{M}_t)\,, \tag{78}$$

but it is illustrative to confirm this also algebraically. First we observe that in view of Lemma 5,

$$\mathscr{C}(\mathbf{W}^{1/2}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}) = \mathscr{C}(\mathbf{W}^{1/2}\mathbf{F}') \cap \mathscr{C}(\mathbf{W}^{1/2}\mathbf{M}_2)\,, \tag{79}$$

and thereby Lemma 7 implies that $\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{M}_2} - \mathbf{P}_{\mathbf{W}^{1/2}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}} = \mathbf{P}_{\mathbf{Z}}$, where

$$\mathscr{C}(\mathbf{Z}) = \mathscr{C}(\mathbf{W}^{1/2}\mathbf{M}_2) \cap \mathscr{C}(\mathbf{W}^{+1/2}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2})^{\perp}. \tag{80}$$

Hence we have the following equivalent inequalities:

$$\mathbf{X}_1'\mathbf{W}^{+1/2}(\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{M}_2} - \mathbf{P}_{\mathbf{W}^{1/2}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}})\mathbf{W}^{+1/2}\mathbf{X}_1 \ge_{\mathrm{L}} \mathbf{0}\,, \tag{81}$$

$$\mathbf{X}_1'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{M}_2}\mathbf{W}^{+1/2}\mathbf{X}_1 \ge_{\mathrm{L}} \mathbf{X}_1'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}}\mathbf{W}^{+1/2}\mathbf{X}_1\,, \tag{82}$$

$$(\mathbf{X}_1'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{M}_2}\mathbf{W}^{+1/2}\mathbf{X}_1)^{+} \le_{\mathrm{L}} (\mathbf{X}_1'\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}}\mathbf{W}^{+1/2}\mathbf{X}_1)^{+}. \tag{83}$$

The equivalence between (82) and (83) is due to the fact that the matrices on each side of (82) have the same rank, which is $\mathrm{r}(\mathbf{X}_1)$; see (73) and (74). The equivalence between (83) and (78) follows by the same argument as that between (41) and (42).

The equality in (82) holds if and only if

$$\mathbf{P}_{\mathbf{Z}}\mathbf{W}^{+1/2}\mathbf{X}_1 = (\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{M}_2} - \mathbf{P}_{\mathbf{W}^{1/2}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}})\mathbf{W}^{+1/2}\mathbf{X}_1 = \mathbf{0}\,, \tag{84}$$

which is equivalent to

$$\mathbf{W}^{1/2}(\mathbf{P}_{\mathbf{W}^{1/2}\mathbf{M}_2} - \mathbf{P}_{\mathbf{W}^{1/2}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}})\mathbf{W}^{+1/2}\mathbf{X}_1 = \mathbf{0}\,. \tag{85}$$

Writing up (85) yields

$$\mathbf{W}\dot{\mathbf{M}}_{2W}\mathbf{X}_1 = \mathbf{W}\mathbf{M}_2(\mathbf{M}_2\mathbf{W}\mathbf{M}_2)^{-}\mathbf{M}_2\mathbf{X}_1 = \mathbf{W}\mathbf{N}(\mathbf{N}'\mathbf{W}\mathbf{N})^{-}\mathbf{N}\mathbf{X}_1\,. \tag{86}$$

We observe that in view of (80) we have

$$\mathscr{C}(\mathbf{Z})^{\perp} = \mathscr{C}(\mathbf{W}^{+1/2}\mathbf{X}_2 : \mathbf{Q}_{\mathbf{W}} : \mathbf{W}^{1/2}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2})\,, \tag{87}$$

where we have used the Lemma 4 giving us $\mathscr{C}(\mathbf{W}^{1/2}\mathbf{M}_2)^{\perp} = \mathscr{C}(\mathbf{W}^{+1/2}\mathbf{X}_2 : \mathbf{Q}_{\mathbf{W}})$. Therefore (84) holds if and only if

$$\mathscr{C}(\mathbf{W}^{+1/2}\mathbf{X}_1) \subset \mathscr{C}(\mathbf{Z})^{\perp} = \mathscr{C}(\mathbf{W}^{+1/2}\mathbf{X}_2 : \mathbf{Q}_{\mathbf{W}} : \mathbf{W}^{1/2}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2})\,. \tag{88}$$

Premultiplying the above inclusion by $\mathbf{W}^{1/2}$ yields an equivalent condition:

$$\begin{aligned}\mathscr{C}(\mathbf{X}_1) \subset \mathscr{C}(\mathbf{X}_2 : \mathbf{W}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}) &= \mathscr{C}(\mathbf{X}_2 : \mathbf{M}_2\mathbf{W}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}) \\ &= \mathscr{C}(\mathbf{X}_2) \oplus [\mathscr{C}(\mathbf{W}\mathbf{F}') \cap \mathscr{C}(\mathbf{W}\mathbf{M}_2)]\,.\end{aligned} \tag{89}$$

Our next step is to prove the equivalence of (89) and the linear sufficiency condition

$$\mathscr{C}(\mathbf{W}\dot{\mathbf{M}}_{2W}\mathbf{X}_1) \subset \mathscr{C}(\mathbf{W}\mathbf{F}')\,. \tag{90}$$

The equality (85), which is equivalent to (89), immediately implies (90). To go the other way, we observe that (90) implies

$$\mathscr{C}[\mathbf{W}\mathbf{M}_2(\mathbf{M}_2\mathbf{W}\mathbf{M}_2)^{-}\mathbf{M}_2\mathbf{X}_1] \subset \mathscr{C}(\mathbf{W}\mathbf{F}') \cap \mathscr{C}(\mathbf{W}\mathbf{M}_2) = \mathscr{C}(\mathbf{W}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2})\,, \tag{91}$$

where we have used Lemma 5. Premultiplying (91) by $\mathbf{M}_2$ and noting that

$$\mathbf{M}_2\mathbf{W}\mathbf{M}_2(\mathbf{M}_2\mathbf{W}\mathbf{M}_2)^{+} = \mathbf{P}_{\mathbf{M}_2\mathbf{W}} \tag{92}$$

yields

$$\mathscr{C}(\mathbf{P}_{\mathbf{M}_2\mathbf{W}}\mathbf{M}_2\mathbf{X}_1) = \mathscr{C}(\mathbf{M}_2\mathbf{X}_1) \subset \mathscr{C}(\mathbf{M}_2\mathbf{W}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2})\,. \tag{93}$$

Using (93) we get

$$\mathscr{C}(\mathbf{X}_1) \subset \mathscr{C}(\mathbf{X}_1 : \mathbf{X}_2) = \mathscr{C}(\mathbf{X}_2 : \mathbf{M}_2\mathbf{X}_1) \subset \mathscr{C}(\mathbf{X}_2 : \mathbf{M}_2\mathbf{W}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}) \,, \tag{94}$$

and thus we have shown that (90) implies (89).

Now we can summarize our findings for further equivalent conditions for $\mathbf{F}\mathbf{y}$ being linearly sufficient for $\mathbf{X}_1\boldsymbol{\beta}_1$:

Theorem 3 *Let $\boldsymbol{\mu}_1 = \mathbf{X}_1\boldsymbol{\beta}_1$ be estimable under $\mathscr{M}_{12}$ and $\mathscr{M}_t$ and let $\mathbf{W} \in \mathscr{W}$. Then*

$$\operatorname{cov}(\tilde{\boldsymbol{\mu}}_1 \mid \mathscr{M}_{12}) \le_{\mathrm{L}} \operatorname{cov}(\tilde{\boldsymbol{\mu}}_1 \mid \mathscr{M}_t) \,. \tag{95}$$

Moreover, the following statements are equivalent:

(a) $\operatorname{cov}(\tilde{\boldsymbol{\mu}}_1 \mid \mathscr{M}_{12}) = \operatorname{cov}(\tilde{\boldsymbol{\mu}}_1 \mid \mathscr{M}_t)$.
(b) $\mathscr{C}(\mathbf{W}\mathbf{M}_{2W}\mathbf{X}_1) \subset \mathscr{C}(\mathbf{W}\mathbf{F}')$.
(c) $\mathscr{C}(\mathbf{X}_1) \subset \mathscr{C}(\mathbf{X}_2 : \mathbf{W}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}) = \mathscr{C}(\mathbf{X}_2 : \mathbf{M}_2\mathbf{W}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2})$.
(d) $\mathscr{C}(\mathbf{X}_1) \subset \mathscr{C}(\mathbf{X}_2) \oplus [\mathscr{C}(\mathbf{W}\mathbf{F}') \cap \mathscr{C}(\mathbf{W}\mathbf{M}_2)]$.
(e) $\mathbf{W}\mathbf{M}_2(\mathbf{M}_2\mathbf{W}\mathbf{M}_2)^{-}\mathbf{M}_2\mathbf{X}_1 = \mathbf{W}\mathbf{N}(\mathbf{N}'\mathbf{W}\mathbf{N})^{-}\mathbf{N}\mathbf{X}_1$, *where* $\mathbf{N} = \mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}$.
(f) *The statistic* $\mathbf{F}\mathbf{y}$ *is linearly sufficient for* $\mathbf{X}_1\boldsymbol{\beta}_1$ *under* $\mathscr{M}_{12}$.

If, in the situation of Theorem 3, we request $\mathbf{F}\mathbf{y}$ to be linearly sufficient for $\mathbf{X}_1\boldsymbol{\beta}_1$ for *any* $\mathbf{X}_1$ (expecting though $\mathbf{X}_1\boldsymbol{\beta}_1$ to be estimable), we get the following corollary.

Corollary 1 *Let $\boldsymbol{\mu}_1 = \mathbf{X}_1\boldsymbol{\beta}_1$ be estimable under $\mathscr{M}_{12}$ and $\mathscr{M}_t$ and let $\mathbf{W} \in \mathscr{W}$. Then the following statements are equivalent:*

(a) *The statistic* $\mathbf{F}\mathbf{y}$ *is linearly sufficient for* $\mathbf{X}_1\boldsymbol{\beta}_1$ *under* $\mathscr{M}_{12}$ *for any* $\mathbf{X}_1$.
(b) $\mathscr{C}(\mathbf{W}) \subset \mathscr{C}(\mathbf{X}_2 : \mathbf{W}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}) = \mathscr{C}(\mathbf{X}_2) \oplus \mathscr{C}(\mathbf{W}\mathbf{F}') \cap \mathscr{C}(\mathbf{W}\mathbf{M}_2)$.

Proof The statistic $\mathbf{F}\mathbf{y}$ is linearly sufficient for $\mathbf{X}_1\boldsymbol{\beta}_1$ under $\mathscr{M}_{12}$ for any $\mathbf{X}_1$ if and only if

$$\mathbf{W}^{+1/2}\mathbf{P}_{\mathbf{Z}}\mathbf{W}^{+1/2} = \mathbf{0} \,. \tag{96}$$

Now (96) holds if and only if

$$\mathscr{C}(\mathbf{W}^{+1/2}) \subset \mathscr{C}(\mathbf{Z})^{\perp} = \mathscr{C}(\mathbf{W}^{+1/2}\mathbf{X}_2 : \mathbf{Q}_{\mathbf{W}} : \mathbf{W}^{1/2}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}) \,. \tag{97}$$

Premultipying (97) by $\mathbf{W}^{1/2}$ yields an equivalent form

$$\mathscr{C}(\mathbf{W}) \subset \mathscr{C}(\mathbf{X}_2 : \mathbf{W}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}) = \mathscr{C}(\mathbf{X}_2) \oplus \mathscr{C}(\mathbf{W}\mathbf{F}') \cap \mathscr{C}(\mathbf{W}\mathbf{M}_2) \,. \tag{98}$$

□

5 Linear Sufficiency Under $\mathscr{M}_1$ vs. $\mathscr{M}_{12}$

Consider the small model $\mathscr{M}_1 = \{\mathbf{y},\ \mathbf{X}_1\boldsymbol{\beta}_1,\ \mathbf{V}\}$ and full model $\mathscr{M}_{12} = \{\mathbf{y},\ \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2,\ \mathbf{V}\}$. Here is a reasonable question: what about comparing conditions for

$$\mathbf{Fy} \in \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_1) \quad \text{versus} \quad \mathbf{Fy} \in \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_{12})\,. \tag{99}$$

For example, under which condition

$$\mathbf{Fy} \in \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_1) \implies \mathbf{Fy} \in \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_{12})\,. \tag{100}$$

There is one crucial matter requiring our attention. Namely in the small model $\mathscr{M}_1$ the response $\mathbf{y}$ is lying in $\mathscr{C}(\mathbf{W}_1)$ but in $\mathscr{M}_{12}$ the response $\mathbf{y}$ can be in a wider subspace $\mathscr{C}(\mathbf{W})$. How to take this into account? What about assuming that

$$\mathscr{C}(\mathbf{X}_2) \subset \mathscr{C}(\mathbf{X}_1 : \mathbf{V})\ ? \tag{101}$$

This assumption means that adding the $\mathbf{X}_2$-part into the model does not carry $\mathbf{y}$ out of $\mathscr{C}(\mathbf{W}_1)$ which seems to be a logical requirement. In such a situation we should find conditions under which

$$\mathscr{C}(\mathbf{X}_1) \subset \mathscr{C}(\mathbf{W}_1\mathbf{F}') \tag{102}$$

implies

$$\mathscr{C}(\mathbf{W}_1\dot{\mathbf{M}}_{2W}\mathbf{X}_1) \subset \mathscr{C}(\mathbf{W}_1\mathbf{F}')\,. \tag{103}$$

We know that under certain conditions the BLUE of $\mathbf{X}_1\boldsymbol{\beta}_1$ does not change when the predictors in $\mathbf{X}_2$ are added into the model. It seems obvious that in such a situation (102) and (103) are equivalent. Supposing that (101) holds, then, e.g., according to Haslett and Puntanen [9, Th. 3.1],

$$\tilde{\boldsymbol{\mu}}_1(\mathscr{M}_{12}) = \tilde{\boldsymbol{\mu}}_1(\mathscr{M}_1) - \mathbf{X}_1(\mathbf{X}_1'\mathbf{W}_1^+\mathbf{X}_1)^-\mathbf{X}_1'\mathbf{W}_1^+\tilde{\boldsymbol{\mu}}_2(\mathscr{M}_{12})\,, \tag{104}$$

and hence

$$\tilde{\boldsymbol{\mu}}_1(\mathscr{M}_{12}) = \tilde{\boldsymbol{\mu}}_1(\mathscr{M}_1) \tag{105}$$

if and only if $\mathbf{X}_1'\mathbf{W}_1^+\tilde{\boldsymbol{\mu}}_2(\mathscr{M}_{12}) = \mathbf{0}$, i.e.,

$$\mathbf{X}_1'\mathbf{W}_1^+\mathbf{X}_2(\mathbf{X}_2'\dot{\mathbf{M}}_1\mathbf{X}_2)^-\mathbf{X}_2'\dot{\mathbf{M}}_1\mathbf{y} = \mathbf{0}\,. \tag{106}$$

Requesting (106) to hold for all $\mathbf{y} \in \mathscr{C}(\mathbf{X}_1 : \mathbf{V})$ and using the assumption $\mathscr{C}(\mathbf{X}_2) \subset \mathscr{C}(\mathbf{X}_1 : \mathbf{V})$, we obtain

$$\mathbf{X}_1'\mathbf{W}_1^+\mathbf{X}_2(\mathbf{X}_2'\dot{\mathbf{M}}_1\mathbf{X}_2)^-\mathbf{X}_2'\dot{\mathbf{M}}_1\mathbf{X}_2 = \mathbf{0}\,, \tag{107}$$

i.e.,

$$\mathbf{X}_1'\mathbf{W}_1^+\mathbf{X}_2\mathbf{P}_{\mathbf{X}_2'} = \mathbf{X}_1'\mathbf{W}_1^+\mathbf{X}_2 = \mathbf{0}\,, \tag{108}$$

where we have used the fact $\mathscr{C}(\mathbf{X}_2'\dot{\mathbf{M}}_1\mathbf{X}_2) = \mathscr{C}(\mathbf{X}_2')$. Thus we have shown the equivalence of (105) and (108).

On the other hand, (102) implies (103) if and only if $\mathscr{C}(\mathbf{W}_1\dot{\mathbf{M}}_{2W}\mathbf{X}_1) \subset \mathscr{C}(\mathbf{X}_1)$, which is equivalent to

$$\mathscr{C}(\mathbf{W}_1\dot{\mathbf{M}}_{2W}\mathbf{X}_1) = \mathscr{C}(\mathbf{X}_1)\,, \tag{109}$$

because we know that $\mathrm{r}(\mathbf{W}_1\dot{\mathbf{M}}_{2W}\mathbf{X}_1) = \mathrm{r}(\mathbf{X}_1)$. Hence neither column spaces in (109) can be a proper subspace of the other. Therefore, as stated by Baksalary [1, p. 23] in the case of $\mathbf{V} = \mathbf{I}_n$, either the classes of statistics which are linearly sufficient for $\boldsymbol{\mu}_1$ are in the models $\mathscr{M}_1$ and $\mathscr{M}_{12}$ exactly the same, or, if not, there exists at least one statistic $\mathbf{Fy}$ such that $\mathbf{Fy} \in \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_1)$ but $\mathbf{Fy} \notin \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_{12})$ and at least one statistic $\mathbf{Fy}$ such that $\mathbf{Fy} \in \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_{12})$ but $\mathbf{Fy} \notin \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_1)$.

Now (102) and (103) are equivalent if and only if (109) holds, i.e.,

$$\mathbf{M}_1\mathbf{W}_1\dot{\mathbf{M}}_{2W}\mathbf{X}_1 = \mathbf{0}\,. \tag{110}$$

Using (57), (110) becomes

$$\mathbf{M}_1\mathbf{X}_2(\mathbf{X}_2'\mathbf{W}_1^+\mathbf{X}_2)^-\mathbf{X}_2'\mathbf{W}_1^+\mathbf{X}_1 = \mathbf{0}\,. \tag{111}$$

Because $\mathrm{r}(\mathbf{M}_1\mathbf{X}_2) = \mathrm{r}(\mathbf{X}_2)$, we can cancel, on account of Marsaglia and Styan [18, Th. 2], the matrix $\mathbf{M}_1$ in (111) and thus obtain

$$\mathbf{X}_2(\mathbf{X}_2'\mathbf{W}_1^+\mathbf{X}_2)^-\mathbf{X}_2'\mathbf{W}_1^+\mathbf{X}_1 = \mathbf{0}\,. \tag{112}$$

Premultiplying (111) by $\mathbf{X}_2'\mathbf{W}_1^+$ shows that (109) is equivalent to

$$\mathbf{X}_2'\mathbf{W}_1^+\mathbf{X}_1 = \mathbf{0}\,. \tag{113}$$

In (113) of course $\mathbf{W}_1^+$ can be replaced with any $\mathbf{W}_1^-$. Thus we have proved the following:

Theorem 4 *Consider the models $\mathscr{M}_{12}$ and $\mathscr{M}_1$ and suppose that $\boldsymbol{\mu}_1 = \mathbf{X}_1\boldsymbol{\beta}_1$ is estimable under $\mathscr{M}_{12}$ and $\mathscr{C}(\mathbf{X}_2) \subset \mathscr{C}(\mathbf{X}_1 : \mathbf{V})$. Then the following statements are equivalent:*

(a) $\mathbf{X}_1'\mathbf{W}_1^+\mathbf{X}_2 = \mathbf{0}$,
(b) $\mathrm{BLUE}(\boldsymbol{\mu}_1 \mid \mathscr{M}_1) = \mathrm{BLUE}(\boldsymbol{\mu}_1 \mid \mathscr{M}_{12})$ *with probability* 1,
(c) $\mathbf{Fy} \in \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_1) \iff \mathbf{Fy} \in \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_{12})$.

Overlooking the problem for $\mathbf{y}$ belonging to $\mathscr{C}(\mathbf{X} : \mathbf{V})$ or to $\mathscr{C}(\mathbf{X}_1 : \mathbf{V})$, we can start our considerations by assuming that (100) holds, i.e.,

$$\mathscr{C}(\mathbf{X}_1) \subset \mathscr{C}(\mathbf{W}_1\mathbf{F}') \implies \mathscr{C}(\mathbf{W}\dot{\mathbf{M}}_{2W}\mathbf{X}_1) \subset \mathscr{C}(\mathbf{W}\mathbf{F}') \,. \tag{114}$$

Choosing $\mathbf{F}' = \mathbf{W}_1^-\mathbf{X}_1$ we observe that $\mathbf{F}\mathbf{y} \in \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_1)$ for any choice of $\mathbf{W}_1^-$. Thus (114) implies that we must also have

$$\mathscr{C}(\mathbf{W}\dot{\mathbf{M}}_{2W}\mathbf{X}_1) \subset \mathscr{C}(\mathbf{W}\mathbf{W}_1^-\mathbf{X}_1) \,. \tag{115}$$

According to Lemma 3 of Baksalary and Mathew [5], (for nonnull $\mathbf{W}\dot{\mathbf{M}}_{2W}\mathbf{X}_1$ and $\mathbf{X}_1$) the inclusion (115) holds for any $\mathbf{W}_1^-$ if and only if

$$\mathscr{C}(\mathbf{W}) \subset \mathscr{C}(\mathbf{W}_1) \tag{116}$$

holds along with

$$\mathscr{C}(\mathbf{W}\dot{\mathbf{M}}_{2W}\mathbf{X}_1) \subset \mathscr{C}(\mathbf{W}\mathbf{W}_1^+\mathbf{X}_1) \,. \tag{117}$$

Inclusion (116) means that $\mathscr{C}(\mathbf{X}_2) \subset \mathscr{C}(\mathbf{X}_1 : \mathbf{V})$, i.e., $\mathscr{C}(\mathbf{W}) = \mathscr{C}(\mathbf{W}_1)$, which is our assumption in Theorem 4. Thus we can also conclude the following.

Corollary 2 *Consider the models $\mathscr{M}_{12}$ and $\mathscr{M}_1$ and suppose that $\boldsymbol{\mu}_1 = \mathbf{X}_1\boldsymbol{\beta}_1$ is estimable under $\mathscr{M}_{12}$. Then the following statements are equivalent:*

(a) $\mathbf{X}_1'\mathbf{W}_1^+\mathbf{X}_2 = \mathbf{0}$ *and* $\mathscr{C}(\mathbf{X}_2) \subset \mathscr{C}(\mathbf{X}_1 : \mathbf{V})$.
(b) $\mathbf{F}\mathbf{y} \in \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_1) \iff \mathbf{F}\mathbf{y} \in \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_{12})$.

We complete this section by considering the linear sufficiency of $\mathbf{F}\mathbf{y}$ versus that of $\mathbf{F}\mathbf{M}_2\mathbf{y}$.

Theorem 5 *Consider the models $\mathscr{M}_{12}$ and $\mathscr{M}_{12\cdot 2}$ and suppose that $\boldsymbol{\mu}_1 = \mathbf{X}_1\boldsymbol{\beta}_1$ is estimable under $\mathscr{M}_{12}$. Then*

(a) $\mathbf{F}\mathbf{y} \in \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_{12}) \implies \mathbf{F}\mathbf{M}_2\mathbf{y} \in \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_{12})$.
(b) *The reverse relation in* (a) *holds* $\iff \mathscr{C}(\mathbf{F}\mathbf{M}_2\mathbf{W}) \cap \mathscr{C}(\mathbf{F}\mathbf{X}_2) = \{\mathbf{0}\}$.
Moreover, the following statements are equivalent:
(c) $\mathbf{F}\mathbf{M}_2\mathbf{y} \in \mathrm{S}(\mathbf{X}_1\boldsymbol{\beta}_1 \mid \mathscr{M}_{12})$,
(d) $\mathbf{F}\mathbf{M}_2\mathbf{y} \in \mathrm{S}(\mathbf{X}_1\boldsymbol{\beta}_1 \mid \mathscr{M}_{12\cdot 2})$,
(e) $\mathbf{F}\mathbf{M}_2\mathbf{y} \in \mathrm{S}(\mathbf{M}_2\mathbf{X}_1\boldsymbol{\beta}_1 \mid \mathscr{M}_{12\cdot 2})$.

Proof To prove (a), we observe that $\mathbf{F}\mathbf{y} \in \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_{12})$ implies (91), i.e.,

$$\mathscr{C}(\mathbf{W}\dot{\mathbf{M}}_{2W}\mathbf{X}_1) \subset \mathscr{C}(\mathbf{W}\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}) \,. \tag{118}$$

Now on account Lemma 5d, we have $\mathbf{M}_2\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2} = \mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2}$. Substituting this into (118) gives $\mathscr{C}(\mathbf{W}\dot{\mathbf{M}}_{2W}\mathbf{X}_1) \subset \mathscr{C}(\mathbf{W}\mathbf{M}_2\mathbf{F}'\mathbf{Q}_{\mathbf{F}\mathbf{X}_2})$, and so

$$\mathscr{C}(\mathbf{W}\dot{\mathbf{M}}_{2W}\mathbf{X}_1) \subset \mathscr{C}(\mathbf{W}\mathbf{M}_2\mathbf{F}') \,, \tag{119}$$

which is the condition for $\mathbf{FM}_2\mathbf{y} \in \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_{12})$, thus confirming our claim (a). For an alternative proof of (a), see Isotalo and Puntanen [10, Cor. 1].

The reverse relation in (a) holds if and only if (119) implies (118), i.e.,

$$\mathscr{C}(\mathbf{WM}_2\mathbf{F}') \subset \mathscr{C}(\mathbf{WM}_2\mathbf{F}'\mathbf{Q}_{\mathbf{FX}_2}) \,, \tag{120}$$

where of course only the equality is possible. Now

$$\mathrm{r}(\mathbf{WM}_2\mathbf{F}'\mathbf{Q}_{\mathbf{FX}_2}) = \mathrm{r}(\mathbf{WM}_2\mathbf{F}') - \dim \mathscr{C}(\mathbf{FM}_2\mathbf{W}) \cap \mathscr{C}(\mathbf{FX}_2) \,, \tag{121}$$

and hence (120) holds if and only if $\mathscr{C}(\mathbf{FM}_2\mathbf{W}) \cap \mathscr{C}(\mathbf{FX}_2) = \{\mathbf{0}\}$ which proves our claim (b).

The condition (c), $\mathbf{FM}_2\mathbf{y} \in \mathrm{S}(\boldsymbol{\mu}_1 \mid \mathscr{M}_{12})$, holds if and only if

$$\mathscr{C}[\mathbf{WM}_2(\mathbf{M}_2\mathbf{WM}_2)^-\mathbf{M}_2\mathbf{X}_1] \subset \mathscr{C}(\mathbf{WM}_2\mathbf{F}') \,. \tag{122}$$

Premultiplying (122) by $\mathbf{M}_2$ yields

$$\mathscr{C}(\mathbf{M}_2\mathbf{X}_1) \subset \mathscr{C}(\mathbf{M}_2\mathbf{WM}_2\mathbf{F}') \,, \tag{123}$$

which means that (e) holds. Premultiplying (123) by $\mathbf{WM}_2(\mathbf{M}_2\mathbf{WM}_2)^-$ yields (122) thus confirming the equivalence of (c) and (e).

Applying Lemma 2b we observe that (d) holds if and only if

$$\mathscr{C}\{\mathbf{M}_2\mathbf{X}_1[\mathbf{X}_1'\mathbf{M}_2(\mathbf{M}_2\mathbf{WM}_2)^-\mathbf{M}_2\mathbf{X}_1]^-\mathbf{X}_1'\mathbf{M}_2\} \subset \mathscr{C}(\mathbf{M}_2\mathbf{WM}_2\mathbf{F}') \,. \tag{124}$$

The fact that the left-hand side of (124) is $\mathscr{C}(\mathbf{M}_2\mathbf{X}_1)$ shows the equivalence of (d) and (c), and thus the proof is completed. □

6 Conclusions

If our interest is in all estimable parametric functions of $\boldsymbol{\beta}_1$, as in Groß and Puntanen [8], Markiewicz and Puntanen [16], and Kala and Pordzik [13], then we could concentrate on estimating $\mathbf{M}_2\mathbf{X}_1\boldsymbol{\beta}_1$. This is due to the fact that $\mathbf{K}_1\boldsymbol{\beta}_1$ is estimable if and only if $\mathscr{C}(\mathbf{K}_1') \subset \mathscr{C}(\mathbf{X}_1'\mathbf{M}_2)$; see, e.g., Groß and Puntanen [8, Lemma 1]. Hence, the BLUE for an arbitrary estimable vector $\mathbf{K}_1\boldsymbol{\beta}_1$ may easily be computed from the BLUE of $\mathbf{M}_2\mathbf{X}_1\boldsymbol{\beta}_1$. We may also mention that in the corresponding way, Baksalary [1, 2, §3.3, §5] considered the linearly sufficient statistics for $\mathbf{X}_1'\mathbf{M}_2\mathbf{X}_1\boldsymbol{\beta}_1$ under $\mathscr{M}_1$ and $\mathscr{M}_{12}$ when $\mathbf{V} = \mathbf{I}_n$.

Our interest in this paper has been focused on the estimation of $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$ and $\boldsymbol{\mu}_1 = \mathbf{X}_1\boldsymbol{\beta}_1$ under the linear model $\mathscr{M}_{12} = \{\mathbf{y}, \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2, \mathbf{V}\}$. Here we need to assume that $\mathbf{X}_1\boldsymbol{\beta}_1$ is estimable (and thereby also $\mathbf{X}_2\boldsymbol{\beta}_2$ is estimable). We have characterized the linearly sufficient statistic $\mathbf{Fy}$ by using the covariance

matrices of the BLUEs under $\mathscr{M}_{12}$ and under its transformed version $\mathscr{M}_t = \{\mathbf{Fy}, \mathbf{FX}_1\boldsymbol{\beta}_1 + \mathbf{FX}_2\boldsymbol{\beta}_2, \mathbf{FVF}'\}$. In particular, certain orthogonal projectors appear useful in our considerations. We have obtained new interesting proofs for some known results, like Lemma 2, and presented some new properties related to linear sufficiency. Particular attention has been paid to the condition under which adding new regressors (in $\mathbf{X}_2$) does not affect the linear sufficiency of $\mathbf{Fy}$. Similarly we have characterized linear sufficiency of $\mathbf{Fy}$ versus that of $\mathbf{FM}_2\mathbf{y}$ under the models $\mathscr{M}_{12}$ and $\mathscr{M}_{12\cdot 2}$.

As one of the referees of this paper stated, our considerations are based on effective matrix and column space properties and hence its relevance for applied data analysts may be a bit limited. However, we believe that in the long run the given column space properties may provide some new insights into the linear estimation theory.

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Hybrid Model for Recurrent Event Data

Ivo Sousa-Ferreira and Ana Maria Abreu

Abstract In the last four decades, there has been an increasing interest in developing survival models appropriate for multiple event data and, in particular, for recurrent event data. For these situations, several extensions of the Cox's regression model have been developed. Some of the most known models were suggested by: Prentice, Williams, and Peterson (PWP); Andersen and Gill (AG); Wei, Lin, and Weissfeld (WLW); and Lee, Wei, and Amato (LWA). These models can handle with situations where exist potentially correlated lifetimes of the same subject (due to the occurrence of more than one event for each subject) which is common in this type of data.

In this chapter we present a new model, which we call hybrid model, with the purpose of minimizing some limitations of PWP model. With this model we obtained an improvement in the precision of the parameters estimates and a better fit to the simulated data.

Keywords Correlated observations · Extensions of Cox model · Hybrid model · Recurrent events · Survival analysis

1 Introduction

A historical landmark that has revolutionized the survival analysis took place in 1972, when Sir David Cox [3] proposed a regression model capable of including factors that are assumed to affect the lifetime of the subjects (known as *prognostic*

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or *risk factors*), which are represented by covariates. Based on this model, new extensions and approaches that seek to respond to the most varied problems have been developed.

Over the last few years there has been an increasing interest in studying the time until the observation of various events that may occur more than once for a given subject. The main feature of multiple events data is the observation of more than one lifetime for each subject, which makes the direct application of the Cox's regression model unfeasible. Therefore, several extensions of the Cox model have been suggested to analyze multiple events, in particular a single type of events that occurs more than once for the same subject. Such outcomes have been termed *recurrent events*. For these situations, the most applied extensions of the Cox model were suggested by: Prentice, Williams, and Peterson (PWP) [10]; Andersen and Gill (AG) [1]; Wei, Lin, and Weissfeld (WLW) [15]; and Lee, Wei, and Amato (LWA) [6].

According to Kelly and Lim [5], these models can be classified based on the dependency structure between events (of the same subject). The PWP and AG models have a conditional dependency structure, since subjects are not considered at risk for a given event unless the previous one has occurred. On the other hand, WLW and LWA models have a marginal dependency structure, by reason of it is considered that subjects are simultaneously at risk for the occurrence of any of events from the initial time, i.e., the occurrence of each event is not conditioned on the prior occurrence of any others. Therefore, the first two models are most appropriate to analyze recurrent events, since they allow to accommodate the orderly nature of such data.

One of the major problems in the application of these four models is related to the strong possibility of occurring within-subject correlation. In the Cox model and its extensions the estimation of regression parameters is made assuming that the observations are independent. In other words, we ignore the existence of within-subject correlation. For this reason, from the point of view of the estimation of the parameters, all of these extensions are also called *marginal models* [13]. Several authors [1, 7, 15] have proven that, under certain regularity conditions, the maximum likelihood estimator obtained thereby is still consistent and with the same asymptotic properties, even in the presence of correlated lifetimes.

Consequently, the estimate of variance for the regression parameters also treats each observation as independent. This means that, when the lifetimes are correlated, the usual estimate of the variance does not correctly evaluate the accuracy of estimated regression parameters. In order to offset this aspect, an adjustment in the estimation of variance should take place. Then, a robust estimator of covariance matrix—"sandwich" estimator—was developed to take that correlation into account [8, 15].

In this chapter we present a hybrid model that will focus on the two models that have a conditional dependency structure between events. The purpose of this hybrid model is an attempt to overcome two limitations pointed out by some authors [2, 13] about the PWP model: (1) the loss of heterogeneity throughout the study; and (2) the violation of the missing completely at random (MCAR) condition. Therefore, in the

next section we present the situations where the PWP and AG models are applied and, afterwards, we formalize the new hybrid model. In Sect. 3, the performance of the hybrid model is analyzed. For this purpose, the simulation of recurrent events was carried out through the R statistical software [11]. Finally, some considerations about the application of this model are discussed.

2 Methodology

The PWP and AG models will be formalized to subsequently construct the PWP-AG hybrid model. The characteristics of each model will be examined in order to understand in which situations the application of each of them is more appropriate. In the first instance, it is necessary to introduce some notation which will enable the construction of these survival models.

2.1 Notation

Suppose that there are n subjects in study and each subject can experience a maximum of S failures. Let $T_{is} = \min\left\{X_{is}, C_{is}\right\}$ be the observation time, where X_{is} and C_{is} represent the true lifetime and the censoring time of the sth event ($s = 1, \ldots, S$) in the ith subject ($i = 1, \ldots, n$), respectively. Define $\delta_{is} = I(X_{is} \leq C_{is})$ as being the indicator censoring variable, where $I(E) = 1$ when the event E holds, and $I(E) = 0$ otherwise. It is assumed that censoring is non-informative. Let $\mathbf{z}_{is}(t) = \left(z_{is1}(t), \ldots, z_{isp}(t)\right)'$ represent the p-vector of time-dependent covariates for the ith subject with respect to the sth event and $\mathbf{z}_i(t) = \left(\mathbf{z}'_{i1}(t), \ldots, \mathbf{z}'_{iS}(t)\right)$ denote his overall covariate vector. The true lifetime vector $\mathbf{X}_i = (X_{i1}, \ldots, X_{iS})'$ and the censoring time vector $\mathbf{C}_i = (C_{i1}, \ldots, C_{iS})'$ are assumed to be independent conditional on the overall covariate vector $\mathbf{z}_i(t)$. If X_{is} or $\mathbf{z}_{is}$ is missing, we set $C_{is} = 0$, which ensures that $T_{is} = 0$ and $\delta_{is} = 0$. We require that such cases are MCAR.

2.2 Prentice, Williams, and Peterson (PWP) Model

In 1981, Prentice et al. [10] suggested one of the earliest extensions of the Cox model for the analysis of multiple events and it is often labeled as the *PWP model*. This model applies to the situations in which events occur in an orderly way, where it is considered that a subject cannot be at risk for the sth event until he has experienced the $s - 1$ order event (Fig. 1). Therefore, it means that the risk set is restrictive.

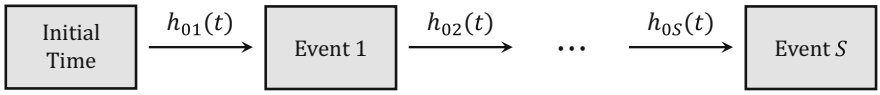

Fig. 1 Schematic representation of the PWP model

Furthermore, it is assumed that the risk of occurrence of the following event is modified by the occurrence of the previous one. This means that it is necessary to stratify the subjects according to the order in which events occur. Thus, if it has been observed s events, then there will be s ordered strata, wherein each of them will be associated a different baseline hazard function $h_{0s}(t)$, $t \geq 0$ and $s = 1, \ldots, S$.

The authors of PWP model have suggested two possible time scales to construct the risk intervals: counting process or gap time formulation. We will only consider the first formulation. Then the hazard function of the ith subject for the sth event is defined as

$$h\big(t; \mathbf{z}_{is}(t)\big) = h_{0s}(t) \exp\big(\boldsymbol{\beta}' \mathbf{z}_{is}(t)\big), \qquad t \geq 0, \tag{1}$$

where $h_{0s}(t) \geq 0$ is the event-specific baseline hazard function and $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_p)'$ is the $p \times 1$ overall vector of unknown regression parameters.

The regression parameters are estimated through the partial likelihood function, where we admit that the observations within the same subject are independent. For a model with stratification, this function is given by

$$L(\boldsymbol{\beta}) = \prod_{i=1}^{n} \prod_{s=1}^{S} \left[\frac{\exp\big(\boldsymbol{\beta}' \mathbf{z}_{is}(t_{is})\big)}{\sum_{j=1}^{n} Y_{js}(t_{is}) \exp\big(\boldsymbol{\beta}' \mathbf{z}_{js}(t_{is})\big)} \right]^{\delta_{is}}, \tag{2}$$

where $Y_{is}(t) = I\big(t_{i(s-1)} < t \leq t_{is}\big)$ is the risk set indicator which represents the counting process formulation and t_{is} is the observation time of the ith subject with respect to the sth event.

Conventionally, the overall maximum likelihood estimator $\widehat{\boldsymbol{\beta}}$ is obtained by adjusting a single vector of covariates, that in this case is the overall covariate vector $\mathbf{z}_i(t)$. However, since there is stratification, it is also possible to obtain the event-specific vector of unknown regression parameters $\boldsymbol{\beta}_s = (\beta_{s1}, \ldots, \beta_{sp})'$, one for each s stratum [7]. For this purpose, it is required to adjust the event-specific covariate vector of each stratum, in such a way that $\mathbf{z}_i(t) = \big(\mathbf{0}, \ldots, \mathbf{0}, \mathbf{z}_{is}(t), \mathbf{0}, \ldots, \mathbf{0}\big)'$, towards $s = 1, \ldots, S$. Thus, we obtain the event-specific estimates $\widehat{\boldsymbol{\beta}}_1, \widehat{\boldsymbol{\beta}}_2 \ldots, \widehat{\boldsymbol{\beta}}_S$.

In the PWP model, the set of subjects at risk is restricted in the sense that subjects who have not experienced the sth event may not be included in the analysis of the $s + 1$ order event. In this way, the risk set will gradually decrease over the study, revealing increasingly less heterogeneous. Consequently, the event-specific parameters estimates will become unreliable. Therneau and Grambsch [13] presented two options to solve this limitation: (1) truncate the data set exactly in the event where

the number of subjects at risk is considered too small; or (2) agglomerate the final strata, starting from that one is considered to have a small number of subjects at risk. The latter option is more attractive, because it has the advantage of not wasting information that may be critical for the analysis.

In addition to the loss of heterogeneity, in a restrictive risk set the choice of subjects that will be at risk for a given event does not occur randomly, because it is determined by observation of the previous event. This leads to another limitation—the violation of the MCAR assumption [2].

2.3 Andersen and Gill (AG) Model

In 1982, Andersen and Gill [1] proposed a simple model for the analysis of recurrent events, usually referred to as *AG model*. This model was suggested in the same line of reasoning of the previous model but has stronger assumptions. The main assumption concerns with the independence of times between events within a subject.

In this model, the events follow a given order, but it is assumed that the events have equal risk of occurring (Fig. 2). Thus, there will be a common hazard function, $h_0(t)$, $t \geq 0$, to all events.

The AG model was conceived for the case where the occurrence of each event does not depend on time elapsed since the last observation, nor the number of events observed previously. This means that although the occurrence of each event is conditioned to the occurrence of previous events, it is considered that the times between the events are independent.

The authors of this model only considered the counting process formulation to construct the risk intervals. The hazard function for the ith subject with respect to the sth event is defined as

$$h\big(t; \mathbf{z}_{is}(t)\big) = h_0(t) \exp\big(\boldsymbol{\beta}' \mathbf{z}_{is}(t)\big), \qquad t \geq 0, \tag{3}$$

where $h_0(t) \geq 0$ is the common baseline hazard function and $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_p)'$ is the $p \times 1$ overall vector of unknown regression parameters.

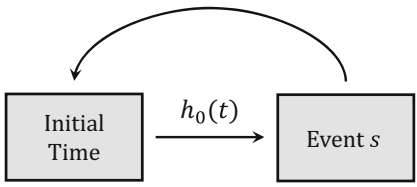

Fig. 2 Schematic representation of the AG model

As in this case there is no stratification, the parameters are estimated through the following partial likelihood function

$$L(\boldsymbol{\beta}) = \prod_{i=1}^{n} \prod_{s=1}^{S} \left[\frac{\exp\left(\boldsymbol{\beta}' \mathbf{z}_{is}(t_{is})\right)}{\sum_{j=1}^{n} \sum_{l=1}^{S} Y_{jl}(t_{is}) \exp\left(\boldsymbol{\beta}' \mathbf{z}_{jl}(t_{is})\right)} \right]^{\delta_{is}}, \tag{4}$$

where $Y_{is}(t) = I\left(t_{i(s-1)} < t \leq t_{is}\right)$ is the risk set indicator and t_{is} is the observation time of the ith subject with respect to the sth event. Since this model has a common hazard function to all events, it is only possible to obtain the overall maximum likelihood estimator $\widehat{\boldsymbol{\beta}}$.

When the PWP and AG models have been suggested, they did not present any adjustment for the within-subject correlation. However, the authors of these models were conscious of this strong possibility and recommended attempt to capture this correlation including time-dependent covariates on the model. A few years later, it was realized that it was possible to take advantage of the fact that these two models are also classified as marginal models from the point of view of the parameters estimation. From this point, the robust estimator of the covariance matrix was applied to take the within-subject correlation into account [7, 13].

In contrast with the previous model, the AG model reveals neither loss of the heterogeneity nor the violation of the MCAR condition because the set of subject at risk is unrestrictive. This means that all risk intervals of all subjects may contribute to the risk set for any given event, regardless of the number of events observed previously for each subject [5].

2.4 PWP-AG Hybrid Model

In order to overcome the limitations pointed for the PWP model, we present a slightly different option from those presented in [13].

In fact, there may exist another reason to agglomerate the final strata. Suppose that, initially, the PWP model has a very heterogeneous risk set, whereby the differences between the hazard functions of the various subjects are due, in particular, to the effect of several covariates with quite different values for each of them. Suppose that the risk set related to the second event (which contains only the subjects that had suffered the first event) no longer contains the subjects who belong to a certain category of a covariate. This means that, in addition to subjects being less heterogeneous, this covariate is no longer important to the model. Thus, its effect on the survival shall be embedded in the baseline hazard functions, which necessarily have to be different from the baseline hazard function of the first event. With that in mind, assume that after a certain event, denoted by S^*, the subjects at risk will be more homogeneous, in such a way that the baseline hazard functions

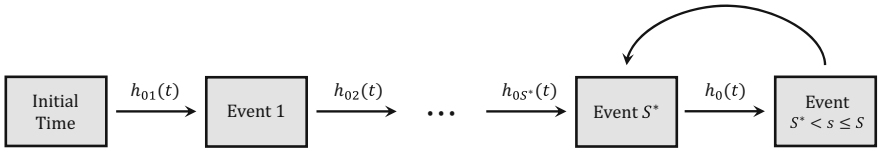

Fig. 3 Schematic representation of the PWP-AG hybrid model

for each event no longer have to be different. Then, instead of continuing to apply the PWP model, the AG model can be implemented after the observation of the S^* event, as illustrated in Fig. 3.

In general, the events $1, 2, \ldots, S^*$ are analyzed with the PWP model (1) and the events $S^* + 1, S^* + 2, \ldots, S$ are analyzed with the AG model (3). The proposal to agglomerate the final strata gives rise to the PWP-AG hybrid model that, as far as we know, has not yet been mathematically formalized in the available literature. Therefore, considering the counting process formulation, the hazard function for the ith subject regarding the sth event is defined as

$$h\big(t; \mathbf{z}_{is}(t)\big) = \begin{cases} h_{0s}(t) \exp\big(\boldsymbol{\beta}' \mathbf{z}_{is}(t)\big), & 0 < s \leq S^* \\ h_0(t) \exp\big(\boldsymbol{\beta}' \mathbf{z}_{is}(t)\big), & S^* < s \leq S \end{cases}, \quad t \geq 0.$$

where $h_{0s}(t) \geq 0$ is the event-specific baseline hazard function, $h_0(t) \geq 0$ is the common baseline hazard function, and $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_p)'$ is the $p \times 1$ overall vector of unknown regression parameters.

Similarly it is necessary to adapt the partial likelihood functions of PWP (2) and AG (4) models to this situation. Admitting that the observations within the same subject are independent, the overall maximum likelihood estimator $\widehat{\boldsymbol{\beta}}$ is obtained through the following function:

$$L(\boldsymbol{\beta}) = \prod_{i=1}^{n} \prod_{s=1}^{S} \left[\frac{\exp\big(\boldsymbol{\beta}' \mathbf{z}_{is}(t_{is})\big)}{\mathbf{Q}_s(\boldsymbol{\beta}, t_{is})^{\Delta_s} \, \overline{\mathbf{Q}}(\boldsymbol{\beta}, t_{is})^{1-\Delta_s}} \right]^{\delta_{is}},$$

where $\mathbf{Q}_s(\boldsymbol{\beta}, t) = \sum_{j=1}^{n} Y_{js}(t) \exp\big(\boldsymbol{\beta}' \mathbf{z}_{js}(t)\big)$, $\overline{\mathbf{Q}}(\boldsymbol{\beta}, t) = \sum_{s=1}^{S} \mathbf{Q}_s(\boldsymbol{\beta}, t)$ and $\Delta_s = I(s \leq S^*)$ denote the indicator model variable which takes the value $\Delta_s = 1$ when the PWP model is considered ($0 < s \leq S^*$) and $\Delta_s = 0$ when the AG model is considered ($S^* < s \leq S$). It should be noted that Δ_s does not depend on the i index, which means that for all subjects we define that the AG model is applied from the S^* event. Furthermore, it is noteworthy that when $\Delta_s = 1$ we can also obtain the event-specific estimators $\widehat{\boldsymbol{\beta}}_1, \widehat{\boldsymbol{\beta}}_2, \ldots, \widehat{\boldsymbol{\beta}}_{S^*}$. The estimation of the event-specific regression parameters is performed by the same procedure described in Sect. 2.2.

3 PWP-AG Hybrid Model with Simulated Data

The application of the marginal models can be easily accomplished by `R`, S-Plus, or SAS statistical software. In this contribution we used the `R` statistical software [11], version 3.4.0, where for the analysis we used the `survival` package [12].

In order to evaluate the performance of the PWP-AG hybrid model, we proceeded with the simulation of a recurrent event data, bearing in mind the characteristics of the situations where this model is applied. The data set was simulated with `survsim` package [9], where we considered that the time to right censoring and to events follows a Weibull distribution. The values of the covariates were simulated from Bernoulli distribution (with probability of success $p = 0.5$), uniform distribution (that takes values in the range [0, 1]), and standard gaussian distribution. Let them be denoted by `x`, `x.1` and `x.2`, respectively. The procedure used for the simulation of this data set was recently presented by Ferreira [4].

Before applying any model, we decided to analyze the evolution of the risk for each event over time. The cumulative hazard functions from Kaplan-Meier estimates on the left side of Fig. 4 show that the first four events have different risks of occurring, but after that the risk is more similar. This was the main reason why we considered the PWP-AG hybrid model with $S^* = 4$ (right side of Fig. 4). Also, in Table 1 it can be seen the number of subjects at risk and observed events in each event number, where the decreasing over the strata becomes obvious. This means that if we want to calculate the event-specific estimates for the PWP model, these will be unreliable or even missing.

The implementation code of the PWP-AG hybrid model is very similar to the code of the PWP model [13, 14], the only difference lies in the way that we define the stratification variable. For the hybrid model it is necessary to define a new

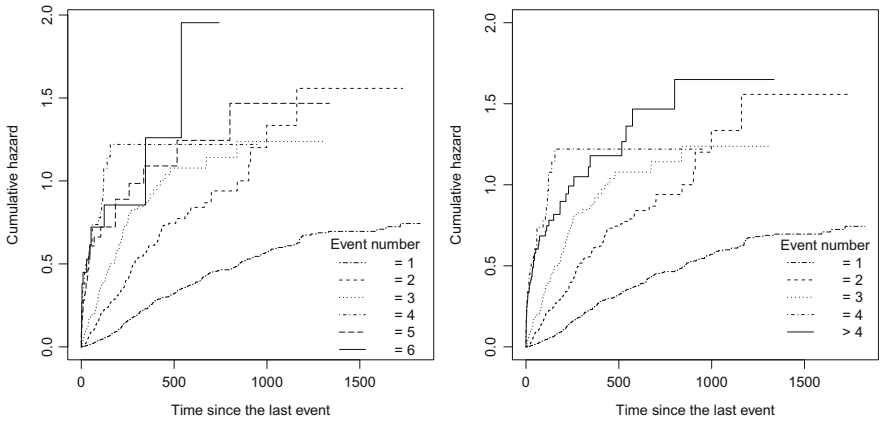

Fig. 4 Cumulative hazards from Kaplan-Meier estimates of the first 6 events (*left*) and of the first 4 events with the following ones agglomerated in the last stratum (*right*)

Table 1 Number of subjects at risk and observed events

	Event number									
	1	2	3	4	5	6	7	8	9	10
Subjects at risk	1000	365	162	87	48	27	15	10	6	3
Observed events	365	162	87	48	27	15	10	6	3	0

Table 2 Overall estimates of the various parameters associated with each model

Covariate/Model	$\widehat{\beta}_j$	$\exp(\widehat{\beta}_j)$	$se(\widehat{\beta}_j)$	$se_r(\widehat{\beta}_j)$	p-value
x					
PWP	0.52734	1.69442	0.08076	0.08624	9.66e−10
PWP-AG	0.52234	1.68598	0.07998	0.08615	1.33e−09
x.2					
PWP	0.67673	1.96742	0.04759	0.05003	<2e−16
PWP-AG	0.67702	1.96800	0.04694	0.04943	<2e−16

stratification variable, where we specified that after the $S^* = 4$ event the last strata are agglomerate in the $S^* + 1 = 5$ event number. So, in the stratification variable of the PWP-AG hybrid model the first four strata remain unchanged and the last strata are agglomerated in the stratum number five. Consequently, there will be an event-specific baseline hazard function for the first four events and a common baseline hazard function for the subsequent events.

The analysis revealed that the covariate `x.1` was not significant in both models (p-value=0.553 and p-value=0.403 in PWP and PWP-AG hybrid models, respectively). Therefore, in Table 2 we present the results of the models with the remaining two covariates. The parameters estimates were similar but the standard errors were slightly smaller in PWP-AG hybrid model, thus improving the accuracy of the estimates. For both models, the robust standard errors were inflated compared to the usual ones. This observed inflation suggests that there is less variation within-subjects than between-subjects [5].

In addition, the value of concordance for both models is 0.722. However, the value of R^2 is better for PWP-AG hybrid model ($R^2 = 0.131$ vs $R^2 = 0.129$).

4 Conclusions and Future Work

The proposed PWP-AG hybrid model revealed to be an alternative to the PWP model. The decision of gathering the last events was mainly based on the similarity of the cumulative hazard functions and not only on the dimension of the risk set. The fact that subjects become more homogeneous does not ensure that the hazard functions corresponding to the subsequent events are the same because the

mechanism that triggers such events may cause differences in these functions. This is the reason why it is important to represent the cumulative hazard function of each event.

On the other hand, the simulation showed that the parameters estimates become more accurate. Moreover, in this case the PWP-AG hybrid model has resulted in a better fit to the simulated data.

Although the PWP-AG hybrid model may not completely overcome the limitations of the PWP model (the loss of heterogeneity and the violation of the MCAR assumption), nevertheless these limitations are reduced. Therefore, the PWP-AG hybrid model is a compromise between PWP and AG models, which allows to compile the features of each of them.

Further work is required with this model, namely a simulation study, which can clarify when this model is more appropriate than the other models for recurrent events.

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A New Look at Combining Information from Stratum Submodels

Radosław Kala

Abstract If an experiment possesses the property of orthogonal block structure, the information contained in the experimental observations can be divided into uncorrelated parts represented by separate stratum submodels. The paper shows that this property is sufficient to obtain the results identical with those established by Nelder (J R Stat Soc Ser B 30:303–311, 1968) under the additional property of general balance. The approach proposed here is direct, quite general, and mainly geometrical.

Keywords Mixed linear models · Treatment contrasts · Stratum submodels · General balance

1 Introduction

The main principles improving the objectivity of inference from planned experiments consist of blocking the experimental units, sampling or randomizing processes, and replications of treatments on which the interest of the experimenter is focused. These principles determine a model of observations resulting from the experiment. The model with fixed effects of treatments and with random effects of various levels of blocking is classified as a mixed model. This paper deals with the issue of combining information on treatment comparisons following from several submodels, also known as stratum models, induced by the orthogonal block structure, possible when some additional assumptions are fulfilled.

The approach proposed here is quite general and mainly geometrical, which simplifies the considerations. In the next section, the basic concepts concerning the treatment parameters in the standard fixed model are recalled. In Sect. 3, the specific and well-known property of the orthogonal block structure, being the source

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of many stratum submodels, is presented. It is shown that this property is sufficient to justify the Nelder equations for estimating the variance components. Section 4 is devoted to the problem of combining information when the design possesses the property of general balance. In the next section three simple but illustrative examples are presented. Some concluding remarks are provided in the final section.

2 Fixed Models

Information delivered by any planned experiment is contained in a set of observations, forming a vector random variable $\boldsymbol{y}$, in a design determining the expectation of $\boldsymbol{y}$, $E(\boldsymbol{y})$, and in the dispersion matrix of $\boldsymbol{y}$, $D(\boldsymbol{y})$. These three elements form the model of observations,

$$\{\boldsymbol{y},\ E(\boldsymbol{y}),\ D(\boldsymbol{y})\}. \tag{1}$$

Usually the expectation of an n-dimensional vector $\boldsymbol{y}$ is directly connected with the set of p treatments through an $n \times p$ design matrix $\boldsymbol{X}$, i.e.,

$$E(\boldsymbol{y}) = \boldsymbol{\mu} = \boldsymbol{X}\boldsymbol{\beta}, \tag{2}$$

where $\boldsymbol{\beta}$ is a p-dimensional vector of fixed treatment parameters. Let the range of $\boldsymbol{X}$, $\mathcal{R}(\boldsymbol{X})$, be called the expectation subspace.

On the dispersion matrix we assume that it belongs to a suitably parametrized set $\mathcal{V}$ of the nonnegative definite matrices of order n, $D(\boldsymbol{y}) \in \mathcal{V}$. In a simplest, but not trivial, fixed model the set $\mathcal{V}$ takes the form $\mathcal{V} = \{\sigma^2\boldsymbol{F}\}$, where σ^2 is an unknown positive scalar, interpreted as a variance of errors, while $\boldsymbol{F}$ is a known nonnegative definite matrix, $\boldsymbol{F} \geq \boldsymbol{0}$. Such a model is represented by the triplet

$$\{\boldsymbol{y},\ \boldsymbol{X}\boldsymbol{\beta},\ \sigma^2\boldsymbol{F}\}. \tag{3}$$

If $\boldsymbol{F}$ is not of full rank, the model is termed singular. If, in addition, the expectation subspace $\mathcal{R}(\boldsymbol{X})$ is contained in $\mathcal{R}(\boldsymbol{F})$, the model is called weakly singular. Such models are of interest in this paper.

If the design matrix $\boldsymbol{X}$ is not of full column rank, only some linear functions of treatment parameters, $\boldsymbol{c}'\boldsymbol{\beta}$, are estimable. This concept, introduced by Bose [7], means that there exists a linear function of $\boldsymbol{y}$, $\boldsymbol{s}'\boldsymbol{y}$, such that $E(\boldsymbol{s}'\boldsymbol{y}) = \boldsymbol{c}'\boldsymbol{\beta}$. Of course, the expectation of $\boldsymbol{y}$, i.e., the vector $\boldsymbol{\mu} = \boldsymbol{X}\boldsymbol{\beta}$, is composed of n estimable functions (it is so, because $E(\boldsymbol{y}) = \boldsymbol{\mu}$ by the model definition). Because each estimable function $\boldsymbol{c}'\boldsymbol{\beta}$ can be replaced by $\boldsymbol{s}'\boldsymbol{X}\boldsymbol{\beta} = \boldsymbol{s}'\boldsymbol{\mu}$, i.e., by a linear function of the expectation of $\boldsymbol{y}$, we can focus our attention on the estimation of $\boldsymbol{\mu}$. For this, it will be convenient to express the model in the form,

$$\{\boldsymbol{y},\ \boldsymbol{P}\boldsymbol{\mu},\ \sigma^2\boldsymbol{F}\}, \tag{4}$$

where $\boldsymbol{P}$ is the orthogonal projector on $\mathcal{R}(\boldsymbol{X})$, i.e., $\boldsymbol{P}^2 = \boldsymbol{P} = \boldsymbol{P}'$ and $\boldsymbol{PX} = \boldsymbol{X}$. In result, $\boldsymbol{P}\boldsymbol{\mu} = \boldsymbol{X}\boldsymbol{\beta}$.

Although the vector $\boldsymbol{y}$ is an unbiased estimator of $\boldsymbol{\mu}$, it is far from being the best. By the best linear unbiased estimator (BLUE) we mean such a linear unbiased statistic which has, irrespective of the unknown variance σ^2, the smallest dispersion matrix according to the Löwner order. Under the condition $\mathcal{R}(\boldsymbol{X}) \subset \mathcal{R}(\boldsymbol{F})$ (i.e., that the model is weakly singular), the best linear unbiased estimator of $\boldsymbol{\mu}$ is obtainable through a solution of the normal equations, which can be expressed as

$$\boldsymbol{P}\boldsymbol{F}^+\boldsymbol{P}\boldsymbol{\mu} = \boldsymbol{P}\boldsymbol{F}^+\boldsymbol{y}, \tag{5}$$

where $\boldsymbol{F}^+$ denotes the Moore–Penrose inverse of $\boldsymbol{F}$. In consequence, the BLUE of $\boldsymbol{\mu}$ takes the form $\widehat{\boldsymbol{\mu}} = \boldsymbol{P}^{\mathbf{F}}\boldsymbol{y}$, where

$$\boldsymbol{P}^{\mathbf{F}} = \boldsymbol{P}(\boldsymbol{P}\boldsymbol{F}^+\boldsymbol{P})^+\boldsymbol{P}\boldsymbol{F}^+. \tag{6}$$

Having the BLUE of $\boldsymbol{\mu}$, one can obtain the BLUE of any estimable function $\boldsymbol{c}'\boldsymbol{\beta}$. Indeed, if $\boldsymbol{c}'\boldsymbol{\beta}$ is estimable, then $\boldsymbol{c}'\boldsymbol{\beta} = \boldsymbol{s}'\boldsymbol{X}\boldsymbol{\beta} = \boldsymbol{s}'\boldsymbol{\mu}$ for some $\boldsymbol{s}$, which, by the linearity property, implies that $\widehat{\boldsymbol{c}'\boldsymbol{\beta}}$ is equal to $\boldsymbol{s}'\widehat{\boldsymbol{\mu}}$.

The matrix $\boldsymbol{P}^{\mathbf{F}}$ is idempotent (i.e., $\boldsymbol{P}^{\mathbf{F}}\boldsymbol{P}^{\mathbf{F}} = \boldsymbol{P}^{\mathbf{F}}$), $\boldsymbol{P}^{\mathbf{F}}\boldsymbol{P} = \boldsymbol{P}$, and $\boldsymbol{P}^{\mathbf{F}}\boldsymbol{F}$ together with $\boldsymbol{F}^+\boldsymbol{P}^{\mathbf{F}}$ are symmetric matrices. The first and second property means that $\boldsymbol{P}^{\mathbf{F}}$ is a projector on the expectation subspace, because $\mathcal{R}(\boldsymbol{P}) = \mathcal{R}(\boldsymbol{X})$. This operator projects along the complementary subspace $\mathcal{R}(\boldsymbol{I}-\boldsymbol{P}^{\mathbf{F}})$, where $\boldsymbol{I}$ denotes the identity matrix, here of order n. The third property has a geometrical sense. Because $(\boldsymbol{I} - \boldsymbol{P}^{\mathbf{F}})'\boldsymbol{F}^+\boldsymbol{P} = \boldsymbol{0}$, the operator $\boldsymbol{P}^{\mathbf{F}}$ is the orthogonal projector on $\mathcal{R}(\boldsymbol{X})$ under the semi-inner product defined with the use of $\boldsymbol{F}^+$.

The operator

$$\boldsymbol{R} = \boldsymbol{I} - \boldsymbol{P}^{\mathbf{F}} \tag{7}$$

is also a projector such that $\boldsymbol{R}\boldsymbol{F} = \boldsymbol{F}\boldsymbol{R}'$ and $\boldsymbol{R}\boldsymbol{P} = \boldsymbol{0}$. It produces the vector of residuals if applied to the vector $\boldsymbol{y}$. The squared length of the vector of residuals under the aforementioned semi-inner product,

$$\mathrm{RSS} = \boldsymbol{y}'\boldsymbol{R}'\boldsymbol{F}^+\boldsymbol{R}\boldsymbol{y}, \tag{8}$$

is known as the residual sum of squares.

The expectation of the RSS can be easily calculated as

$$E(\mathrm{RSS}) = \sigma^2\mathrm{tr}(\boldsymbol{F}\boldsymbol{R}'\boldsymbol{F}^+\boldsymbol{R}) + \boldsymbol{\mu}'\boldsymbol{R}'\boldsymbol{F}^+\boldsymbol{R}\boldsymbol{\mu} = \sigma^2\mathrm{tr}(\boldsymbol{F}\boldsymbol{F}^+\boldsymbol{R}) = \sigma^2 d, \tag{9}$$

where $d = \mathrm{rank}(\boldsymbol{F}) - \mathrm{rank}(\boldsymbol{X})$. In consequence, the mean square error (i.e., the RSS divided by the degrees of freedom d) provides the well-known unbiased estimator of the error variance σ^2.

A replacement of the matrix $\boldsymbol{F}$ in the model (3) by the identity matrix $\boldsymbol{I}$ results in so-called the simple model $\{\boldsymbol{y}, \boldsymbol{X\beta}, \sigma^2\boldsymbol{I}\}$. This replacement means that the observations given in $\boldsymbol{y}$ are uncorrelated. In this case the projector (6) reduces to $\boldsymbol{P}$ which depends only on the matrix spanning the expectation subspace.

The projector $\boldsymbol{P}$, ignoring the form of the dispersion matrix, can be applied also in the model (3). Then the estimator $\boldsymbol{Py}$ is unbiased for $\boldsymbol{\mu}$, but is not the BLUE. Its dispersion matrix, $\sigma^2\boldsymbol{PFP}$, is greater, in the Löwner order, than that of the BLUE for $\boldsymbol{\mu}$, $D(\widehat{\boldsymbol{\mu}}) = \sigma^2\boldsymbol{P}(\boldsymbol{PF}^+\boldsymbol{P})^+\boldsymbol{P}$, which means that $\boldsymbol{PFP} - \boldsymbol{P}(\boldsymbol{PF}^+\boldsymbol{P})^+\boldsymbol{P} \geq \boldsymbol{0}$. The statistic $\boldsymbol{Py}$ is called the least squares estimator, LSE. The problem of equality between the BLUE and LSE focused the attention of many authors [1, 17, 19–21]. A more complete review of the results concerning this issue is presented in the paper by Baksalary et al. [6]. One of such results states that the BLUE of $\boldsymbol{\mu}$ coincides with the LSE of $\boldsymbol{\mu}$ if and only if the expectation subspace is an invariant subspace of the dispersion matrix $\boldsymbol{F}$, the condition of which can be expressed by the equality $\boldsymbol{PF} = \boldsymbol{FP}$ (see, e.g., [5]).

3 Mixed Models

The mixed models differ from fixed models in forms of the dispersion matrices. The model is termed variance component model if the set of dispersion matrices has the form

$$\mathcal{V} = \{\boldsymbol{V} = \alpha_1\boldsymbol{V}_1 + \alpha_2\boldsymbol{V}_2 + \cdots + \alpha_l\boldsymbol{V}_l \geq \boldsymbol{0}\}, \tag{10}$$

where $\boldsymbol{V}_1, \boldsymbol{V}_2, \ldots, \boldsymbol{V}_l$ are known nonnegative definite matrices, while $\alpha_1, \alpha_2, \ldots, \alpha_l$ are unknown positive scalars. Usually, the matrix $\boldsymbol{V}_l = \boldsymbol{I}$, and then the component $\alpha_l = \sigma^2$ is interpreted as the error variance of measurements. In designed experiments, the other matrices $\boldsymbol{V}_i, i = 1, 2, \ldots, l-1$, reflect the randomization processes in relation with the structure of blocking of experimental units.

Under a specific condition satisfied by the matrices $\boldsymbol{V}_i, i = 1, 2, \ldots, l$, the set $\mathcal{V}$ can be reparametrized in such a way that

$$\mathcal{V} = \{\boldsymbol{F} = \sigma_1^2\boldsymbol{\phi}_1 + \sigma_2^2\boldsymbol{\phi}_2 + \cdots + \sigma_k^2\boldsymbol{\phi}_k\}, \tag{11}$$

where $\sigma_1^2, \sigma_2^2, \ldots, \sigma_k^2$ are linear functions of $\alpha_1, \alpha_2, \ldots, \alpha_l$ and $\boldsymbol{\phi}_1, \boldsymbol{\phi}_2, \ldots, \boldsymbol{\phi}_k$ are mutually orthogonal projectors and such that

$$\boldsymbol{\phi}_1 + \boldsymbol{\phi}_2 + \cdots + \boldsymbol{\phi}_k = \boldsymbol{I}. \tag{12}$$

A design with such property is said that it possesses the orthogonal block structure (OBS) (see [2, 3, 12–14]). The resulting model may be written in a form

similar to the fixed model, i.e.,

$$\{\boldsymbol{y},\ \boldsymbol{P}\boldsymbol{\mu},\ \sigma^2\boldsymbol{F}_{\boldsymbol{\delta}}\}. \tag{13}$$

where $\boldsymbol{\delta} = (\sigma_1^2/\sigma^2, \sigma_2^2/\sigma^2, \ldots, \sigma_k^2/\sigma^2)'$ and $\boldsymbol{F}_{\boldsymbol{\delta}} = \delta_1\boldsymbol{\phi}_1 + \delta_2\boldsymbol{\phi}_2 + \cdots + \delta_k\boldsymbol{\phi}_k$. Of course, for any positive scalar σ^2, we have $\sigma^2\boldsymbol{F}_{\boldsymbol{\delta}} = \boldsymbol{F}$, where $\boldsymbol{F}$ is defined in (11).

The existence of the BLUE for $\boldsymbol{\mu}$ under the model (13) is very limited. Actually, for any given vector $\boldsymbol{\delta}$ with positive entries, the triplet (13) defines a fixed model. In each such fixed model the BLUE of $\boldsymbol{\mu}$ exists, but it is a local BLUE, because it is determined by the value of $\boldsymbol{\delta}$. In view of (12), the vector $\boldsymbol{\delta} = (1, 1, \ldots, 1)'$ induces the simple model $\{\boldsymbol{y},\ \boldsymbol{P}\boldsymbol{\mu},\ \sigma^2\boldsymbol{I}\}$ in which the BLUE and the LSE for $\boldsymbol{\mu}$ are the same statistics. Of course none of the local BLUE, as dependent on $\boldsymbol{\delta}$, is the overall BLUE in the model (13).

The OBS property provides another possibility. Post-multiplying (12) by $\boldsymbol{y}$ leads to the equality

$$\boldsymbol{y} = \boldsymbol{y}_1 + \boldsymbol{y}_2 + \cdots + \boldsymbol{y}_k, \tag{14}$$

where $\boldsymbol{y}_j = \boldsymbol{\phi}_j\boldsymbol{y}$, $j = 1, 2, \ldots, k$, are uncorrelated random variables. This means that the information contained in the vector $\boldsymbol{y}$ is divided into uncorrelated parts. The part j, represented by the vector $\boldsymbol{y}_j$, leads to the model

$$\{\boldsymbol{y}_j,\ \boldsymbol{\phi}_j\boldsymbol{P}\boldsymbol{\mu},\ \sigma_j^2\boldsymbol{\phi}_j\}, \tag{15}$$

in which the expectation subspace $\mathcal{R}(\boldsymbol{\phi}_j\boldsymbol{P}) = \mathcal{R}(\boldsymbol{\phi}_j\boldsymbol{X})$ is the projection of $\mathcal{R}(\boldsymbol{X})$ by the projector $\boldsymbol{\phi}_j$ while the dispersion matrix follows from the symmetric transformation: $\sigma^2\boldsymbol{F}_{\boldsymbol{\delta}} \to \boldsymbol{\phi}_j\boldsymbol{F}\boldsymbol{\phi}_j = \sigma_j^2\boldsymbol{\phi}_j$.

The triplet (15) represents the so-called jth stratum submodel. Its expectation subspace is contained in the range of the singular dispersion matrix, $\mathcal{R}(\boldsymbol{\phi}_j)$, which means that the model is weakly singular. The BLUE of the expectation in this model can be obtained by solving the normal equation, which is presented here in the form as in Houtman and Speed ([12] equation NE_α),

$$\boldsymbol{P}\boldsymbol{\phi}_j\boldsymbol{P}\boldsymbol{\mu} = \boldsymbol{P}\boldsymbol{\phi}_j\boldsymbol{y}. \tag{16}$$

Actually, such stratum BLUE follows by the least squares procedure, because for each stratum submodel the expectation subspace $\mathcal{R}(\boldsymbol{\phi}_j\boldsymbol{P})$ is an invariant subspace of the corresponding dispersion matrix $\boldsymbol{\phi}_j$.

Now, let us assume that the entries of $\boldsymbol{\delta}$ are known. Then, one can pose the question, how to combine the information from the various strata to obtain the BLUE of $\boldsymbol{\mu}$ in the overall model (13). The answer is easy. It was exploited by many authors (see, e.g., [8–12]). Actually, it is sufficient to note that the weighted sum of

the normal equations related to all strata,

$$\sum_{j=1}^{k} \delta_j^{-1} \boldsymbol{P}\boldsymbol{\phi}_j \boldsymbol{P}\boldsymbol{\mu} = \sum_{j=1}^{k} \delta_j^{-1} \boldsymbol{P}\boldsymbol{\phi}_j \boldsymbol{y}, \tag{17}$$

leads to the overall normal equations

$$\boldsymbol{P}\boldsymbol{F}_{\boldsymbol{\delta}}^{+}\boldsymbol{P}\boldsymbol{\mu} = \boldsymbol{P}\boldsymbol{F}_{\boldsymbol{\delta}}^{+}\boldsymbol{y}, \tag{18}$$

because

$$\sum_{j=1}^{k} \delta_j^{-1} \boldsymbol{\phi}_j = \boldsymbol{F}_{\boldsymbol{\delta}}^{+}. \tag{19}$$

This property suggests that the optimal estimator of $\boldsymbol{\mu}$, even if the vector $\boldsymbol{\delta}$ is unknown, should also be delivered by the projector of the form (6) with $\boldsymbol{F}^{+}$ replaced by $\boldsymbol{F}_{\boldsymbol{\delta}}^{+}$. Of course, the vector $\boldsymbol{\delta}$ should be chosen properly. This issue means a necessity of estimating the stratum variances, what was exactly stated in Nelder [15, at the end of Section 2].

To this aim, let us consider the overall residual sum of squares. It takes the form

$$\mathrm{RSS} = \boldsymbol{y}'\boldsymbol{R}_{\boldsymbol{\delta}}'\boldsymbol{F}_{\boldsymbol{\delta}}^{+}\boldsymbol{R}_{\boldsymbol{\delta}}\boldsymbol{y}, \tag{20}$$

where $\boldsymbol{R}_{\boldsymbol{\delta}} = \boldsymbol{I} - \boldsymbol{P}^{\mathbf{F}_{\boldsymbol{\delta}}}$. Of course, its expectation follows as in (9), i.e., $E(\mathrm{RSS}) = \sigma^2 tr(\boldsymbol{F}_{\boldsymbol{\delta}}\boldsymbol{F}_{\boldsymbol{\delta}}^{+}\boldsymbol{R}_{\boldsymbol{\delta}})$. Now, let us assume that all δ's, except δ_j, in the matrix $\boldsymbol{F}_{\boldsymbol{\delta}}$ converge to zero. Then $\boldsymbol{F}_{\boldsymbol{\delta}}$ converges to $\delta_j\boldsymbol{\phi}_j$, i.e., to the matrix proportional to the dispersion matrix of the jth stratum submodel. In consequence,

$$\mathrm{RSS} = \boldsymbol{y}'\boldsymbol{R}_{\boldsymbol{\delta}}'\boldsymbol{F}_{\boldsymbol{\delta}}^{+}\boldsymbol{R}_{\boldsymbol{\delta}}\boldsymbol{y} \;\to\; \delta_j^{-1}\boldsymbol{y}'\boldsymbol{R}_{\boldsymbol{\delta}}'\boldsymbol{\phi}_j\boldsymbol{R}_{\boldsymbol{\delta}}\boldsymbol{y}, \tag{21}$$

and

$$E(\mathrm{RSS}) = \sigma^2\mathrm{tr}(\boldsymbol{F}_{\boldsymbol{\delta}}\boldsymbol{F}_{\boldsymbol{\delta}}^{+}\boldsymbol{R}_{\boldsymbol{\delta}}) \;\to\; \sigma^2\mathrm{tr}(\boldsymbol{\phi}_j\boldsymbol{R}_{\boldsymbol{\delta}}). \tag{22}$$

Comparing the right-hand sides of (21) and (22), also for the other subscripts j, i.e., with respect to all stratum submodels, leads to a system of k nonlinear equations

$$\boldsymbol{y}'\boldsymbol{R}_{\boldsymbol{\delta}}'\boldsymbol{\phi}_j\boldsymbol{R}_{\boldsymbol{\delta}}\boldsymbol{y} = \sigma_j^2\mathrm{tr}(\boldsymbol{\phi}_j\boldsymbol{R}_{\boldsymbol{\delta}}), \quad j = 1, 2, \ldots, k, \tag{23}$$

written also as

$$\left\|\boldsymbol{\phi}_j\boldsymbol{R}_{\boldsymbol{\delta}}\boldsymbol{y}\right\|^2 = \sigma_j^2\mathrm{tr}(\boldsymbol{\phi}_j\boldsymbol{R}_{\boldsymbol{\delta}}), \quad j = 1, 2, \ldots, k.$$

They are actually the same as those first established by Nelder [15] in the context of the generally balanced designs if, however, the simplification following from Lemma (ii) in Houtman and Speed [12] is taken into account. They also coincide, as it was observed by Patterson and Thompson [16], with the equations following from their maximum likelihood approach under the assumption that $\boldsymbol{y}$ has a multivariate normal distribution.

Equations (23) can also be established directly by considering the orthogonal projections of the residual vector $\boldsymbol{R}_{\boldsymbol{\delta}}\boldsymbol{y}$ onto the subspaces $\mathcal{R}(\boldsymbol{\phi}_j)$, $j = 1, 2, \ldots, k$. The quadratic length of each such vector takes the form

$$\mathrm{RSS}_j = \boldsymbol{y}'\boldsymbol{R}'_{\boldsymbol{\delta}}\boldsymbol{\phi}_j\boldsymbol{R}_{\boldsymbol{\delta}}\boldsymbol{y}. \tag{24}$$

Its expectation can be obtained exactly in the same way as in (9), i.e.,

$$E(\mathrm{RSS}_j) = \sigma^2\mathrm{tr}(\boldsymbol{F}_{\boldsymbol{\delta}}\boldsymbol{R}'_{\boldsymbol{\delta}}\boldsymbol{\phi}_j\boldsymbol{R}_{\boldsymbol{\delta}}) + \boldsymbol{\mu}'\boldsymbol{R}'_{\boldsymbol{\delta}}\boldsymbol{\phi}_j\boldsymbol{R}_{\boldsymbol{\delta}}\boldsymbol{\mu} = \sigma_j^2\mathrm{tr}(\boldsymbol{\phi}_j\boldsymbol{R}_{\boldsymbol{\delta}}), \tag{25}$$

because $\boldsymbol{F}_{\boldsymbol{\delta}}\boldsymbol{R}'_{\boldsymbol{\delta}}$ is a symmetric matrix and $\boldsymbol{F}_{\boldsymbol{\delta}}\boldsymbol{\phi}_j = \delta_j\boldsymbol{\phi}_j$. In consequence, it appears that for any fixed vector $\boldsymbol{\delta}$, the expectation of the right-hand side in (21) really equals to the right-hand side in (22), which again justifies Eq. (23).

The set of Eqs. (23) can be solved iteratively starting with any initial values of δ's in the residual projector $\boldsymbol{R}_{\boldsymbol{\delta}}$. The simplest starting point is $\boldsymbol{\delta} = (1, 1, \ldots, 1)$. This choice means that the initial projector $\boldsymbol{R}_{\boldsymbol{\delta}}$ coincides with $\boldsymbol{I} - \boldsymbol{P}$, where $\boldsymbol{P}$ is the simple least squares operator. The iteration process is continued until its convergence.

When the final values σ_j^2, $j = 1, 2, \ldots, k$, are correctly established, then summing up Eqs. (23) premultiplied by δ_j^{-1}, $j = 1, 2, \ldots, k$, respectively, leads to the equality

$$\boldsymbol{y}'\boldsymbol{R}'_{\boldsymbol{\delta}}\left(\sum_{j=1}^{k}\delta_j^{-1}\boldsymbol{\phi}_j\right)\boldsymbol{R}_{\boldsymbol{\delta}}\boldsymbol{y} = \sigma^2\mathrm{tr}\left(\boldsymbol{R}_{\boldsymbol{\delta}}\sum_{j=1}^{k}\boldsymbol{\phi}_j\right),$$

which, in view of (12) and (19), can be written as

$$\boldsymbol{y}'\boldsymbol{R}'_{\boldsymbol{\delta}}\boldsymbol{F}_{\boldsymbol{\delta}}^{+}\boldsymbol{R}_{\boldsymbol{\delta}}\boldsymbol{y} = \sigma^2\mathrm{tr}\left(\boldsymbol{R}_{\boldsymbol{\delta}}\right). \tag{26}$$

This equality holds for any positive σ^2. Taking $\sigma^2 = 1$ leads to the conclusion that the mean square error in the model with estimated variance components from Eqs. (23) is equal to one. This fact may be utilized to control the convergence of the iteration process.

Finally note that Eqs. (23) give a reasonable bases for estimating the unknown stratum variances even if the design is not generally balanced [see, e.g. 9, Section 3.2]. The evaluation presented here is fully geometrical, distribution free and requires only that the design has the orthogonal block structure.

4 Generally Balanced Designs

The property of general balance can be characterized simply as a commutativity of the information matrices of the stratum submodels, i.e., the design is generally balanced if and only if the matrices $\boldsymbol{P}\boldsymbol{\phi}_i\boldsymbol{P}$ and $\boldsymbol{P}\boldsymbol{\phi}_j\boldsymbol{P}$ commute, for all $i, j = 1, 2, \ldots, k, i \neq j$. This condition means that all these matrices have a set of common eigenvectors.

However, in view of Eq. (12), pre- and post-multiplied by $\boldsymbol{P}$, the following equality

$$\boldsymbol{P}\boldsymbol{\phi}_1\boldsymbol{P} + \boldsymbol{P}\boldsymbol{\phi}_2\boldsymbol{P} + \cdots + \boldsymbol{P}\boldsymbol{\phi}_k\boldsymbol{P} = \boldsymbol{P} \tag{27}$$

holds. Because the projector $\boldsymbol{P}$ also commutes with all matrices on the left-hand side of (27), each common eigenvector $\boldsymbol{q}_s$ fulfills the equality

$$\begin{aligned} &\boldsymbol{P}\boldsymbol{\phi}_1\boldsymbol{P}\boldsymbol{q}_s + \boldsymbol{P}\boldsymbol{\phi}_2\boldsymbol{P}\boldsymbol{q}_s + \cdots + \boldsymbol{P}\boldsymbol{\phi}_k\boldsymbol{P}\boldsymbol{q}_s = \\ &= \epsilon_{s1}\boldsymbol{q}_s + \epsilon_{s2}\boldsymbol{q}_s + \cdots + \epsilon_{sk}\boldsymbol{q}_s = \boldsymbol{P}\boldsymbol{q}_s = \boldsymbol{q}_s \neq \boldsymbol{0}, \end{aligned} \tag{28}$$

where ϵ_{sj} is the eigenvalue of $\boldsymbol{P}\boldsymbol{\phi}_j\boldsymbol{P}$ corresponding to the eigenvector $\boldsymbol{q}_s$. In consequence, if $\epsilon_{sj} = 0$, then $\boldsymbol{P}\boldsymbol{\phi}_j\boldsymbol{P}\boldsymbol{q}_s = \boldsymbol{0}$, i.e., $\boldsymbol{\phi}_j\boldsymbol{q}_s = \boldsymbol{0}$, because $\boldsymbol{P}\boldsymbol{q}_s = \boldsymbol{q}_s$ for all non-zero $\boldsymbol{q}_s$. Actually, the number of non-zero eigenvectors $\boldsymbol{q}_s$ is equal to $r = \mathrm{rank}(\boldsymbol{X})$, because $\boldsymbol{P}$ has the eigenvalue equal to one with multiplicity equal to $\mathrm{rank}(\boldsymbol{X})$. The latter property implies that

$$\epsilon_{i1} + \epsilon_{i2} + \cdots + \epsilon_{ik} = 1, \tag{29}$$

for all $i = 1, 2, \ldots, r$. These eigenvalues, summing up to one, are considered as the efficiency factors measuring the usefulness of each stratum submodel in estimation of a given linear function $\boldsymbol{q}_s'\boldsymbol{\mu}$.

Now, come back to Eq. (17). Taking into account the simultaneous spectral decomposition of all matrices $\boldsymbol{P}\boldsymbol{\phi}_j\boldsymbol{P}$, one obtains

$$\sum_{j=1}^{k}\delta_j^{-1}\sum_{i=1}^{r}\epsilon_{ij}\boldsymbol{q}_i\boldsymbol{q}_i'\boldsymbol{\mu} = \sum_{i=1}^{r}\gamma_i\boldsymbol{q}_i\boldsymbol{q}_i'\boldsymbol{\mu} = \sum_{j=1}^{k}\delta_j^{-1}\boldsymbol{P}\boldsymbol{\phi}_j\boldsymbol{y} \tag{30}$$

where

$$\gamma_i = \sum_{j=1}^{k}\delta_j^{-1}\epsilon_{ij}. \tag{31}$$

In consequence, the projector $\boldsymbol{P}^{\mathbf{F}_\delta}$ takes the form

$$\boldsymbol{P}^{\mathbf{F}_\delta} = \boldsymbol{P}\left(\sum_{i=1}^{r}\gamma_i \boldsymbol{q}_i\boldsymbol{q}_i'\right)^{+}\sum_{j=1}^{k}\delta_j^{-1}\boldsymbol{P}\boldsymbol{\phi}_j. \tag{32}$$

If some $\epsilon_{sl} = 1$, then the lth stratum submodel is the only one in which the function $\boldsymbol{q}_s'\boldsymbol{\mu}$ is estimated with full efficiency. The equality $\epsilon_{sl} = 1$ implies that $\gamma_s = \delta_l^{-1}$. In result, the statistic $\boldsymbol{q}_s'\widehat{\boldsymbol{\mu}}$ reduces as follows:

$$\boldsymbol{q}_s'\boldsymbol{P}^{\mathbf{F}_\delta}\boldsymbol{y} = \boldsymbol{q}_s'\boldsymbol{P}\left(\sum_{i=1}^{r}\gamma_i^{-1}\boldsymbol{q}_i\boldsymbol{q}_i'\right)\sum_{j=1}^{k}\delta_j^{-1}\boldsymbol{P}\boldsymbol{\phi}_j\boldsymbol{y} =$$

$$= \delta_l\,\boldsymbol{q}_s'\sum_{j=1}^{k}\delta_j^{-1}\boldsymbol{\phi}_j\boldsymbol{y} = \delta_l\,\boldsymbol{q}_s'\delta_l^{-1}\boldsymbol{\phi}_l\boldsymbol{y} = \boldsymbol{q}_s'\boldsymbol{y}_l = \boldsymbol{q}_s'\boldsymbol{y}, \tag{33}$$

where the final equalities take place as $\boldsymbol{\phi}_l\boldsymbol{q}_s = \boldsymbol{q}_s$ and $\boldsymbol{\phi}_j\boldsymbol{q}_s = \boldsymbol{0}$ for $j \neq s$. Therefore, the statistic $\boldsymbol{q}_s'\boldsymbol{y}_l = \boldsymbol{q}_s'\boldsymbol{y}$ is the local BLUE for $\boldsymbol{q}_s'\boldsymbol{\mu}$ in the lth stratum submodel and, simultaneously, is the BLUE for $\boldsymbol{q}_s'\boldsymbol{\mu}$ in the overall model. The last conclusion can also be confirmed by the criterion of Zyskind [21] that $\boldsymbol{q}_s'\boldsymbol{y}$ is the BLUE for its expectation if and only if the vector $\boldsymbol{F}_\delta\boldsymbol{q}_s$ is contained in the expectation subspace of the model. It is so, because $\boldsymbol{F}_\delta\boldsymbol{q}_s = \boldsymbol{F}_\delta\boldsymbol{\phi}_l\boldsymbol{q}_s = \delta_l\boldsymbol{\phi}_l\boldsymbol{q}_s = \delta_l\boldsymbol{q}_s \in \mathcal{R}(\boldsymbol{P})$.

The variances of $\boldsymbol{q}_s'\boldsymbol{y}_l$ and of $\boldsymbol{q}_s'\boldsymbol{y}$ are obviously the same,

$$var(\boldsymbol{q}_s'\boldsymbol{y}_l) = \sigma_l^2 = var(\boldsymbol{q}_s'\boldsymbol{y}).$$

The estimate of σ_l^2 can be obtained from the lth Eq. in (23),

$$\boldsymbol{y}'\boldsymbol{R}_\delta'\boldsymbol{\phi}_l\boldsymbol{R}_\delta\boldsymbol{y} = \sigma_l^2\mathrm{tr}(\boldsymbol{\phi}_l\boldsymbol{R}_\delta),$$

or from the similar equation related to the lth stratum submodel,

$$\boldsymbol{y}'\boldsymbol{R}_l\boldsymbol{y} = \sigma_l^2\mathrm{tr}(\boldsymbol{R}_l),$$

where $\boldsymbol{R}_l = \boldsymbol{\phi}_l - \boldsymbol{\phi}_l\boldsymbol{P}(\boldsymbol{P}\boldsymbol{\phi}_l\boldsymbol{P})^{+}\boldsymbol{P}\boldsymbol{\phi}_l$ is the corresponding residual projector. These equations do not lead, however, to the same solution. It can be shown that $\boldsymbol{R}_\delta'\boldsymbol{\phi}_l\boldsymbol{R}_\delta - \boldsymbol{R}_l \geq \boldsymbol{0}$ and, simultaneously, $\mathrm{tr}(\boldsymbol{\phi}_l\boldsymbol{R}_\delta) \geq \mathrm{tr}(\boldsymbol{R}_l)$. In consequence, it is not possible to predict which model provides the smaller estimate of σ_l^2.

When ϵ_{sl} is less than one, the information about $\boldsymbol{q}_s'\boldsymbol{\mu}$ splits into at least two stratum submodels and the estimation of all variance components is necessary to obtain a reasonable estimate. The estimates of variance components can be obtained by solving Eqs. (23). The final estimator is not the BLUE, but it combines

information from various strata taking into account their efficiency factors as well as stratum variances. Another question is, whether the function $\boldsymbol{q}_s' \boldsymbol{P}^{\mathbf{F}_\delta} \boldsymbol{y}$ brings an interesting information about the treatment comparisons. It depends on the blocking structure of the design. A comprehensive discussion on this topic is contained in the paper by Bailey [4]. Some simple examples in the next section exhibit some aspects of this issue.

5 Three Examples

The examples require some computations. In this matter, it is important to note that in almost all formulas instead of the Moore–Penrose inverse one can use any g-inverse. This follows from the invariance property as, e.g., in Rao and Rao [18, Corollary 8.2.5]. Moreover, instead of solving Eqs. (5), (16), or (18) with respect to $\boldsymbol{\mu}$, it is easier to solve the standard normal equations with respect to $\boldsymbol{\beta}$. Similarly, Eq. (27) can be replaced by the equivalent equation

$$\boldsymbol{X}'\boldsymbol{\phi}_1\boldsymbol{X} + \boldsymbol{X}'\boldsymbol{\phi}_2\boldsymbol{X} + \cdots + \boldsymbol{X}'\boldsymbol{\phi}_k\boldsymbol{X} = \boldsymbol{X}'\boldsymbol{X}. \tag{34}$$

In this case, the commutativity of the matrices $\boldsymbol{X}'\boldsymbol{\phi}_j\boldsymbol{X}$, $j = 1, 2, \ldots, k$, with respect to the inverse of $\boldsymbol{X}'\boldsymbol{X}$ is the necessary and sufficient condition for the general balance property. In consequence, the simultaneous spectral decomposition of all matrices $\boldsymbol{X}'\boldsymbol{\phi}_j\boldsymbol{X}$, $j = 1, 2, \ldots, k$, is based on the set of common eigenvectors considered with respect to $\boldsymbol{X}'\boldsymbol{X}$. Such approach reduces the order of matrices involved to the number of fixed parameters.

After the above remarks, it is worth to consider the simple but instructive examples. The first two follow from the mixed model of the form

$$\{\boldsymbol{y},\ \boldsymbol{X}\boldsymbol{\beta},\ \sigma_b^2\boldsymbol{Z}\boldsymbol{D}\boldsymbol{Z}' + \sigma_0^2\boldsymbol{I}\}, \tag{35}$$

where $\boldsymbol{Z}$ represents a design matrix for blocks, $\boldsymbol{D}$, being a diagonal matrix with non-zero entries related to the block sizes, represents a dispersion matrix for block effects, while σ_b^2 and σ_0^2 are the variances of random block effects and measurements, respectively. This model has the form parallel to that of Patterson and Thompson [16] with $\boldsymbol{D} = \gamma\boldsymbol{I}$ and $\sigma_b^2 = \gamma\sigma_0^2$.

In the first example, it is assumed that

$$\boldsymbol{y} = \begin{bmatrix} 10 \\ 14 \\ 15 \\ 9 \\ 12 \end{bmatrix}, \quad \boldsymbol{X} = \begin{bmatrix} 1\,0\,0 \\ 0\,1\,0 \\ 0\,0\,1 \\ 1\,0\,0 \\ 0\,1\,0 \end{bmatrix}, \quad \boldsymbol{Z} = \begin{bmatrix} 1\,0 \\ 1\,0 \\ 1\,0 \\ 0\,1 \\ 0\,1 \end{bmatrix}, \quad \boldsymbol{D} = \begin{bmatrix} 2\,0 \\ 0\,3 \end{bmatrix}, \tag{36}$$

i.e., the design relates five observations of three treatments with two blocks, one complete and the other without the third treatment. Such design has the orthogonal block structure with $\boldsymbol{\phi}_1 = \boldsymbol{Z}(\boldsymbol{Z}'\boldsymbol{Z})^{-1}\boldsymbol{Z}'$, $\sigma_1^2 = 6\sigma_b^2 + \sigma_0^2$, $\boldsymbol{\phi}_2 = \boldsymbol{I} - \boldsymbol{\phi}_1$, and $\sigma_2^2 = \sigma_0^2$. Moreover, this design is generally balanced. In this place, it is worth to note that any design with orthogonal block structure and only two strata possess generally balance property.

As a consequence, the information matrices of the intra-block and inter-block stratum of the model (36) have the simultaneous spectral decomposition leading to the following basic contrasts and their efficiencies:

Basic contrasts	Inter-block eff.	Intra-block eff.
$\boldsymbol{c}_1 = (1, \ -1, \ \ 0)'$	$*$	1
$\sqrt{5}\,\boldsymbol{c}_2 = (1, \ \ 1, \ -2)'$	1/6	5/6

As it is easy to observe, only the basic contrast $\boldsymbol{c}_1'\boldsymbol{\beta}$ can be estimated with full efficiency. This can be done in the intra-block stratum. The information about the other contrast, $\boldsymbol{c}_2'\boldsymbol{\beta}$, splits into both strata.

To illustrate the considerations of the previous sections, the estimates of the basic and elementary contrasts together with their variances were obtained. The results following from the both strata as well as those generated by the proposed direct iteration procedure, utilizing the approach of Nelder [15] and of Houtman and Speed [12] (denoted here as NHS iteration), are presented in the following table:

Contrasts	Inter-block		Intra-block		Simple model		NHS iteration	
$\beta_2 - \beta_1$			3.500	0.250	3.500	1.250	3.500	0.250
$\beta_2 - \beta_3$					−2.000	1.875	−1.333	0.431
$\beta_3 - \beta_1$					5.500	1.875	4.833	0.431
$\beta_1 + \beta_2 - 2\beta_3$	−15.000	$*$	−6.000	1.500	−7.500	6.250	−6.167	1.472

In the inter-block stratum the residual sum of squares is equal to zero. It is so, because in this simple model the vector of transformed observations belongs directly to the expectation subspace. In consequence, the corresponding estimate of variance is denoted by the asterisk. In the intra-block stratum the variance of errors is estimated with only one degree of freedom. The first contrast estimated here is also the BLUE in the overall model. The next set of results represents the first step in the NHS iteration. Actually, the estimates obtained here correspond to the simple model, i.e., a model in which the blocks are ignored. The last set contains the final estimates. They were obtained after fourth step of iteration when the precision up to 10^{-4} was achieved.

In the second example there are also five observations and three treatments. The treatments were allocated into three blocks, two of size two and one with only one treatment. The vector of observations and the matrices describing the model are as follows:

$$\boldsymbol{y} = \begin{bmatrix} 11 \\ 15 \\ 17 \\ 18 \\ 12 \end{bmatrix}, \quad \boldsymbol{X} = \begin{bmatrix} 1\,0\,0 \\ 0\,1\,0 \\ 0\,1\,0 \\ 0\,0\,1 \\ 1\,0\,0 \end{bmatrix}, \quad \boldsymbol{Z} = \begin{bmatrix} 1\,0\,0 \\ 1\,0\,0 \\ 0\,1\,0 \\ 0\,1\,0 \\ 0\,0\,1 \end{bmatrix}, \quad \boldsymbol{D} = \begin{bmatrix} 1\,0\,0 \\ 0\,1\,0 \\ 0\,0\,2 \end{bmatrix}. \tag{37}$$

This design has also the orthogonal block structure, is generally balanced and the information matrices of the intra-block and inter-block stratum have two common basic contrasts. They are presented below with their efficiency factors:

Basic contrasts	Inter-block eff.	Intra-block eff.
$\sqrt{15-5\sqrt{5}}\,\boldsymbol{c}_1 = (\ \sqrt{5}-3,\ \ 2,\ \ 1-\sqrt{5}\ )'$	$(3-\sqrt{5})/8$	$(5+\sqrt{5})/8$
$\sqrt{15+5\sqrt{5}}\,\boldsymbol{c}_2 = (-\sqrt{5}-3,\ \ 2,\ \ 1+\sqrt{5}\ )'$	$(3+\sqrt{5})/8$	$(5-\sqrt{5})/8$

It is easy to notice that both contrasts $\boldsymbol{c}_1'\boldsymbol{\beta}$ and $\boldsymbol{c}_2'\boldsymbol{\beta}$ are far from elementary and the combination of information from both strata is necessary. The results are as follows:

Contrasts	Inter-block		Intra-block		Simple model		NHS iteration	
$\beta_2-\beta_1$					4.500	1.250	4.055	0.109
$\beta_2-\beta_3$					−2.000	1.875	−1.056	0.112
$\beta_3-\beta_1$					6.500	1.875	5.111	0.216
$-0.8\beta_1+2\beta_2-1.2\beta_3$	−7.125	*	1.820	*	0.966	4.775	1.792	0.229
$-5.2\beta_1+2\beta_2+3.2\beta_3$	33.125	*	24.180	*	30.034	32.725	24.650	3.909

In the inter-block stratum as well as in the intra-block stratum there are no enough degrees of freedom for estimating the error variance. In the simple model the results are overestimated. The NHS iteration gives the results after very long process of 39 steps, giving precision up to 10^{-3}. This is due to very unusual form of the basic contrasts which seems to be hardly acceptable by the experimenter. Fortunately, the design used in this model is also far from the standards.

The last example is based on the row-column design mentioned in Bailey [4, p. 176]. This design supplemented by a vector of observations, indispensable for illustrative purposes, leads to the following mixed model

$$\{\boldsymbol{y},\ \boldsymbol{X}\boldsymbol{\beta},\ \sigma_r^2\boldsymbol{R}\boldsymbol{R}'+\sigma_c^2\boldsymbol{C}\boldsymbol{C}'+\sigma_0^2\boldsymbol{I}\}, \tag{38}$$

where

$$\boldsymbol{y} = \begin{bmatrix} 47 \\ 48 \\ 44 \\ 30 \\ 44 \\ 31 \\ 30 \\ 45 \\ 49 \end{bmatrix}, \quad \boldsymbol{X} = \begin{bmatrix} 1\,0\,0 \\ 1\,0\,0 \\ 0\,1\,0 \\ 0\,0\,1 \\ 0\,1\,0 \\ 0\,0\,1 \\ 0\,0\,1 \\ 0\,1\,0 \\ 1\,0\,0 \end{bmatrix}, \quad \boldsymbol{R} = \begin{bmatrix} 1\,0\,0 \\ 1\,0\,0 \\ 1\,0\,0 \\ 0\,1\,0 \\ 0\,1\,0 \\ 0\,1\,0 \\ 0\,0\,1 \\ 0\,0\,1 \\ 0\,0\,1 \end{bmatrix}, \quad \boldsymbol{C} = \begin{bmatrix} 1\,0\,0 \\ 0\,1\,0 \\ 0\,0\,1 \\ 1\,0\,0 \\ 0\,1\,0 \\ 0\,0\,1 \\ 1\,0\,0 \\ 0\,1\,0 \\ 0\,0\,1 \end{bmatrix}. \tag{39}$$

This design relates nine observations of three treatments with three rows and three columns. It has orthogonal block structure but is not generally balanced. The stratum contrasts and their efficiency factors, as established in Bailey [4], are presented in the following table:

Contrasts	Row eff.	Column eff.	Plot eff.
$\beta_1 - \beta_3$	4/9	*	*
$\beta_2 - \beta_3$	*	4/9	*
$\beta_1 - \beta_2$	*	*	7/9
$\beta_1 + \beta_2 - 2\beta_3$	*	*	3/9

It is easy to notice that each elementary contrast is estimated in separate stratum and that the plot stratum provides the information about two contrasts. The detailed results after seventh iteration are as follows:

Contrasts	Rows		Columns		Plots		Simple model		NHS iteration	
$\beta_1 - \beta_3$	17.00	1.33					17.667	0.370	17.566	0.155
$\beta_2 - \beta_3$			15.00	1.33			14.000	0.370	13.494	0.162
$\beta_1 - \beta_2$					4.14	0.11	3.667	0.370	4.072	0.095
$\beta_1 + \beta_2 - 2\beta_3$					31.00	0.76	31.667	1.111	31.061	0.540

Simple comparisons of the estimated variances show that in this generally unbalanced case the smallest variances for all contrasts were obtained from the NHS iteration. It is worth also to notice that the simple least squares approach gives here better results than that following from the rows stratum and the columns stratum treated separately. It is not the case for the comparison $\beta_1 - \beta_2$ in the plots stratum submodel where the efficiency factor is the largest.

6 Concluding Remarks

The considerations conducted in the previous sections supported by the three simple examples lead to some final conclusions. First of all, it should be noted that for applying the direct approach to estimate the variance components it is sufficient that the design has the orthogonal block structure. The property of the general balance is not necessary. However, if the design is generally balanced, the usefulness of each stratum with respect to each basic contrast can be evaluated and the existence of the BLUE for some contrasts may be uncovered. On the other hand, the basic contrasts, as it is well known and also confirmed here in the second example, may not be satisfactory to the experimenter.

The NHS iteration may also be applied when the block designs have unequal block sizes, similarly as in the maximum likelihood method of Patterson and Thompson [16]. But the present approach is distribution free as it uses only geometrical arguments.

The iteration process leading to the final empirical estimates is simple. In each step all stratum variances are directly established, giving the base for the next step with no need of evaluation of any weights as in the original Nelder [15] approach (see also [11] where real experimental data generated from the nested block design were analyzed).

The rate of convergence of the iteration process depends heavily on the property of the design. Only if the design is regular, with equal replications and equal block sizes on various blocking levels, one can expect that the iteration process will terminate rapidly. Otherwise, the iteration can last much longer, as happened in the second example.

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Ingram Olkin (1924–2016): An Appreciation for a People Person

Simo Puntanen and George P. H. Styan

Abstract Ingram Olkin, Professor Emeritus of Statistics and Education at Stanford University, Master of multivariate statistical analysis, linear algebra, inequalities, majorization, and meta-analysis, passed away on 28 April 2016 at home in Palo Alto, California, after complications from colon cancer. In the words of his daughter Julia Olkin [7]

> My father, Ingram Olkin, died peacefully on Thursday evening, April 28, 2016, with his daughter Rhoda and wife Anita by his side. He had absolutely no regrets ... both personally and professionally, and led a full, wonderful life. He valued all his friendships with everyone. Thank you for being a part of his life ...

Richard W. Cottle, Professor Emeritus of Management Science & Engineering and a close friend of Olkin, said [4]:

> He was a man of remarkable intelligence and affability. His nearly boundless energy was generously used for the welfare of others. It is hard to capture in words the goodness that Ingram showed in his everyday life.

In the conversation part of the *Olkin Festschrift* [8], Ingram described himself:

> You also know that I'm generally a people person, which is one of the reasons why I've enjoyed students and collaborators. Over the years, the professional contacts have merged with the personal contacts.

We deeply miss you, a truly outstanding and unforgettable *People Person*, Ingram Olkin.

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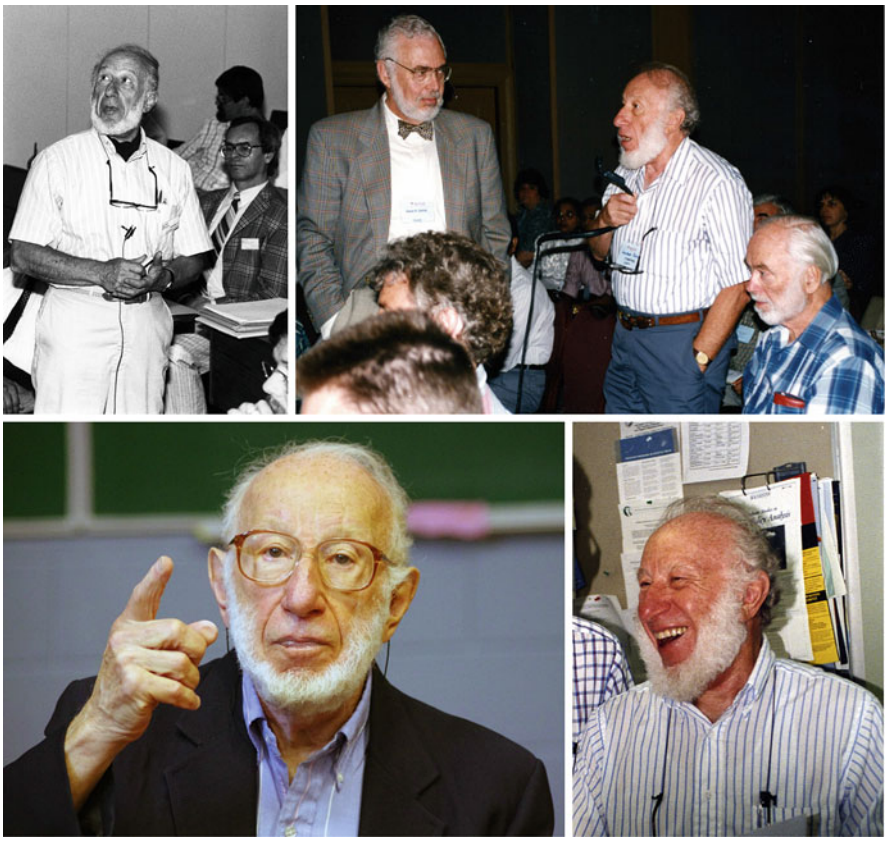

1 IWMS

Now let's go back to some personal memories of Ingram and memorable experiences that we shared with him. One important activity for us was his role in the International Workshop on Matrices and Statistics (IWMS) series [29]. Ingram was a frequent participant at IWMS meetings, and at the IWMS-2004 in Poland we celebrated Ingram's 80th Birthday. On 4 June 2003 his reply to our invitation was this e-mail [Ingram usually used only lowercase letters in his e-mails.]:

> dear all ... wow !!!! how about celebrating my 80th but call it my 60th ... thanks so much to all of you ... would be pleased to attend.

When Ingram learnt that the IWMS-2014 was to be held in Ljubljana, he immediately, on 22 October 2013, sent this e-mail:

> ... in any case next year is my 90th and what better than to visit ljubljana ... so i do hope to attend. as i see my strength at this point i should be in good shape by then. so please include me in the program.

It was always great news for the event organizers to have Ingram around: a guarantee of lively colorful sessions, Ingram sitting in the front row and asking questions after each talk. Ingram's role in meetings is nicely described in the Olkin-biography article [9]:

> At most statistics meetings, you will find Ingram in constant conversation—perhaps promoting a new journal, encouraging progress of a key committee, or giving advice about seeking grants or allocating funds. His public accomplishments are many and impressive, but equally important are his behind-the-scenes contributions.

The first IWMS was held in Tampere, Finland, 6–8 August 1990. Ingram gave an invited talk entitled *Interface between statistics and linear algebra*, which was one of his favorite topics and he practically knew everything about it [22, 24]. For the IWMS-2013 in Toronto he prepared an excellent "linear algebra biography," which was presented there as a poster; see also [25]:

> I gave a brief biography of my introduction to linear algebra and my interaction with some of the linear algebraists at that time.

At the IWMS-1990 in Tampere, Ingram also gave a talk about Gustav Elfving (1908–1984), a famous Finnish statistician, probabilist, and mathematician who was a frequent visitor to Stanford. For more about Elfving, see Nordström [19]. On 19 March 2013 Ingram sent this e-mail to Simo:

> i am cleaning my files and i found folder marked elfving which contains mimeographed notes entitled bayes statistics. it consists of about 40 pages ... so one possibility is that i scan these and send to you ... assuming you want this material ... please advise.

Elja Arjas then found out that these notes were a basis for Elfving's paper [5] published in *Skandinavisk Aktuarietidskrift* in 1968.

As for Elfving, on 20 May 2011 Ingram wrote the following:

> ... my only concern is how to handle the mixture of beer and aquavit. I don't have the right DNA. I once visited gustav elfving and he took me to a meeting of students where they drank beer and aquavit and talked and drank and sang and drank ... i barely made it back to the hotel. So Finland can be a very dangerous country ... but i am willing to take a chance.

Ingram's performances in Tampere in 1990 can be seen in videos online at YouTube [38]. When we asked for Ingram's permission to show these videos, he replied:

> these are wonderful ... an absolutely great addition to the conference archives. however, you ask for me to give permission to make these public. the answer is in the negative unless you can add some hair and make me look more like james bond. of course, if you do that then i would be glad to grant permission !!!!!

Kimmo Vehkalahti had agreed to host Ingram and Michael Greenacre in Helsinki, 1–3 July 2011, directly after the IWMS-2011 in Tartu, Estonia. With the kind courtesy of Kimmo, we copy here part of Ingram's travelling protocol.

> dear kimmo: on the basis of my previous experiences in finland I suggest that we just go to a Sauna, drink some beer and listen to michael [Greenacre] sing some of his compositions.. . .
> meanwhile my very best,
> ingram.
> ps. michael ... why don't you write a song with the first three words: sauna, sauna, sauna.

Before coming to Tartu in June 2011, Ingram first went to Vilnius, Lithuania. Just recently, on 27 June 2016, when Simo was leaving for the 10th Tartu Multivariate Conference, he received the following email from Remigijus Leipus:

> Browsing the Tartu conference program I found out that Ingram Olkin is not with us anymore. This was sad news also for Lithuanian mathematicians. In June 2011 Ingram visited Vilnius University where he presented two talks on June 21 and 22. As you know, Ingram's father came from Vilnius, and his mother from Warsaw (later they met there, in Warsaw).
>
> During his stay in Vilnius, with Ingram we were trying to find out information about his father. We visited a Jewish community center and a Jewish cultural center in Vilnius. It was difficult to find any data in such a short time. ... In any case, the time we spent with Ingram in Vilnius was very interesting, I will never forget his energy, sense of humor, attention. ...

The IWMS-2008 was held in Tomar, Portugal (22–26 July 2008) in celebration of the 90th birthday of T. W. Anderson, mentor of George and grand-mentor of Simo, and a long-time Stanford colleague of Ingram's. We invited Ingram as an after-dinner speaker. On 8 April 2008 he wrote:

> i replied that i didn't want to give an after-dinner talk. i was going over my files and i found the after-dinner talk that i gave in 1998 in florida ... so what would you think if i gave the same talk ... maybe with some modest updates. i also kept the photos on transparencies which are different from what simo has.

Unfortunately Ingram was unable to attend the IWMS-2008 in Tomar. On 7 July 2008 he wrote to the IWMS organizers:

> i think that it may make it easier for everyone if i send you the after-dinner speech that i had in mind. simo is pretty [serious a guy compared with the others][1] so he may be a good choice [to present this after-dinner speech].

Let us borrow a paragraph from Ingram's after-dinner speech:

> I was once interviewed and asked who makes the decisions in our family. I knew the answer in a flash—I make all the big decisions, Anita makes all the small decisions. The only problem is that we haven't had a big decision yet in my 63 years of marriage.

Ingram's title for his (technical) invited talk in Tomar was *Moment Inequalities, Mean Inequalities, Matrix Inequalities, and Probability Inequalities: An Inequality Bouillabaisse*. Ingram, if anybody, was a Michelin-calibre chef able to cook a delicious Inequality Bouillabaisse!

Section 20.5 in our 2011 *Matrix Tricks* book [32] deals with *How Deviant Can You Be?*— the deviation of any particular observation from the mean, building on Ingram's paper [23], Jensen and Styan [14] and Samuelson [34].

In December 2011 we (Simo and George) had an interesting and pleasant task: we were to prepare a supporting letter to nominate Ingram Olkin for the Hans Schneider Prize in Linear Algebra. For additional support, we contacted Grace Wahba, Professor of Statistics at the University of Wisconsin–Madison, and on 31

[1] Wording changed.

December 2011 she wrote us:

> I wholeheartedly support the proposal that Ingram Olkin be considered for the Hans Schneider Prize in Linear Algebra. Absolutely he has to get it!

Though Ingram did not ultimately receive this particular Prize, on 2 August 2012, he kindly sent us a thank-you e-mail:

> simo: thanks for your message and in particular i forgot about the award ... however, i am signing George up to write my obituary (assuming he outlives me !!!!!!!) ... I can always count on him. my best, ingram.

In the IWMS-2013 in Toronto, Ingram was supposed to be the first speaker on Monday, 12 August. However, on Saturday, 10 August, we received the following email from Ingram:

> dear simo and ejaz: it is now 4 p.m. in california and it is evident that i am not in condition to travel. i don't have a life threatening problem, but i do have a problem ... one of which is that they are not sure what is causing the problem.
>
> i apologize for all the trouble this will cause you. if you do decide to have someone read the talk and i can help, please do let me know.
>
> please convey my regrets to all my friends ... i had looked forward to once again seeing everyone.
>
> my best, ingram

George presented Ingram's talk in Toronto.

2 Inequalities: Theory of Majorization

In our supporting letter for the Hans Schneider Prize we pointed out that in our view Ingram's most significant contribution in linear algebra was the book *Inequalities: Theory of Majorization and Its Applications,* with Albert W. Marshall, first published in 1979 [17]. We now have the second edition, with Barry Arnold [18], of the highly praised classic, without which we know that some people never leave home: now these faithful ones must take into account that the second edition has 909 pages (vs. 569) and its shipping weight is 3.2 pounds (vs. 2.2).

At the end of the first edition of *Inequalities: Theory of Majorization and Its Applications* [17] there is a section on "Biographies" with a photograph of Issai Schur (1875–1941) on page 525. This was the first photograph of Schur that we found and George used it, with the permission of the "publisher and the authors" of [17], in his article on "Schur complements and linear statistical models" [36]; see also [27, 28].

Fuzhen Zhang wrote us on 11 May 2016:

> Dating back to 1984, I went to Beijing Normal University as a graduate student. The first math book in English we used as a text was Ingram's (with Marshall), the 1st edition. I learned and benefited so much from the book. The book has become classical, famous and standard as a reference in this area of research. In 2012, I had the privilege of writing a review for the 2nd edition of the book (published in [39]).

In passing we may mention that Simo wrote of brief review [26] of [18].

Ingram had a number of Chinese connections, among them was Kai-Tai Fang. In [16, p. 16], which appears in [13], he tells the following, which is a nice example of Ingram's organizational generosity!

> During my visit to Stanford University (1981–1982), Professor Ingram Olkin organized a small seminar group on 'multivariate multiple comparisons' which met every week. The participants included T. W. Anderson, Mary Ellen Bock, Zhongguo Cheng and me. ... Then in 1985–1986, upon Professor Ingram Olkin's recommendation, I taught two subjects in the Swiss Federal Institute (ETH, Zürich) as a Guest Professor.

As a further interesting link between Ingram Olkin and Kai-Tai Fang we wish to mention Pao-Lu Hsu, a UK-educated Chinese mathematician, who changed the course of probability and statistics in China; see [3]. To go back a little, Hsu was employed at the University of North Carolina at Chapel Hill in 1946–1947, then returned to China. In 1948–1951 Ingram was working for his Ph.D. dissertation [20] at Chapel Hill. His supervisors were S. N. Roy and Harold Hotelling, and as Ingram says in the interview part of [8], "Chapel Hill had a galaxy of stars on the faculty." In [33] and [25] Ingram says:

> I had never taken multivariate. I had no idea why I wanted to take multivariate, but I did. I went to Hotelling and I told him that I wanted to take multivariate, and he said, 'Well, why don't you get P. L. Hsu's notes from last year, and study them on your own'. ... Hsu's proofs were elegant examples of the use of linear algebra in statistics. My thesis in 1951 came out of these lectures.

Interestingly, Pao-Lu Hsu was a supervisor of Kai-Tai Fang in Beijing in the early 1960s. In [16] Kai-Tai Fang tells how Hsu's insistence in fulfilling his teaching obligations, despite his weak physical condition, and his dedication to research exerted a great influence on his own future academic career.

George thinks that he first met Ingram at a colloquium in the Department of Mathematical Statistics at Columbia University in the mid-1960s and at that time may well have served Ingram a cup of tea! Ingram then introduced George to "correlation structure," such as when all the correlation coefficients are equal (intraclass correlation) but the variances are not necessarily all equal. This led to George's Ph.D. thesis [35]. See also Ingram's paper on "correlations revisited" (with discussion) [21].

George spent the summer of 1970 at Stanford and he believes it was probably there that Ingram introduced him to the seminal paper by Fan and Hoffman [6] in which it is proved that for any $n \times n$ matrix $\mathbf{A}$

$$\mathrm{ch}_j(\mathbf{A} + \mathbf{A}^*)/2 \;\le\; \mathrm{ch}_j^{1/2}(\mathbf{A}\mathbf{A}^*), \qquad j = 1, 2, \ldots, n. \tag{1}$$

Here ch_j denotes the jth largest eigenvalue. See also Marshall and Olkin [17, p. 240, eq. 4]. The inequalities (1) were then used by Grossman and Styan in their article on Theil's BLUS residuals [10]. And last, but not least, George is most grateful to Ingram for supporting George's appointment as Editor of *The IMS Bulletin*, 1987–1992 [37].

3 Fire and a Good Story

Here is a descriptive piece of conversation between the interviewer Allan R. Sampson and Ingram Olkin, see [33]:

Sampson: You've been involved with these various forms of applied problems for a long time. But what keeps you still so fired-up?
Olkin: This question about the "fire" is one I have trouble answering.
Sampson: It may precede your beginnings in statistics—perhaps something in your upbringing.
Olkin: I suspect that's true. My mother had fire until she was 98.
Sampson: Amen!
Olkin: The "fire" was mostly addressed to me. And I think there may be some genetics because my daughters have a certain amount of that transmitted.
Sampson: When you were a child, were you as intense and as passionate in whatever you were doing then as you are now?
Olkin: Let me put it this way ...

In the "Biographies" section (pp. 528–529) of *Inequalities: Theory of Majorization and Its Applications* [17] there are three photographs of Godfrey Harold Hardy (1877–1947), who with John Edensor Littlewood (1885–1977) and George Pólya (1887–1985) wrote the seminal book *Inequalities* [11], first published in 1934. G. H. Hardy is featured in *The Man Who Knew Infinity* [2], a recent British biographical drama film based on the book [15] by Robert Kanigel. The film stars Dev Patel as Srinivasa Ramanujan (1887–1920) and Jeremy Irons as G. H. Hardy. George E. Andrews in his review [1] wrote: "I sincerely hope that every mathematician goes to see this movie," while Allan Hunter [12] in his review of the movie wrote

> It tells such a good story that it is hard to resist.

We agree! Would a movie about Ingram, *The Man Who Knew Inequalities: Theory of Majorization,* similarly make a good story, hard to resist?

Acknowledgements Warm thanks go to Elja Arjas, Kai-Tai Fang, Michael Greenacre, Harold V. Henderson, Jeffrey J. Hunter, Remigijus Leipus, Peter Šemrl, Evelyn Matheson Styan, Kimmo Vehkalahti, Grace Wahba, and Fuzhen Zhang for their help.

Photographs: Top left p_{11} at IWMS-1990 Tampere (with Jerzy K. Baksalary and Yadolah Dodge, photograph courtesy University of Tampere); top right p_{12} at IWMS-1995 Montréal (with Gene H. Golub and T. W. Anderson, photograph by Simo Puntanen); bottom left p_{21} at IWMS-2011 Tartu, Estonia (photograph by Jeffrey J. Hunter); bottom right p_{22} at IWMS-1995 Montréal (photograph by Simo Puntanen).

The original, shorter version of this appreciation of Ingram Olkin appeared in [30]. A shortened version also appeared in [31].

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A Notion of Positive Definiteness for Arithmetical Functions

Mika Mattila and Pentti Haukkanen

Abstract In the theory of Fourier transform some functions are said to be positive definite based on the positive definiteness property of a certain class of matrices associated with these functions. In the present article we consider how to define a similar positive definiteness property for arithmetical functions, whose domain is not the set of real numbers but merely the set of positive integers. After finding a suitable definition for this concept we shall use it to construct a partial ordering on the set of arithmetical functions. We shall study some of the basic properties of our newly defined relations and consider a couple of well-known arithmetical functions as examples.

Keywords Arithmetical function · GCD matrix · Positive definite function · Positive semidefinite ordering · Dirichlet convolution · Möbius function

1 Introduction

A complex valued function $f : \mathbb{R} \to \mathbb{C}$ is said to be a *positive definite function* if the matrix $[f(x_i - x_j)]$ is positive semidefinite for all choices of points $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}$ and all $n = 1, 2, \ldots$. A positive definite function is under mild restrictions the Fourier transform of a nonnegative real-valued function $g : \mathbb{R} \to \mathbb{R}_{\geq 0}$; see [3] or [5, Article 192B] for Bochner's theorem (note that the notion of a "positive semidefinite function" is not a term usually employed). By using the definition it is possible to prove several basic properties for a positive definite function f:

- $f(-x) = \overline{f(x)}$ for all $x \in \mathbb{R}$
- $f(0) \in \mathbb{R}$ and $f(0) \geq 0$

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- f is a bounded function, and $|f(x)| \leq f(0) \quad \forall x \in \mathbb{R}$
- If f is continuous at 0, then it is continuous everywhere
- If $f_1, f_2, \ldots, f_n$ are positive definite functions and $a_1, a_2, \ldots, a_n$ are nonnegative real numbers, then the function $a_1 f_1 + a_2 f_2 + \cdots + a_n f_n$ is a positive definite function
- If f is a positive definite function, then so are $\overline{f}$ and $|f|^2$

Functions $\cos x$ (but not $\sin x$), e^{aix} $(a \in \mathbb{R})$, $\dfrac{1}{1-ix}$, $\dfrac{1}{1+x^2}$ and $\dfrac{1}{\cosh x}$ are all examples of positive definite functions (for more information, see [9, pp. 400–401] and [3, Section 3]).

In this article we are interested in *arithmetical functions*, which are real-valued (or sometimes complex-valued) functions on $\mathbb{Z}^+ = \{1, 2, 3, \ldots\}$. There are various operations defined on the set of arithmetical functions, see [2, 12]. For our purposes the most important are:

- The usual sum: $(f + g)(m) = f(m) + g(m) \quad \forall m \in \mathbb{Z}^+$
- The usual product: $(fg)(m) = f(m)g(m) \quad \forall m \in \mathbb{Z}^+$
- The Dirichlet convolution: $(f * g)(m) = \displaystyle\sum_{d \mid m} f(d) g\left(\frac{m}{d}\right) \quad \forall m \in \mathbb{Z}^+$

One of the main goals of this article is to consider how to define positive definiteness property for arithmetical functions. The original definition is a bit problematic since it would require the function to be defined on negative integers as well. There are a couple of ways how one may try to get around this problem, and we shall discuss them in Sect. 2. In Sect. 3 we shall introduce our final definition and in Sect. 4 we investigate some of the basic properties of our newly defined positive definiteness concept. In Sect. 5 we use our positive definiteness relation to define a partial order on the set of arithmetical functions and then study the properties of this relation. We also present several examples concerning some fundamental arithmetical functions. In Sect. 6 we give some concluding remarks.

2 Defining Positive Definiteness of Arithmetical Functions by Using the Original Definition

The most obvious way to define positive definiteness for arithmetical functions would be to expand the domain of arithmetical functions and to define the concept by using the matrix $[f(x_i - x_j)]$. First it should be noted that without loss of generality, we may assume that $x_1 < x_2 < \cdots < x_n$. If $x_i = x_j$ for some indices i and j with $i \neq j$, then the respective rows (and respective columns) are identical and the multiplicity of eigenvalue zero is increased by one. After eliminating identical rows and columns we can permute the rows and respective columns of the matrix $[f(x_i - x_j)]$ so that $x_1 < x_2 < \cdots < x_n$ is satisfied and the eigenvalues are still the

same (if P is any permutation matrix, then $P^{-1} = P^T$ and the matrices $P^T A P$ and A share the same spectrum).

For an arithmetical function f it is customary to assume that $f(x) = 0$ whenever $x \notin \mathbb{Z}^+$. Under this assumption the matrix $[f(x_i - x_j)]$ takes the form

$$\begin{bmatrix} f(x_1-x_1) & f(x_1-x_2) & f(x_1-x_3) & \dots \\ f(x_2-x_1) & f(x_2-x_2) & f(x_2-x_3) & \dots \\ f(x_3-x_1) & f(x_3-x_2) & f(x_3-x_3) & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \dots \\ f(x_2-x_1) & 0 & 0 \dots \\ f(x_3-x_1) & f(x_3-x_2) & 0 \dots \\ \vdots & \vdots & \vdots \ddots \end{bmatrix}.$$

But since the concept of positive definiteness is defined only on Hermitian matrices, the positive definiteness of the above matrix actually implies that all the elements of the matrix are equal to zero. Thus f must be the constant function 0, which is the only positive definite function according to this definition. It appears that for the purposes of arithmetical functions the classical definition of positive definite function is quite useless.

If f is a real-valued arithmetical function, then another rather obvious attempt would be to define $f(-m) = f(m)$ for all $m \in \mathbb{Z}^+$, which makes the matrix $[f(x_i - x_j)]$ symmetric. In this case the matrix $[f(x_i - x_j)]$ takes the form

$$\begin{bmatrix} f(0) & f(x_2-x_1) & f(x_3-x_1) & \dots \\ f(x_2-x_1) & f(0) & f(x_3-x_2) & \dots \\ f(x_3-x_1) & f(x_3-x_2) & f(0) & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}.$$

This is still problematic since $f(0)$ remains undefined. However, the value $f(0)$ is crucial to the positive definiteness of the matrix $[f(x_i - x_j)]$. As was the case with the usual positive definite functions, also this definition implies that $|f(i)| \leq f(0)$ for all $i \in \mathbb{Z}^+$. It becomes quite clear that this approach does not work either, and therefore there seems to be no natural way to define positive definiteness of arithmetical functions by using the matrix $[f(x_i - x_j)]$.

Since the two most natural ways to extend the domain of arithmetical functions do not serve our purposes very well, it seems that we need to use a different class of matrices in order to define positive definiteness for arithmetical functions. It would also make sense to define this concept without extending the domain of arithmetical functions, since many operations such as the Dirichlet convolution are defined intrinsically only on $\mathbb{Z}^+$. These kind of technical difficulties can be avoided if we base our definition on GCD matrices.

3 Defining Positive Definiteness by Using GCD Matrices

Let $\mathscr{A}$ denote the set of arithmetical functions and let $f \in \mathscr{A}$. Let

$$S = \{x_1, x_2, \ldots, x_n\}$$

be a finite subset of $\mathbb{Z}^+$ with $x_1 < x_2 < \cdots < x_n$. The GCD matrix $(S)_f$ of the set S with respect to the function f is the $n \times n$ matrix with $f(\gcd(x_i, x_j))$ as its ij entry. This definition originates from the seminal paper [17] by H. J. S. Smith published in 1876. For more information about GCD and related matrices, see [1, 8, 13, 16].

Definition 1 An arithmetical function $f : \mathbb{Z}^+ \to \mathbb{R}$ is positive definite if the GCD matrix $[f(\gcd(x_i, x_j))]$ is positive semidefinite for all choices of points $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{Z}^+$ and all $n = 1, 2, \ldots$

Remark 1 Arithmetical function f is positive definite if and only if the GCD matrix $(S)_f$ succeeds the corresponding zero matrix with respect to the Löwner order for all finite nonempty sets $S \subset \mathbb{Z}$.

Example 1 Let $\delta \in \mathscr{A}$ with $\delta(1) = 1$ and $\delta(m) = 0$ for all $m > 1$ (the function δ is the identity element with respect to the Dirichlet convolution). Let $S = \{1, 2\}$. Then

$$(S)_\delta = \begin{bmatrix} \delta(\gcd(1,1)) & \delta(\gcd(1,2)) \\ \delta(\gcd(2,1)) & \delta(\gcd(2,2)) \end{bmatrix} = \begin{bmatrix} \delta(1) & \delta(1) \\ \delta(1) & \delta(2) \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}.$$

This matrix is not positive semidefinite, since $\det(S)_\delta = -1$, and thus δ is not a positive definite function.

Example 2 The Möbius function μ is defined as follows:

- $\mu(m) = (-1)^k$ if $p^2 \nmid m$ for any prime number p and k is the number of the prime factors of m,
- $\mu(m) = 0$ if $p^2 \mid m$ for some prime number p.

Take any prime number p and set $S = \{p\}$. We obtain $(S)_\mu = [\mu(p)] = [-1]$. Thus the function μ is not positive definite.

Example 3 Let $\alpha \in \mathbb{R}$. We define $N^\alpha(m) = m^\alpha$ for all $m \in \mathbb{Z}^+$.

(a) Let $\alpha > 0$. It is a well-known fact (see, e.g., [4]) that in this case the matrix $(S)_{N^\alpha} = [\gcd(x_i, x_j)^\alpha]$ is positive definite for all finite nonempty sets $S \subset \mathbb{Z}^+$. Thus N^α is a positive definite function for all $\alpha > 0$.

(b) Let $\alpha < 0$ and $S = \{x_1, x_2\}$ with $x_1 \mid x_2$. In this case

$$(S)_{N^\alpha} = \begin{bmatrix} N^\alpha(x_1) & N^\alpha(x_1) \\ N^\alpha(x_1) & N^\alpha(x_2) \end{bmatrix} = \begin{bmatrix} x_1^\alpha & x_1^\alpha \\ x_1^\alpha & x_2^\alpha \end{bmatrix}.$$

Now $\det(S)_{N^\alpha} = (x_1 x_2)^\alpha - (x_1^2)^\alpha < 0$. Thus N^α is not a positive definite function for any $\alpha < 0$.

(c) For $\alpha = 0$ we denote $N^0 = \zeta$ and have $\zeta(m) = 1$ for all $m \in \mathbb{Z}^+$ (the function ζ is the identity element with respect to the usual product). For any finite nonempty set $S \subset \mathbb{Z}$ the matrix $(S)_\zeta$ is an $n \times n$ matrix with all elements equal to 1. It has two distinct eigenvalues: 0 with multiplicity $n - 1$ and n with multiplicity 1. The matrix $(S)_\zeta$ is positive semidefinite and thus ζ is a positive definite function.

4 Positive Definiteness Properties for Arithmetical Functions

In this section we investigate various basic properties that follow directly from the definition of a positive definite arithmetical function. We continue to assume that S is ordered as in the previous section: $x_1 < x_2 < \cdots < x_n$.

Theorem 1 *Let $f \in \mathscr{A}$ be a positive definite function. Then*

(a) $f(m) \geq 0$ for all $m \in \mathbb{Z}^+$,
(b) $k \mid m \Rightarrow f(k) \leq f(m)$ for all $k, m \in \mathbb{Z}^+$.

Proof Let $m \in \mathbb{Z}^+$. The part (a) follows by setting $S = \{m\}$, which yields the 1×1 GCD matrix $(S)_f = [f(m)]$. This matrix needs to be positive semidefinite, and therefore $f(m) \geq 0$.

Next we prove part (b). Suppose that $k \mid m$. In this case we choose $S = \{k, m\}$ to obtain the GCD matrix

$$(S)_f = \begin{bmatrix} f(k) & f(k) \\ f(k) & f(m) \end{bmatrix}.$$

The determinant of this matrix is equal to $f(k)f(m) - f(k)^2 = f(k)(f(m) - f(k)) \geq 0$. From this we deduce by distinguishing the cases in which $f(k)$ is 0 and $\neq 0$, that $f(m) \geq f(k)$.

Corollary 1 *If $f \in \mathscr{A}$ is a positive definite function, then $f(m) \geq f(1) \geq 0$ for all $m \in \mathbb{Z}^+$.*

Theorem 2 *A function $f \in \mathscr{A}$ is positive definite if and only if the GCD matrix $(S_m)_f$ of the set $S_m = \{1, 2, \ldots, m\}$ is positive semidefinite for all $m = 1, 2, \ldots$.*

Proof The implication $\Rightarrow$ is trivial, and thus it suffices to show the direction $\Leftarrow$. Suppose that the matrix $(S_m)_f$ of the set $S_m = \{1, 2, \ldots, m\}$ is positive semidefinite for all $m = 1, 2, \ldots$. Let $S = \{x_1, x_2, \ldots, x_n\}$ be an arbitrary subset of $\mathbb{Z}^+$. Let m be a positive integer with $x_n \leq m$. Now the GCD matrix $(S)_f$ of the set S is a principal submatrix of the GCD matrix $(S_m)_f$ of the set $\{1, 2, \ldots, m\}$. Since every principal submatrix of a positive semidefinite matrix is positive semidefinite, see [9, Observation 7.1.2], we may deduce that the matrix $(S)_f$ is positive semidefinite.

Theorem 3 *A function $f \in \mathscr{A}$ is positive definite if and only if $(f * \mu)(k) \geq 0$ for all $k \in \mathbb{Z}^+$.*

Proof By Theorem 2, it suffices to show that the GCD matrix $(S_m)_f$ of the set $S_m = \{1, 2, \ldots, m\}$ is positive semidefinite for all $m \in \mathbb{Z}^+$ if and only if $(f * \mu)(k) \geq 0$ for all $k \in \mathbb{Z}^+$. Let $m \in \mathbb{Z}^+$. First we recall the well-known factorization

$$(S_m)_f = EDE^T,$$

where E is the $m \times m$ matrix with

$$e_{ij} = \begin{cases} 1 & \text{if } j \mid i, \\ 0 & \text{otherwise} \end{cases}$$

and $D = \operatorname{diag}((f*\mu)(1), (f*\mu)(2), \ldots, (f*\mu)(m))$. Since E is a triangular matrix with all of its diagonal elements equal to 1, by Sylvester's Law of Inertia (see [9, Theorem 4.5.8]) we may deduce that the matrix $(S_m)_f$ is positive semidefinite if and only if the matrix D is positive semidefinite. The claim follows from this.

Remark 2 Neither the argument used in the proof of Theorem 2 nor the idea of using LDL^T factorization in determining the inertias of GCD type matrices is entirely new—both of them appear in the article [14] from the year 2004 by J. S. Ovall. The LDL^T factorization itself originates from [15] and [4]. The factorization has also other applications, see, e.g., [11].

Theorem 4 *Let $f, g \in \mathscr{A}$ be positive definite functions. Then*

(a) af is a positive definite function for all $a \geq 0$,
(b) $f + g$ is a positive definite function,
(c) fg is a positive definite function,
(d) $f * g$ is a positive definite function.

Proof It is clear that $(S)_{af} = a(S)_f$ and $(S)_{f+g} = (S)_f + (S)_g$. Thus parts (a) and (b) follow from the fact that every nonnegative linear combination of positive semidefinite matrices is positive semidefinite. Since $(S)_{fg} = (S)_f \circ (S)_g$, the part (c) follows from the observation that the Hadamard product of two positive semidefinite matrices is positive semidefinite—see [9, Theorem 7.5.3]. We prove part (d) by showing that $((f * g) * \mu)(k) \geq 0$ for all $k \in \mathbb{Z}^+$. The associativity of the Dirichlet convolution yields

$$((f * g) * \mu)(k) = (f * (g * \mu))(k) = \sum_{d \mid k} \underbrace{f(d)}_{\geq 0} \underbrace{(g * \mu)\left(\frac{k}{d}\right)}_{\geq 0} \geq 0.$$

Remark 3 It is easy to see that in the proof of Theorem 4 (d) it suffices that one of the functions f and g is positive definite and the values of the other are nonnegative.

The following corollary is an immediate consequence of Theorem 4.

Corollary 2 *Suppose that $f \in \mathscr{A}$ is positive definite. Then the functions*

$$f^r = \underbrace{f \cdot f \cdots f}_{r \text{ times}} \qquad \text{and} \qquad f^{*r} = \underbrace{f * f * \cdots * f}_{r \text{ times}}$$

are positive definite for all $r = 1, 2, 3, \ldots$.

It is also interesting to consider how positive definiteness of arithmetical functions behaves with respect to different inverse operations.

Theorem 5 *Let $f \in \mathscr{A}$ be a positive definite function.*

(a) If $-f$ is also a positive definite function, then $f(m) = 0$ for all $m \in \mathbb{Z}^+$.
(b) If $f^{-1} = \frac{1}{f}$ exists and is also a positive definite function, then there exists $a \in \mathbb{R}$ such that $f(m) = a$ for all $m \in \mathbb{Z}^+$.
(c) If $f^{*(-1)}$ (the Dirichlet inverse of f) exists, then it cannot be positive definite.

Proof

(a) The first part follows directly from the simple fact that if both A and $-A$ are positive definite, then A must be equal to the zero matrix. And if the GCD matrix of any finite nonempty set $S \subset \mathbb{Z}^+$ with respect to the function f is the zero matrix, then f must be the constant function zero.

(b) If the function $\frac{1}{f}$ exists and is positive definite, then we must have $f(m) > 0$ for all $m \in \mathbb{Z}^+$. Let m be an arbitrary integer greater than 1 and let $S = \{1, m\}$. Since f and $\frac{1}{f}$ are positive definite, both of the GCD matrices

$$(S)_f = \begin{bmatrix} f(1) & f(1) \\ f(1) & f(m) \end{bmatrix} \quad \text{and} \quad (S)_{\frac{1}{f}} = \begin{bmatrix} \frac{1}{f(1)} & \frac{1}{f(1)} \\ \frac{1}{f(1)} & \frac{1}{f(m)} \end{bmatrix}$$

are positive semidefinite. The determinants of these matrices must be nonnegative, in other words,

$$f(1)(f(m) - f(1)) \geq 0 \quad \text{and} \quad \frac{1}{f(1)}\left(\frac{1}{f(m)} - \frac{1}{f(1)}\right) \geq 0.$$

Since $f(1) > 0$, the first inequality yields $f(m) \geq f(1)$ and the second implies that $f(1) \geq f(m)$. Thus we must have $f(m) = f(1)$ for any positive integer m.

(c) If $f^{*(-1)}$ exists and f is positive definite, then we have $f(1) > 0$ and $f^{*(-1)}(1) = \frac{1}{f(1)} > 0$. If $f(m) = 0$ for all $m > 1$, then there exists a positive real number a such that $f = a\delta$, where δ is the arithmetical function defined in Example 1. Like the function δ, the function f is not positive definite.

Assume next that $f(m) > 0$ for some $m > 1$. Let m_0 be the smallest positive integer such that $m_0 > 1$ and $f(m_0) > 0$. We obtain

$$0 = \delta(m_0) = (f * f^{*(-1)})(m_0) = \sum_{d \mid m_0} f(d) f^{*(-1)}\left(\frac{m_0}{d}\right)$$
$$= \underbrace{f(1)}_{>0} f^{*(-1)}(m_0) + \underbrace{f(m_0)}_{>0} \underbrace{f^{*(-1)}(1)}_{>0}.$$

This means that we must have $f^{*(-1)}(m_0) < 0$, and therefore $f^{*(-1)}$ cannot be positive definite.

5 A Partial Order on the Set of Arithmetical Functions

Notation 1 *Let f and g be arithmetical functions. If the function $g - f$ is positive definite, we shall write $f \preceq g$.*

Theorem 6 *$f \preceq g$ if and only if the matrix $(S)_g - (S)_f$ is positive semidefinite for all finite nonempty sets $S \subset \mathbb{Z}^+$ (in other words, $f \preceq g$ if and only if $(S)_f \leqslant (S)_g$ for all finite nonempty sets $S \subset \mathbb{Z}^+$, where $\leqslant$ is the Löwner order).*

Proof By definition, $g - f$ is positive definite if and only if the matrix $(S)_{g-f} = (S)_g - (S)_f$ is positive semidefinite for all sets $S = \{x_1, x_2, \ldots, x_n\} \subset \mathbb{Z}^+$ and for all $n = 1, 2, \ldots$. Furthermore, this is equivalent to the statement that the matrix $(S)_f$ precedes the matrix $(S)_g$ in the sense of the Löwner order.

Theorem 7 *The relation $\preceq$ is a partial order.*

Proof

- For any $f \in \mathscr{A}$ the matrix $(S)_f - (S)_f = \mathbf{0}$ is positive semidefinite for all finite nonempty sets $S \subset \mathbb{Z}^+$. Thus $\preceq$ is reflexive.
- Suppose that $f \preceq g$ and $g \preceq f$. Thus for any finite nonempty set $S \subset \mathbb{Z}^+$ both of the matrices $(S)_g - (S)_f$ and $(S)_f - (S)_g$ are positive semidefinite, which implies that $(S)_f = (S)_g$. Therefore $f(x_i) = g(x_i)$ for all $x_i \in S$ and we must have $f = g$ (since S is an arbitrary set). Thus $\preceq$ is symmetric.
- Suppose that $f \preceq g$ and $g \preceq h$. Let $S \subset \mathbb{Z}^+$. Now the matrices $(S)_g - (S)_f$ and $(S)_h - (S)_g$ are positive semidefinite and

$$(S)_h - (S)_f = ((S)_h - (S)_g) + ((S)_g - (S)_f).$$

Thus $(S)_h - (S)_f$ is positive semidefinite and we must have $f \preceq h$. Thus $\preceq$ is transitive.

The following results now follow directly from Theorems 1 and 3.

Corollary 3 *Suppose that* $f \preceq g$. *Then*

(a) $f(m) \leq g(m)$ *for all* $m \in \mathbb{Z}^+$,
(b) $k \mid m \Rightarrow g(k) - f(k) \leq g(m) - f(m)$ *for all* $k, m \in \mathbb{Z}^+$.

Corollary 4 *Function* $f \preceq g$ *if and only if*

$$((g - f) * \mu)(k) = (g * \mu)(k) - (f * \mu)(k) \geq 0$$

for all $k \in \mathbb{Z}$.

At this point it is natural to consider how our newly defined relation $\preceq$ relates to different function operations.

Theorem 8 *Suppose that* $0 \preceq f_1 \preceq g_1$ *and* $0 \preceq f_2 \preceq g_2$. *Then*

(a) $0 \preceq f_1 f_2 \preceq g_1 g_2$,
(b) $0 \preceq f_1 * f_2 \preceq g_1 * g_2$.

Proof

(a) We need to show that for any finite nonempty set $S \subset \mathbb{Z}^+$ the matrix

$$(S)_{f_1 f_2} - (S)_{g_1 g_2} = (S)_{f_1} \circ (S)_{f_2} - (S)_{g_1} \circ (S)_{g_2}$$

is positive semidefinite. Since $\mathbf{0} \preceq (S)_{f_1} \preceq (S)_{g_1}$ and $\mathbf{0} \preceq (S)_{f_2} \preceq (S)_{g_2}$, the claim follows from [9, p. 475, Problem 4].

(b) In the second case it is more convenient to use Corollary 4 and show that for all $k \in \mathbb{Z}^+$ we have

$$((f_1 * f_2) * \mu)(k) \leq ((g_1 * g_2) * \mu)(k).$$

Let $k \in \mathbb{Z}^+$. By using the associativity of the Dirichlet convolution and Corollaries 3 and 4 we obtain

$$((f_1 * f_2) * \mu)(k) = (f_1 * (f_2 * \mu))(k) = \sum_{d \mid k} \overbrace{\underbrace{f_1(d)}_{\leq g_1(d)}}^{\geq 0} \overbrace{\underbrace{(f_2 * \mu)\left(\frac{k}{d}\right)}_{\leq (g_2 * \mu)\left(\frac{k}{d}\right)}}^{\geq 0}$$

$$\leq \sum_{d \mid k} g_1(d)(g_2 * \mu)\left(\frac{k}{d}\right) = (g_1 * (g_2 * \mu))(k) = ((g_1 * g_2) * \mu)(k).$$

Thus we have shown that $f_1 * f_2 \preceq g_1 * g_2$. The property $0 \preceq f_1 * f_2$ follows from Theorem 4.

Corollary 5 *Suppose that* $0 \preceq f \preceq g$. *Then for all* $r = 1, 2, \ldots$ *we have*

(a) $0 \preceq f^r \preceq g^r$,
(b) $0 \preceq f^{*r} \preceq g^{*r}$.

Example 4 Recall that $\delta(1) = 1$ and $\delta(m) = 0$ for all $m > 1$ and that $\zeta(m) = 1$ for all $m \in \mathbb{Z}^+$. Since $\zeta(2) = 1 > 0 = \delta(2)$, clearly $\zeta \not\preceq \delta$. Let us show that also $\delta \not\preceq \zeta$. Consider the set $S = \{2, 3, 6\}$. We obtain

$$(S)_{\zeta-\delta} = (S)_\zeta - (S)_\delta = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}.$$

The eigenvalues of this matrix are 1, $1+\sqrt{2}$, and $1-\sqrt{2} < 0$. Therefore the matrix $(S)_{\zeta-\delta}$ is not positive semidefinite and thus we cannot have $\delta \preceq \zeta$. It is also possible to consider the set $S = \{1, 2, 3, 4, 5, 6\}$. In this case

$$(S)_{\zeta-\delta} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 \end{bmatrix}.$$

The smallest eigenvalue of this matrix is approximately -0.4812, and therefore the matrix is not positive semidefinite and we may deduce that $\delta \not\preceq \zeta$.

Definition 2 Arithmetical function f is said to be multiplicative if

$$f(km) = f(k)f(m)$$

for all $k, m \in \mathbb{Z}^+$ with $\gcd(k, m) = 1$.

The values of a multiplicative function are completely determined by the values on prime powers. In fact, if $m = p_1^{a_1} p_2^{a_2} \cdots p_r^{a_r}$, then

$$f(m) = f(p_1^{a_1} p_2^{a_2} \cdots p_r^{a_r}) = f(p_1^{a_1}) f(p_2^{a_2}) \cdots f(p_r^{a_r}).$$

The Möbius function μ is multiplicative, and the Dirichlet convolution of multiplicative functions is also multiplicative, see, e.g., [2, Section 2.10] and [12, Chapter 1]. Thus if $f \in \mathscr{A}$ is multiplicative and we wish to show that f is positive definite, i.e. that $(f * \mu)(k) \geq 0$ for all $k \in \mathbb{Z}^+$, then it suffices to show that $(f * \mu)(p^a) \geq 0$ for any prime number p and for all $a \in \mathbb{Z}^+$.

Example 5 The Jordan totient function J_α is defined as

$$J_\alpha(m) = m^\alpha \prod_{p \mid m} \left(1 - \frac{1}{p^\alpha}\right),$$

where $m = p_1^{a_1} p_2^{a_2} \cdots p_r^{a_r}$. If $\alpha \geq 1$, then for any $a \geq 2$ we have

$$\begin{aligned}(J_\alpha * \mu)(p^a) &= \sum_{d \mid p^a} J_\alpha(d)\mu\left(\frac{p^a}{d}\right) = J_\alpha(p^a) - J_\alpha(p^{a-1}) \\ &= p^{\alpha a} - p^{\alpha(a-1)} - p^{\alpha(a-1)} + p^{\alpha(a-2)} = p^{\alpha(a-2)}(p^{2\alpha} - 2p^\alpha + 1) \\ &= p^{\alpha(a-2)}(p^\alpha - 1)^2 \geq 0\end{aligned}$$

and for $a = 1$ we obtain

$$(J_\alpha * \mu)(p) = J_\alpha(p) - 1 = p^\alpha - 1 - 1 = p^\alpha - 2 \geq 0.$$

By multiplicativity this shows that J_α is positive definite for $\alpha \geq 1$. In particular, the Euler totient function $\phi = J_1$ is positive definite. Since $(J_\alpha * \mu)(2) = 2^\alpha - 2 < 0$ for $\alpha < 1$, we see that J_α is not positive definite for $\alpha < 1$.

By utilizing multiplicativity in a similar manner it is possible to show that for $\alpha, \beta \geq 0$,

$$J_\alpha \preceq J_\beta \Leftrightarrow (J_\alpha * \mu)(k) \leq (J_\beta * \mu)(k)\ \forall k \in \mathbb{Z}^+ \Leftrightarrow \alpha \leq \beta.$$

Example 6 In Example 3 it was shown that the power function N^α is positive definite for all $\alpha \geq 0$. With the aid of multiplicativity (as in Example 5) it is possible to show that for $\alpha, \beta \geq 0$,

$$N^\alpha \preceq N^\beta \Leftrightarrow \alpha \leq \beta.$$

Example 7 The divisor function σ_α is defined as $\sigma_\alpha(m) := \sum_{d \mid m} d^\alpha$, or alternatively $\sigma_\alpha = N^\alpha * \zeta$. The function σ_α is positive definite for all $\alpha \in \mathbb{R}$, and for any $\alpha, \beta \in \mathbb{R}$ we have

$$\sigma_\alpha \preceq \sigma_\beta \Leftrightarrow \alpha \leq \beta.$$

The positive definiteness of the function σ_α can easily be shown by using Theorem 3, since

$$\sigma_\alpha * \mu = (N^\alpha * \zeta) * \mu = N^\alpha * (\zeta * \mu) = N^\alpha$$

and $N^{\alpha}(k) \geq 0$ for all $\alpha \in \mathbb{R}$ and $k \in \mathbb{Z}^{+}$. The other claim follows similarly, since

$$(\sigma_{\beta} - \sigma_{\alpha}) * \mu = (\sigma_{\beta} * \mu) - (\sigma_{\alpha} * \mu) = N^{\beta} - N^{\alpha}$$

and the values of this function are nonnegative if and only if $\alpha \leq \beta$.

Example 8 Let $\Omega(m)$ denote the total number of prime divisors of m each counted according to its multiplicity (note that $\Omega(1) = 0$). We prove the positive definiteness of the function Ω by showing that $(\Omega * \mu)(k) \geq 0$ for all $k \in \mathbb{Z}^{+}$.

If $k = 1$, then $(\Omega * \mu)(k) = 0$. Let $k = p_1^{a_1} p_2^{a_2} \cdots p_r^{a_r} \neq 1$ $(r \geq 1)$ be the canonical factorization of k. Then

$$\begin{aligned}(\Omega * \mu)(k) = (\mu * \Omega)(k) &= \sum_{d \mid k} \mu(d) \Omega\left(\frac{k}{d}\right) \\ &= (a_1 + a_2 + \cdots + a_r) \\ &\quad - ((a_1 - 1) + a_2 + \cdots + a_r) - (a_1 + (a_2 - 1) + \cdots + a_r) - \cdots \\ &\qquad - (a_1 + a_2 + \cdots + (a_r - 1)) \\ &\quad + ((a_1 - 1) + (a_2 - 1) + a_3 + \cdots + a_r) + \cdots \\ &\qquad + (a_1 + \cdots + a_{r-2} + (a_{r-1} - 1) + (a_r - 1)) \\ &\quad - \cdots\end{aligned}$$

Denote $s = a_1 + a_2 + \cdots + a_r$. Then

$$\begin{aligned}(\Omega * \mu)(k) &= s - \binom{r}{1}(s-1) + \binom{r}{2}(s-2) + \cdots + (-1)^r \binom{r}{r}(s-r) \\ &= \sum_{i=0}^{r} (-1)^i \binom{r}{i}(s-i) = s \sum_{i=0}^{r} (-1)^i \binom{r}{i} - \sum_{i=0}^{r} (-1)^i \binom{r}{i} i.\end{aligned}$$

By the binomial theorem, $\sum_{i=0}^{r} (-1)^i \binom{r}{i} = 0$ $(r \geq 1)$ and by formula (1.69) of [7],

$$\sum_{i=0}^{r} (-1)^i \binom{r}{i} i = \begin{cases} -1 & \text{if } r = 1, \\ 0 & \text{if } r \geq 2 \end{cases}$$

(this can also be shown by utilizing formula (5.6) of [6]). Thus $(\Omega * \mu)(k) = 1$ if $r = 1$ (i.e., k is a prime power $(\neq 1)$), and $(\Omega * \mu)(k) = 0$ otherwise.

Example 9 Also for the generalized Liouville function $\lambda_{\alpha}(m) = \alpha^{\Omega(m)}$ it is possible to show that λ_{α} is positive definite if and only if $\alpha \geq 1$ and that for $\alpha, \beta \geq 1$,

$$\alpha \leq \beta \Leftrightarrow \lambda_{\alpha} \preceq \lambda_{\beta}.$$

In particular, the usual Liouville function $\lambda = \lambda_{-1}$ is not positive definite. These results can be proved by utilizing multiplicativity. Since the function Ω is positive definite by the previous example, the positive definiteness of λ_α for $\alpha \geq 1$ can also be deduced from the results of [10, Section 6.3]. The Liouville function λ gives the parity of the number of prime factors and is related, e.g., to the Riemann hypothesis.

Example 10 For the generalized Dedekind function $\Psi_\alpha = N^\alpha * \mu^2$, where $\mu^2 = \mu \cdot \mu = |\mu|$, it can be shown that Ψ_α is positive definite if and only if $\alpha \geq 0$ and that for $\alpha, \beta \geq 0$,

$$\alpha \leq \beta \Leftrightarrow \Psi_\alpha \preceq \Psi_\beta.$$

In particular, the usual Dedekind function $\Psi = \Psi_1$ is positive definite. Also these results can be shown by using multiplicativity. The function Ψ was introduced by Richard Dedekind in connection with modular functions. It has also connections to the Riemann hypothesis.

Example 11 For $\alpha \geq 0$, we have

$$J_\alpha \preceq N^\alpha \preceq \Psi_\alpha \preceq \sigma_\alpha.$$

For $\alpha \geq 1$, we obtain

$$\lambda_\alpha \preceq J_\alpha \preceq N^\alpha \preceq \Psi_\alpha \preceq \sigma_\alpha.$$

These can be verified by applying the multiplicativity of the functions $\lambda_\alpha * \mu$, $J_\alpha * \mu$, $N^\alpha * \mu = J_\alpha$, $\Psi_\alpha * \mu$ and $\sigma_\alpha * \mu$. In particular (for $\alpha = 1$),

$$\phi(= J_1) \preceq N(= N^1) \preceq \Psi(= \Psi_1) \preceq \sigma(= \sigma_1).$$

6 Conclusions

As we saw in Sect. 2, defining positive definiteness of arithmetical functions by using GCD matrices appears to be the best way to proceed. Positive definite arithmetical functions seem to possess several properties that one could expect them to have. For example, addition, usual multiplication, and Dirichlet convolution all preserve positive definiteness. On the other hand, in some cases positive definiteness of arithmetical functions behaves quite unexpectedly (for example, the function δ is not positive definite, although it is the identity element with respect to the Dirichlet convolution). Positive definiteness also makes it possible to define a partial order on the set of arithmetical functions, and by making use of multiplicativity we are able to compare various fundamental arithmetical functions with each other.

The study of positive definiteness of arithmetical functions offers many possibilities for further research. One could analyze thoroughly the properties of positive definite arithmetical functions, and there might still be a possibility to utilize some other matrix class and find an alternative definition for positive definite arithmetical functions. Yet another possibility would be to generalize the concept of positive definiteness on real-valued functions defined on any meet semilattice P. In this case one only needs to consider the so-called meet matrix of the set S with respect to the function f (instead of GCD matrix).

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Some Issues in Generalized Linear Modeling

Alan Agresti

Abstract This chapter discusses cautions, questions, challenges, and proposals regarding five issues that arise in generalized linear modeling. With primary emphasis on categorical data, we summarize (1) bias that can occur in using ordinary linear models with ordinal response variables, (2) a new proposal about simple ways to interpret effects in generalized linear models that use nonlinear link functions, (3) problems with using Wald significance tests and confidence intervals, (4) a question about the behavior of residuals for generalized linear models, and (5) a new approach in using generalized estimating equations (GEE) methods for marginal multinomial models.

Keywords GEE methods · Multinomial models · Ordinal models · Residuals · Wald inference

1 Introduction

This chapter discusses several issues about generalized linear models that I believe deserve more attention, either in terms of additional research or greater awareness of already existing literature. I discuss these issues, with primary emphasis on categorical data, in the style of cautions, questions, challenges, and proposals. I became aware of these issues in recent years while writing a book on linear and generalized linear models [4] and while revising two books on categorical data analysis [1, 3].

Section 2 explains the floor and ceiling bias that can occur with modeling ordinal response variables by assigning scores to the outcome categories and using ordinary linear models. Section 3 proposes a simple way to interpret effects in generalized linear models that use nonlinear link functions, by comparing groups

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using a probability summary about the higher response. Section 4 summarizes problems with using Wald significance tests and confidence intervals in modeling binary response variables and suggests related research for other types of response variables. Section 5 raises questions about the behavior of ordinary residuals for generalized linear models, and argues that a standardized residual is more relevant than the popular Pearson residual. Section 6 summarizes some awkward aspects of standard generalized estimating equations (GEE) methods for marginal multinomial models and presents a recently proposed approach that is now available with R software.

Most of this chapter has the style of a tutorial or survey paper. But it is hoped that the material is relevant for a conference that has general consideration of topics related to linearity and modeling.

2 Bias in Ordinary Linear Modeling of Ordinal Responses

Ordinal categorical response variables are common in many disciplines, especially the social sciences with sample survey data. An example is one's report of political ideology, selected from the categories (very liberal, slightly liberal, moderate, slightly conservative, very conservative). Many ordinal variables have a rather subjective outcome choice, such as in medical assessments of patient quality of life (excellent, good, fair, poor) or amount of pain (none, little, considerable, severe).

With ordinal response variables, many methodologists assign monotone scores to the ordered outcome categories and then apply ordinary regression methods. That is, they use least squares to estimate parameters in a linear model for the mean response for the chosen scores. This is sometimes problematic because of requiring the choice of scores, which can be quite unclear when the categories are highly subjective. Are categories such as (excellent, good, fair, poor) equally distant, and if not, how does one decide on relative distances? But here we discuss a less known but perhaps more worrisome problem, that *floor effects* or *ceiling effects* due to the boundedness of the discrete ordinal scale can result in seriously biased estimates of effect magnitudes.

We illustrate this potential problem using an example with an assumed connection between an observed ordinal variable and an underlying continuous latent variable. For an ordinal response variable y, it is often realistic to assume the existence of an underlying continuous latent variable y^* that we would ideally observe if we could measure the response in a more refined manner. For instance, for variables such as political ideology or quality of life, there is nothing sacred about a particular choice of categories, and it's easy to imagine increasing the number of categories until the variable becomes essentially continuous. Our example uses the simple normal linear latent variable model for observation i,

$$y_i^* = 20.0 + 0.6x_i - 40z_i + \epsilon_i$$

in which we take $x_i \sim$ uniform(0, 100), $P(z_i = 0) = P(z_i = 1) = 0.50$ independent of x_i, and $\epsilon_i \sim N(0, 10^2)$. We randomly generate $n = 100$ observations from this model and focus on the issue of comparing the two groups represented by the values of z in terms of the effect of the covariate x.

Now, suppose that the variable we actually observe for subject i is directly related to this latent variable by

$$y_i = 1 \text{ if } y_i^* \leq 20, \quad y_i = 2 \text{ if } 20 < y_i^* \leq 40, \quad y_i = 3 \text{ if } 40 < y_i^* \leq 60,$$

$$y_i = 4 \text{ if } 60 < y_i^* \leq 80, \quad y_i = 5 \text{ if } y_i^* > 80.$$

That is, cutpoints chop up the continuous scale for $y*$, yielding five ordered categories with corresponding values for the observed y. Figure 1 shows the connection between the observed variable y and the latent variable y^*. The first scatterplot in the figure shows the 100 observations on y^* and x, each data point labelled by the category for z. The plot also shows the regression lines that generated the data.

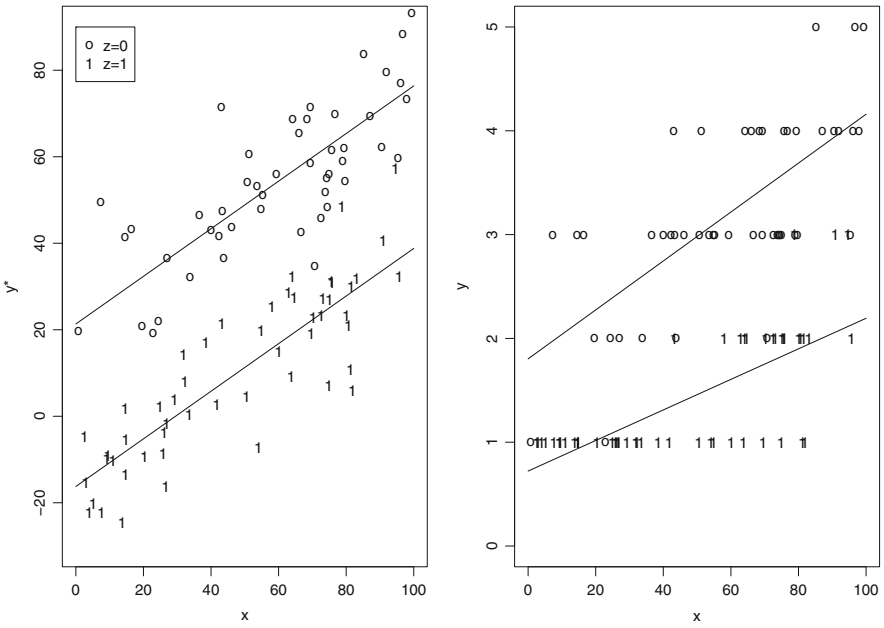

Fig. 1 Ordered categorical data (in second panel) for which ordinary regression suggests interaction, because of a floor effect, but ordinal modeling does not. The data were generated (in first panel) from a normal main-effects regression model with continuous (x) and binary (z) explanatory variables. When the continuous response y^* is categorized and y is measured as (1, 2, 3, 4, 5), the observations labelled '1' for the category of z have a linear x effect with only half the slope of the observations labelled '0' for the category of z

Now, for the observed data, suppose we fit the linear model

$$y_i = \alpha + \beta_1 x_i + \beta_2 z_i + \beta_3 (x_i \cdot z_i) + \epsilon_i$$

using the scores $(1, 2, 3, 4, 5)$, to study the effect of x for the two groups and to analyze whether interaction occurs between x and z in their effects on y. The right panel of the figure shows the result, plotting the least squares fit. For the observed response, the slope of the line is about twice as high when $z = 0$ as when $z = 1$. Why? When $x_i < 50$ with $z_i = 1$, $P(y_i^* \leq 20) = P(y_i = 1)$ is relatively high. As x gets lower, the underlying value y^* can continue to tend to get lower, but the observed ordinal response cannot fall below 1, resulting in a floor effect. This interaction effect is caused by the observations when $z = 1$ tending to fall in category $y = 1$ whenever x takes a relatively low value.

For the observed data, the interaction is statistically and practically significant. Analyzing the data with an ordinary linear model, we would conclude that an effect exists that actually does not. Such spurious effects would not occur if we instead fitted a proper ordinal model, such as the *cumulative logit model*

$$\text{logit}[P(y_i \leq j)] = \alpha_j + \beta_1 x_i + \beta_2 z_i$$

or the *cumulative probit model*

$$\Phi^{-1}[P(y_i \leq j)] = \alpha_j + \beta_1 x_i + \beta_2 z_i$$

with Φ being the standard normal cdf, with $j = 1, 2, 3, 4$ for the four cumulative probabilities. In fact, we'll note in the next section that such models are implied for this latent variable model. The models account for the ordinality by using cumulative probabilities for y without needing to assign scores and assume linearity on that scale.

We are not suggesting that it is always inappropriate to use ordinary linear models with ordinal response variables. With several outcome categories and observations spread among them without high concentrations in boundary categories, such a model can be adequate. Using such a model can be helpful for relatively unsophisticated methodologists who may be comfortable with linear modeling but not with models that imply more complex effect summaries, such as odds ratios. However, in using this strategy, one should be aware of the potential bias that can result.

3 Interpreting Effects in GLMs with Nonlinear Link Function

For an $n \times 1$ vector $\boldsymbol{y}$ of response observations with $\boldsymbol{\mu} = E(\boldsymbol{y})$, consider a generalized linear model

$$g(\boldsymbol{\mu}) = \boldsymbol{X}\boldsymbol{\beta}$$

for link function g and model matrix $\boldsymbol{X}$ with a set of explanatory variables. For many standard link functions, the interpretation of $\boldsymbol{\beta}$ is difficult for non-statisticians and for methodologists who are mainly familiar with ordinary linear models.

For instance, suppose y is ordinal as we considered in the previous section. Let c denote the number of outcome categories for y. For observation i, let x_{ik} denote the value of explanatory variable k. Consider the *cumulative link model*

$$\text{link}[P(y_i \leq j)] = \alpha_j + \sum_k \beta_k x_{ik}, \quad j = 1, \ldots, c-1,$$

for links such as the logit, probit, or complementary log-log. For the probit link (i.e., the inverse of the standard normal cdf), β_k represents the change in $\Phi^{-1}[P(y_i \leq j)]$ for a 1-unit increase in x_k, adjusting for the other explanatory variables. This is a rather obscure interpretation, as very few people can make sense of effects on the scale of an inverse of a cdf.

One way used to interpret such effects relies more on using means for underlying latent variable models. For the observed ordinal response y and for an underlying continuous response y^*, suppose we assume that $y_i^* = \boldsymbol{\beta}^T \boldsymbol{x}_i + \epsilon_i$, where ϵ_i has some parametric cdf G with mean 0. Suppose that there are thresholds (cutpoints) $-\infty = \alpha_0 < \alpha_1 < \ldots < \alpha_c = \infty$ such that

$$y_i = j \text{ if } \alpha_{j-1} < y_i^* \leq \alpha_j.$$

Then, at a fixed value $\boldsymbol{x}$,

$$P(y_i \leq j) = P(y_i^* \leq \alpha_j) = P(y_i^* - \boldsymbol{\beta}^T \boldsymbol{x}_i \leq \alpha_j - \boldsymbol{\beta}^T \boldsymbol{x}_i)$$

$$= P(\epsilon_i \leq \alpha_j - \boldsymbol{\beta}^T \boldsymbol{x}_i) = G(\alpha_j - \boldsymbol{\beta}^T \boldsymbol{x}_i).$$

This implies the model

$$G^{-1}[P(y_i \leq j \mid \boldsymbol{x}_i)] = \alpha_j - \boldsymbol{\beta}^T \boldsymbol{x}_i$$

with G^{-1} as the link function. In particular, one obtains the cumulative probit model when G is the standard normal cdf Φ; then Φ^{-1} is the probit link. (In practice, whether we use $+$ or $-$ for the coefficient of the linear predictor $\boldsymbol{\beta}^T \boldsymbol{x}_i$ merely

affects the sign of the estimates, and varies among the common software packages.) Thus, the cumulative probit model fits well when an ordinary normal linear model holds for an underlying continuous response variable. For this model, β_k has the interpretation that a 1-unit increase in x_k corresponds to a change in $E(y^*)$ of β_k standard deviations, adjusting for the other explanatory variables [9, 20]. But this interpretation can still be rather obscure for non-methodologists who do not think of effects in terms of multiples of standard deviations. Moreover, the latent variable model may not be appropriate in some applications.

We suggest next a simpler interpretation, proposed by Agresti and Kateri [6]. We formulate it in terms of a summary for comparing two groups, adjusting for the other explanatory variables. Let z be an indicator variable for the two groups. At any potential setting $(x_1, \ldots, x_p)$ of p explanatory variables, let y_1^* and y_2^* denote independent latent variables when $z = 1$ and when $z = 0$, respectively. For the latent variable model that generates the cumulative probit model

$$\Phi^{-1}[P(y \le j)] = \alpha_j - \beta z - \beta_1 x_1 - \cdots - \beta_p x_p,$$

the difference between the conditional means of y_1^* and y_2^* is β, and

$$P(y_1^* > y_2^*) = P[(y_1^* - y_2^*) > 0]$$

$$= P\left[\frac{(y_1^* - y_2^*) - \beta}{\sqrt{2}} > \frac{-\beta}{\sqrt{2}}\right] = 1 - \Phi(-\beta/\sqrt{2}) = \Phi(\beta/\sqrt{2}).$$

That is, $P(y_1^* > y_2^*) = \Phi(\beta/\sqrt{2})$ at any setting of the p explanatory variables. Differences between the normal conditional means for the two groups of $\beta = (0, 0.5, 1, 2, 3)$ standard deviations correspond to $P(y_1^* > y_2^*)$ values of (0.50, 0.64, 0.76, 0.92, 0.98).

In practice, the probit link is used much less than the logit link, especially in biostatistics. The cumulative logit model

$$\text{logit}[P(y \le j)] = \alpha_j - \beta z - \beta_1 x_1 - \cdots - \beta_p x_p$$

is implied when an underlying latent variable has a logistic distribution. The derivation just shown for a normal latent variable does not have an exact analog for a logistic latent variable, as the difference between two independent standard logistic random variables does not have a logistic distribution. However, the distribution can be very closely approximated by the logistic with mean 0 and double the variance. This generates the approximation

$$P(y_1^* > y_2^*) \approx \frac{\exp(\beta/\sqrt{2})}{[1 + \exp(\beta/\sqrt{2})]}$$

in terms of the β parameter from the cumulative logit model. This approximation is adequate for practical application. Because of the very close similarity of logit and probit models, another good approximation is to fit also the cumulative probit model and use the exact expression $P(y_1^* > y_2^*) = \Phi(\beta/\sqrt{2})$ for the β parameter from that model.

In practice, it is often sensible to assume a latent variable distribution that, unlike the normal and the logistic, is skewed and has a long tail. For the ordinal model with log-log link, the underlying latent variable has the extreme-value (Gumbel) distribution. The difference between two independent random variables of this type has the standard logistic distribution. So, in this case,

$$P(y_1^* > y_2^*) = \frac{\exp(\beta)}{[1 + \exp(\beta)]}$$

in terms of the β parameter for the cumulative link model with log-log link.

For any of these cumulative link models, ordinary confidence intervals for the β coefficient of the indicator variable induce confidence intervals for $P(y_1^* > y_2^*)$. The measures and the related inferences are presented by Agresti and Kateri [6]. They also proposed analogous measures for the observed ordinal scale that do not require a latent variable connection, and they have available R functions for confidence intervals for the measures.

Such probability-based measures may be especially helpful for practitioners who cannot easily interpret odds ratios and other measures that result from nonlinear link functions. For instance, for a medical researcher, reading that at fixed values for the explanatory variables, the estimated probability the response to drug ($z = 1$) is better than response to placebo ($z = 0$) is 0.72 probably has greater meaning than reading that (1) the estimated cumulative odds for drug is $\exp(\hat{\beta}) = 2.7$ times the estimated cumulative odds for placebo (i.e., the interpretation for the cumulative logit model), or (2) that the estimated cumulative probits differ by $\hat{\beta} = 0.8$ or an underlying mean for drug is $\hat{\beta} = 0.8$ standard deviations better than for placebo (i.e., the interpretation for the cumulative probit model), or (3) that the estimated probability that the response for drug is worse than a particular outcome category is the power $\exp(\hat{\beta}) = 1.7$ of the estimated probability that response for placebo is worse than that category (i.e., interpretation of cumulative link model with complementary log-log link).

This type of probability measure for comparing groups is also relevant for ordinary normal linear models. With constant error variance σ^2 and potential response outcomes (y_1, y_2) for two groups at some setting of explanatory variables, the corresponding measure is

$$P(y_1 > y_2) = \Phi\left(\frac{\beta}{\sqrt{2}\sigma}\right),$$

for coefficient β of the indicator variable for the two groups. This would seem to be a useful summary in many applications. For two groups with no explanatory

variables, a related popular effect size measure is $\beta/\sigma = (\mu_1 - \mu_2)/\sigma$ [13]. One can derive a confidence interval for β/σ in linear models with explanatory variables using the noncentral t distribution, and such an interval induces one for $P(y_1 > y_2)$. For details and an example using R, see Agresti and Kateri [6].

4 Wald Inference When Effects for Binary Data Are Large

To introduce this topic, we start with a toy example that illustrates an awkward aspect that often occurs in using logistic regression, namely that at least one of the maximum likelihood (ML) estimates of model parameters is infinite. This happens when *complete separation* or *quasi-complete separation* occurs in the space of the explanatory variables [7].

For six observations, suppose that $y = 1$ at $x = 1, 2, 3$, and $y = 0$ at $x = 4, 5, 6$, a simple example of complete separation. When we use R to fit the ordinary logistic regression model, $\text{logit}[P(y = 1)] = \alpha + \beta x$, we obtain:

```
------------------------------------------------------------
> x <- c(1,2,3,4,5,6);  y <- c(1,1,1,0,0,0)
> fit <- glm(y ~ x, family = binomial(link = logit))

> summary(fit)
Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept)    165.3   407521.4       0        1
x              -47.2   115264.4       0        1

Number of Fisher Scoring iterations: 25
------------------------------------------------------------
```

After 25 iterations, Fisher scoring converges, as the log-likelihood function is essentially flat at that stage. The fit looks nearly identical to a step function that takes value 1 below $x = 3.5$ and takes value 0 above $x = 3.5$. The maximized log-likelihood value is essentially 0, reflecting the basically perfect fit. Although in fact $\hat{\beta} = -\infty$, R reports $\hat{\beta} = -47.2$. R also reports a huge standard error, reflecting that the unrestricted ML estimate of the standard error (SE) is based on the Fisher information, which summarizes the curvature of the log-likelihood function at $\hat{\beta}$. A perhaps surprising consequence is that $z = \hat{\beta}/SE = 0$, yielding a P-value of 1.0 when we use this ratio as a test statistic for testing H_0: $\beta = 0$. By contrast, the model fit gives evidence of a potentially very strong effect. The likelihood-ratio test statistic equals 8.32 with $df = 1$ and yields P-value = 0.004.

The statistic $z = \hat{\beta}/(SE)$ is an example of a *Wald test*. This approach uses the fact that an ML estimator has an asymptotic normal distribution by testing H_0: $\beta = 0$ with $z = \hat{\beta}/(SE)$, or else treating z^2 as an approximate chi-squared random variable with, $df = 1$. The corresponding confidence interval has the form $\hat{\beta} \pm z(SE)$ for the appropriate standard normal percentile z, for instance with $z = 1.96$ for 95% confidence. A classic result shown by Hauck and Donner [14] is that as $|\beta|$ in a

logistic regression model increases (for fixed n), the Fisher information decreases so quickly that SE grows faster than β. The result is poor performance of Wald methods when effects are large.

The poor performance of Wald methods shows up even in very simple contexts, such as a single binomial response variable without any explanatory variables. For a binomial random variable y based on n independent trials with parameter π, in the context of logistic regression the model is $\text{logit}(\pi) = \beta$. To test H_0: $\beta = 0$ (i.e., $\pi = 0.50$), $\hat{\beta} = \text{logit}(\hat{\pi})$ with $\hat{\pi} = y/n$ has asymptotic variance $[n\pi(1-\pi)]^{-1}$. The Wald chi-squared statistic is

$$(\hat{\beta}/SE)^2 = [\text{logit}(\hat{\pi})]^2[n\hat{\pi}(1-\hat{\pi})].$$

Now, suppose $n = 25$. For testing H_0: $\pi = 0.50$, $\hat{\pi} = \frac{24}{25}$ is stronger evidence against H_0 than $\hat{\pi} = \frac{23}{25}$. Yet the Wald statistic equals 9.7 when $\hat{\pi} = 24/25$ and equals 11.0 when $\hat{\pi} = 23/25$. By comparison, the likelihood-ratio statistic takes values 26.3 and 20.7.

With large or infinite effects, likelihood-ratio (LR) tests and test-based confidence intervals remain valid and behave well because of the concavity of the log-likelihood function. For example, when $\hat{\beta} = -\infty$, a confidence interval consists of a range of plausible values from $-\infty$ to some finite upper bound. With infinite ML estimates, one can alternatively smooth the data and produce finite estimates and finite endpoints of intervals using a Bayesian approach. Or, one can use a penalized likelihood approach with the aim of reducing bias [11], which corresponds to using a Bayesian posterior mode with Jeffreys prior to generate a point estimate.

The poor performance of the Wald test implies poor performance also of corresponding confidence intervals. This has been shown for a variety of measures for categorical data, such as proportions, differences of proportions, odds ratio, and relative risk, particularly when probabilities are near 0 or 1. For a summary of these and various other cases involving categorical data, see Agresti [2]. For example, again for a single binomial parameter π, the 95% Wald confidence interval for π is

$$\hat{\pi} \pm 1.96\sqrt{\hat{\pi}(1-\hat{\pi})/n}.$$

In terms of achieving close to the nominal coverage probability, this interval performs much worse than the interval based on inverting a likelihood-ratio test or inverting the score test of H_0: $\pi = \pi_0$, which has test statistic

$$z = \frac{\hat{\pi} - \pi_0}{\sqrt{\pi_0(1-\pi_0)/n}}.$$

It also behaves much more poorly than a simple approximation to the score confidence interval that (in the 95% case) adds 2 "successes" and 2 "failures" before forming the Wald confidence interval [5].

An important question that could be addressed in future research is whether the poor Wald performance for binary data holds also for various other generalized linear models for other types of data, with nonlinear link functions. For some theoretical work in this direction, see Brown et al. [10].

5 Behavior of Residuals for GLM Fits

For an $n \times 1$ vector $\boldsymbol{y}$ of response observations with $\boldsymbol{\mu} = E(\boldsymbol{y})$, $\boldsymbol{V} = \text{var}(\boldsymbol{y})$, consider an arbitrary generalized linear model

$$\boldsymbol{\eta} = g(\boldsymbol{\mu}) = \boldsymbol{X}\boldsymbol{\beta}$$

with link function g and model matrix $\boldsymbol{X}$. Denote the maximum likelihood fitted values by $\hat{\boldsymbol{\mu}}$.

The ordinary linear model uses identity link $\boldsymbol{\mu} = \boldsymbol{X}\boldsymbol{\beta}$, and assumes $\boldsymbol{V} = \sigma^2\boldsymbol{I}$. For that model, standard results exploit the orthogonal decomposition

$$\boldsymbol{y} = \hat{\boldsymbol{\mu}} + (\boldsymbol{y} - \hat{\boldsymbol{\mu}}) \quad \text{(i.e., data = fit + residual).}$$

With generalized linear models, $\hat{\boldsymbol{\mu}}$ and $(\boldsymbol{y} - \hat{\boldsymbol{\mu}})$ are not orthogonal when we depart from identity link and constant variance. Then, Pythagoras's Theorem does not apply, because maximizing the likelihood does not correspond to minimizing $\|\boldsymbol{y} - \hat{\boldsymbol{\mu}}\|$. With a nonlinear link function, although the space of linear predictor values $\boldsymbol{\eta}$ that satisfy a particular model is a linear vector space, the corresponding set of $\boldsymbol{\mu} = g^{-1}(\boldsymbol{\eta})$ values is not.

Despite the lack of orthogonality, conventional wisdom seems to be that as n increases, $(\boldsymbol{y} - \hat{\boldsymbol{\mu}})$ is asymptotically uncorrelated with $\hat{\boldsymbol{\mu}}$. If this truly holds, then one can obtain an asymptotic covariance matrix for the residuals, because then

$$\boldsymbol{V} = \text{var}(\boldsymbol{y}) \approx \text{var}(\hat{\boldsymbol{\mu}}) + \text{var}(\boldsymbol{y} - \hat{\boldsymbol{\mu}}).$$

It then follows from standard results using the delta method (e.g., see [4, p. 136]) that

$$\text{var}(\boldsymbol{y} - \hat{\boldsymbol{\mu}}) \approx \boldsymbol{V}^{1/2}[\boldsymbol{I} - \boldsymbol{H}]\boldsymbol{V}^{1/2},$$

where $\boldsymbol{H}$ is a generalized hat matrix

$$\boldsymbol{H} = \boldsymbol{W}^{1/2}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{W}^{1/2}$$

incorporating a diagonal weight matrix

$$\boldsymbol{W} = \text{diag}\{(\partial\mu_i/\partial\eta_i)^2/\text{var}(y_i)\}.$$

But why, and under what conditions, is $(\boldsymbol{y} - \hat{\boldsymbol{\mu}})$ asymptotically uncorrelated with $\hat{\boldsymbol{\mu}}$? And for small-to-moderate n, is $\text{corr}(\boldsymbol{y} - \hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\mu}})$ close enough to 0 that we can safely ignore it? When I was recently writing a book on generalized linear models [4], I was surprised not to find literature about this. It seems that we should consider two types of asymptotics: Traditional asymptotics with $n \to \infty$, and the alternative with n fixed and asymptotics applying to individual components, such as binomial indices and Poisson expected counts in a contingency table. For the alternative (called *small-dispersion asymptotics* by Jørgensen [15]), with individual y_i asymptotically normal, $(\boldsymbol{y} - \boldsymbol{\mu})$ and $(\hat{\boldsymbol{\mu}} - \boldsymbol{\mu})$ jointly have an asymptotic normal distribution, as does their difference.

When I asked several statisticians if they knew of the existence of a general result about residuals and fitted values being asymptotically uncorrelated, G. Lovison gave me a heuristic solution. In Lovison [19], he discussed this point in an article that dealt with analogs of linear model results for generalized linear models. He argued that if $(\boldsymbol{y} - \hat{\boldsymbol{\mu}})$ and $\hat{\boldsymbol{\mu}}$ were not asymptotically uncorrelated, one could construct an asymptotically unbiased and more efficient estimator of $\boldsymbol{\mu}$ using $\hat{\boldsymbol{\mu}}^* = [\hat{\boldsymbol{\mu}} + \boldsymbol{L}(\boldsymbol{y} - \hat{\boldsymbol{\mu}})]$ for a matrix $\boldsymbol{L}$. But this would then contradict the ML estimator $\hat{\boldsymbol{\mu}}$ being asymptotically efficient. This argument is sort of an asymptotic version for ML estimators of one in the Gauss–Markov Theorem that unbiased estimators other than least squares estimator have difference from that estimator that is uncorrelated with it. The Lovison argument is heuristic, not distinguishing between the two possible types of asymptotics, and there still seems to be scope for a formal proof of the general result.

Interestingly, in his article, Lovison shows that a weighted version of adjusted responses that has approximately constant variance has orthogonality of fitted values and residuals. On the original scale, such a residual is the "Pearson residual" $e_i = (y_i - \hat{\mu}_i)/\sqrt{v(\hat{\mu}_i)}$ for variance function v evaluated at the model fit. For contingency tables, the Pearson residual is popular, because it results from the decomposition of the Pearson chi-squared statistic. For example, with Poisson counts $\{y_i\}$, the Pearson statistic satisfies

$$X^2 = \sum_i \frac{(y_i - \hat{\mu}_i)^2}{\hat{\mu}_i} = \sum_i e_i^2 \quad \text{with} \quad e_i = \frac{y_i - \hat{\mu}_i}{\sqrt{v(\hat{\mu}_i)}} = \frac{y_i - \hat{\mu}_i}{\sqrt{\hat{\mu}_i}}.$$

As an editorial comment, however, I believe it is strongly preferable to use *standardized residuals* rather than Pearson residuals. The standardized residual is

$$r_i = \frac{y_i - \hat{\mu}_i}{\text{std. error}(y_i - \hat{\mu}_i)} = \frac{y_i - \hat{\mu}_i}{\sqrt{v(\hat{\mu}_i)(1 - \hat{h}_{ii})}} = \frac{e_i}{\sqrt{1 - \hat{h}_{ii}}}$$

for "leverage" $\hat{h}_{ii}$ from the estimated hat matrix $\widehat{\boldsymbol{H}}$. For small-dispersion asymptotics, r_i is asymptotically standard normal when the model holds. This is not true of the Pearson residual e_i, because the denominator ignores the fact that $\hat{\mu}_i$ is random. The standardized residual appropriately recognizes redundancies in

data. For example, for the independence model assuming Poisson or multinomial sampling for a 2×2 table of counts $\{y_{ij}\}$, the fitted values are

$$\{\hat{\mu}_{ij} = np_{i+}p_{+j}\} \text{ for } p_{i+} = (\sum_j y_{ij})/n,\ p_{+j} = (\sum_i y_{ij})/n,$$

and so these two forms of residual then have expressions

$$e_{ij} = \frac{y_{ij} - \hat{\mu}_{ij}}{\sqrt{\hat{\mu}_{ij}}}, \quad r_{ij} = \frac{y_{ij} - \hat{\mu}_{ij}}{\sqrt{\hat{\mu}_{ij}(1 - p_{i+})(1 - p_{+j})}}.$$

For 2×2 tables, $df = 1$, reflecting that all four $|y_{ij} - \hat{\mu}_{ij}|$ are identical, so it seems sensible to have a single value for lack of fit. Yet, all four Pearson residuals can take different values. By contrast, $r_{11} = -r_{12} = -r_{21} = r_{22}$ and each $r_{ij}^2 = X^2$.

6 Improved Marginal Modeling of Multinomial Data

The final topic we consider deals with analyzing correlated observations using marginal models. Suppose that each subject has a cluster of correlated observations $\boldsymbol{y}_i = (y_{i1}, y_{i2}, \ldots, y_{iT})^T$, such as in a longitudinal study or an experiment with repeated measures. (The dimension T could vary by cluster, but for simplicity our notation uses a common value.) For each y_{it} marginally, we assume a model $g(\mu_{it}) = \boldsymbol{x}_{it}^T\boldsymbol{\beta}$.

For discrete data, ML for such a model is awkward because of the lack of a simple multivariate distribution that is characterized by pairwise correlations. For $E(\boldsymbol{y}_i) = \boldsymbol{\mu}_i$ and $\text{var}(\boldsymbol{y}_i) = \boldsymbol{V}_i$, it is common in practice to use estimates that are solutions of *generalized estimating equations* (GEE),

$$\sum_{i=1}^{n} \boldsymbol{D}_i^T \boldsymbol{V}_i^{-1}(\boldsymbol{y}_i - \boldsymbol{\mu}_i) = \boldsymbol{0}.$$

with $\boldsymbol{D}_i = \partial\boldsymbol{\mu}_i/\partial\boldsymbol{\beta}$. The GEE provide a multivariate generalization of quasi-likelihood methods, generalizing likelihood equations for univariate response without specifying a full multivariate distribution. Such an approach is useful when one's primary interest is modeling the marginal distribution of each y_{it} in terms of explanatory variables, rather than modeling dependence among $(y_{i1}, y_{i2}, \ldots, y_{iT})$.

In the estimating equations, in $\boldsymbol{V}_i$ GEE methods assume a "working" correlation structure (e.g., exchangeable, autoregressive) for $\boldsymbol{y}_i$. The resulting estimate of $\boldsymbol{\beta}$ is consistent even if the correlation structure is misspecified, when the marginal model is correct. However, standard errors are not appropriate. The method uses empirical robust estimates of the standard errors that are valid even when the correlation structure is misspecified, based on a "sandwich" covariance matrix. The

GEE method was originally specified by Liang and Zeger [16] for univariate y_{it} (e.g., binomial, Poisson), but extensions exist for multinomial models with $c > 2$ response categories. This has mainly been for ordinal responses, as in Lipsitz et al. [17].

In the multinomial context, let $y_{ijt} = 1$ if subject i makes response j for observation t. Then, for each pair (s, t) of times, one chooses a working corr(y_{ijs}, y_{ikt}), such as exchangeable (= ρ_{jk} for all s, t). However, Touloumis et al. [21] showed that certain correlation patterns do not correspond to a legitimate joint multinomial distribution, especially with large c. They argued that it is more sensible to model the covariance based on structure for local odds ratios, both for ordinal and nominal responses. In the binary case, this was suggested by Lipsitz et al. [18]. Structure specified in terms of local odds ratios using adjacent rows and adjacent columns is compatible with all possible multinomial joint distributions and their margins, and it can be used both with ordinal and nominal response variables.

Specifically, for any $s < t$, one supposes that the marginal $P(y_{ias} = 1, y_{ibt} = 1)$ has expected frequencies

$$\log \mu_{ab}^{(st)} = \lambda^{(st)} + \lambda_a^{(s)} + \lambda_b^{(t)} + \beta^{(st)} u_a u_b,$$

for some set of scores $\{u_j\}$. This is a special case of the *linear-by-linear association* loglinear model, in which row and column scores are identical. For this model, the local log odds ratios satisfy

$$\log \left[\frac{\mu_{ab}^{(st)} \mu_{a+1,b+1}^{(st)}}{\mu_{a,b+1}^{(st)} \mu_{a+1,b}^{(st)}} \right] = \beta^{(st)} (u_{a+1} - u_a)(u_{b+1} - u_b).$$

For an ordinal response variable, one takes $\{u_a\}$ to be fixed, monotone scores. For example, scores $\{u_a = a\}$ imply a uniform local log odds ratio that is merely $\beta^{(st)}$ (the so-called *uniform association model*). Exchangeable structure for the T responses then uses the same $\beta^{(st)}$ for each s, t. For a nominal response variable, one treats $\{u_a\}$ as parameters. This pairwise association structure is then a special case of Goodman's [12] *RC model* and relates to Anderson's [8] *stereotype model*.

With this multinomial GEE approach, Touloumis et al. noted strong efficiency gains over an independence working structure for studies with strong correlation and time-varying covariates. Touloumis has implemented ordinal and nominal local odds ratio structures with his recently developed *multgee* R package. See

http://cran.r-project.org/web/packages/multgee/multgee.pdf.

This package seems to have convergence problems and improper results much less often than existing R multinomial GEE routines. Also, other existing GEE multinomial packages in R do not handle nominal responses.

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Orthogonal Block Structure and Uniformly Best Linear Unbiased Estimators

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Abstract Models with orthogonal block structure, OBS, have variance covariance matrices that are linear combinations $\sum_{j=1}^{m} \gamma_j Q_j$ of known pairwise orthogonal–orthogonal projection matrices that add up to $\boldsymbol{I}_n$. We are interested in characterizing such models with least square estimators that are best linear unbiased estimator whatever the variance components, assuming that $\boldsymbol{\gamma} \in \nabla_{\geq}$, with $\nabla_{\geq}$ the set of vectors with nonnegative components of a subspace ∇. This is an extension of the usual concept of OBS in which we require $\boldsymbol{\gamma} \in \mathbb{R}^m_{\geq}$. Thus as we shall see it is usual when we apply our results to mixed models.

Keywords Best linear unbiased estimator · Least square estimators · Orthogonal block structure · Uniformly minimum variance unbiased estimator

1 Introduction

If a model has the family

$$\nu = \left\{ \sum_{i=1}^{w} \theta_i \boldsymbol{M}_i; \quad \boldsymbol{\theta} \in \Theta \right\} \tag{1}$$

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of variance–covariance matrices it suffices that $\boldsymbol{T}$, the projector onto the column space of matrix $\boldsymbol{X}_0$, commutes with $\boldsymbol{M}_1, \ldots, \boldsymbol{M}_w$ for the least square estimators, LSE, to be best linear unbiased estimator, BLUE, whatever $\boldsymbol{\theta} = \theta_1, \ldots, \theta_w$. Following [12] and [11], we say that, then, the LSE are uniformly best linear unbiased estimator, UBLUE.

When the model has only one variance component θ, then having variance–covariance matrix $\theta \boldsymbol{M}$, $\boldsymbol{T}$ commuting with $\boldsymbol{M}$ is, see [13] and [14], a necessary and sufficient condition for the LSE to be UBLUE. Then matrix $\boldsymbol{M}$ has the spectral decomposition

$$\boldsymbol{M} = \sum_{j=1}^{m} b_j \boldsymbol{Q}_j \tag{2}$$

with $\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_m$ pairwise orthogonal–orthogonal projection matrices, POOPM, and the family of variance–covariance matrices can be written as

$$v = \left\{ \sum_{j=1}^{m} \gamma_j \boldsymbol{Q}_j; \quad \boldsymbol{\gamma} \in R(\boldsymbol{b})_{\geq} \right\}, \tag{3}$$

where $R(\boldsymbol{U})$ is the range space of matrix $\boldsymbol{U}$, $\boldsymbol{b}$ $[\boldsymbol{\gamma}]$ has components $b_1, \ldots, b_m$ $[\gamma_1, \ldots, \gamma_m]$ and $\triangle_{\geq}$ is the family of vectors of subspace $\triangle$ with nonnegative components. We say that those models have $rank$ 1, since $rank(\boldsymbol{b}) = 1$. We intend to extend the necessary and sufficient conditions obtained for $rank$ 1 models to models with

$$v = \left\{ \sum_{j=1}^{m} \gamma_j \boldsymbol{Q}_j; \quad \boldsymbol{\gamma} \in \bigtriangledown_{\geq} \right\}, \tag{4}$$

where $dim(\bigtriangledown) = r \geq 1$. These models will have rank r. When $\bigtriangledown = \mathbb{R}^m$ all the matrices $\sum_{j=1}^{m} \gamma_j \boldsymbol{Q}_j$ with nonnegative coefficients may be variance–covariance matrices and we say the model is full rank. Moreover if

$$\sum_{j=1}^{m} \boldsymbol{Q}_j = \boldsymbol{I}_n \tag{5}$$

the model will have orthogonal block structure, OBS, see [8, 9]. These models continue to play a prominent role in the theory of randomized block designs, see [2, 3].

An interesting case studied by [1] is the case where the family of possible variance–covariance matrices, while still commutative, no longer forms an orthogonal block structure.

In the next section we present results on commutative Jordan algebras (of symmetric matrices), CJA, and describe the algebraic structure of the model. Finally, in the third section, we characterize the models with OBS whose LSE are UBLUE, this is they are BLUE whatever the variance components.

2 Algebras and Structure

A CJA is a linear space constituted by symmetric matrices that commute and containing the squares of its matrices. Each one of these algebras, say $\mathcal{A}$, has a unique basis, the principal basis, $pb(\mathcal{A})$, constituted by POOPM, see [10]. For a family $\boldsymbol{W} = \{\boldsymbol{W}_1, \ldots, \boldsymbol{W}_u\}$ of symmetric matrices to be contained in a CJA, see, e.g., [5], it is necessary and sufficient that its matrices commute. Moreover, intersecting all the CJA that contain $\boldsymbol{W}$ we obtain the least CJA, $\mathcal{A}(\boldsymbol{W})$, that contains $\boldsymbol{W}$, this will be the CJA generated by $\boldsymbol{W}$. If the $n \times n$ matrices in $pb(\mathcal{A})$ add up to $\boldsymbol{I}_n$, the CJA will be complete. For a CJA to contain invertible matrices it is necessary and sufficient that it is complete, see [5].

Let us consider the mixed model

$$\boldsymbol{Y} = \sum_{i=0}^{w} \boldsymbol{X}_i \boldsymbol{\beta}_i, \tag{6}$$

where $\boldsymbol{\beta}_0$ is fixed and the $\boldsymbol{\beta}_1, \ldots, \boldsymbol{\beta}_w$ are random, independent, with null mean vectors and variance–covariance matrices $\boldsymbol{\theta}_1 \boldsymbol{I}_{c_1}, \ldots, \boldsymbol{\theta}_w \boldsymbol{I}_{c_w}$. If the matrices $\boldsymbol{M}_i = \boldsymbol{X}_i \boldsymbol{X}_i^\top, i = 1, \ldots, w$ commute, they will generate $\mathcal{A} = \mathcal{A}(\underline{\boldsymbol{M}})$, where $\underline{\boldsymbol{M}} = \{\boldsymbol{M}_1, \ldots, \boldsymbol{M}_w\}$. With $\underline{\boldsymbol{Q}} = \{\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_m\} = pb(\mathcal{A})$, we will have

$$\boldsymbol{M}_i = \sum_{j=1}^{m} b_{i,j} \boldsymbol{Q}_j, i = 1, \ldots, w \tag{7}$$

and so we will have the variance–covariance matrices

$$\boldsymbol{V}(\boldsymbol{\theta}) = \sum_{i=1}^{w} \theta_i \boldsymbol{M}_i = \sum_{j=1}^{m} \left(\sum_{i=1}^{w} b_{i,j} \theta_i \right) \boldsymbol{Q}_j = \sum_{j=1}^{m} \gamma_j \boldsymbol{Q}_j = \boldsymbol{V}(\boldsymbol{\gamma}), \tag{8}$$

with

$$\boldsymbol{\gamma}_j = \sum_{i=1}^{w} b_{i,j} \theta_i, j = 1, \ldots, m, \tag{9}$$

and so $\boldsymbol{\gamma} \in R(\boldsymbol{B}^\top)_{\geq}$, where $\boldsymbol{B} = [b_{i,j}]$.

Let us establish

Proposition 1 *If* $R([\boldsymbol{X}_1 \ldots \boldsymbol{X}_w]) = \mathbb{R}^n$ *and the matrices* $\boldsymbol{M}_i, i = 1, \ldots, w$, *commute, the model has OBS.*

Proof Since the $\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_m$ are POOPM we have only to show that $\sum_{j=1}^{m} \boldsymbol{Q}_j = \boldsymbol{I}_n$, this is that $\mathcal{A}$ is complete. Now

$$rank\left(\sum_{i=1}^{w} \boldsymbol{M}_i\right) = rank(R[\boldsymbol{X}_1 \ldots \boldsymbol{X}_w]) = n,$$

so $\sum_{i=1}^{w} \boldsymbol{M}_i$, being an $n \times n$ matrix with rank n, is invertible and since $\sum_{i=1}^{w} \boldsymbol{M}_i \in \mathcal{A}$, $\mathcal{A}$ is complete. □

We point out that $\boldsymbol{V}(\boldsymbol{\theta}_1) = \boldsymbol{V}(\boldsymbol{\theta}_2)$ implies $\boldsymbol{\theta}_1 = \boldsymbol{\theta}_2$ if and only if the matrices $\boldsymbol{M}_1, \ldots, \boldsymbol{M}_w$ are linearly independent so the row vectors of matrix $\boldsymbol{B}$. From now on we make this assumption of linear independence so $\boldsymbol{B}$ will be a $w \times m$ matrix with rank w.

If the model has OBS and $\boldsymbol{T}$ commutes with $\boldsymbol{M}$, the model will have commutative OBS and we say that it has COBS. The models with COBS were introduced in [6]. We now have the

Proposition 2 *A model with OBS has COBS if and only if* $\boldsymbol{T}$ *commutes with the* $\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_m$.

Proof We have only to establish the part of the thesis for COBS since the proof for OBS is identical. For this, it is sufficient to show that $\boldsymbol{T}$ commutes with $\boldsymbol{M}_1, \ldots, \boldsymbol{M}_w$ if and only if it commutes with $\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_m$. Now, if $\boldsymbol{T}$ and the $\boldsymbol{M}_1, \ldots, \boldsymbol{M}_w$ commute, the matrices of $\underline{\boldsymbol{M}^*} = \{\boldsymbol{T}, \boldsymbol{M}_1, \ldots, \boldsymbol{M}_w\}$ generate a CJA, $\mathcal{A}^*$, that contains $\mathcal{A}(\underline{\boldsymbol{M}})$, since $\underline{\boldsymbol{M}} \subseteq \underline{\boldsymbol{M}^*}$. Namely we will have $\boldsymbol{T}, \boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_m \in \mathcal{A}^*$ so $\boldsymbol{T}\boldsymbol{Q}_j = \boldsymbol{Q}_j\boldsymbol{T}, j = 1, \ldots, m$. The inverse is easy to establish since $\boldsymbol{M}_i = \sum_{j=1}^{m} b_{i,j}\boldsymbol{Q}_j, i = 1, \ldots, w$, thus $\boldsymbol{T}\boldsymbol{Q}_j = \boldsymbol{Q}_j\boldsymbol{T}, j = 1, \ldots, m$ implies $\boldsymbol{T}\boldsymbol{M}_i = \boldsymbol{M}_i\boldsymbol{T}, i = 1, \ldots, w$. □

Corollary 1 *A model with OBS has COBS if and only if their matrices* $\boldsymbol{Q}_j^* = \boldsymbol{Q}_j\boldsymbol{T}, j = 1, \ldots, m$, *are orthogonal projection matrices (we point out that* $\boldsymbol{0}_{n\times n}$ *is an orthogonal projection matrix).*

Proof The thesis follows directly from Proposition 2 since the $\boldsymbol{Q}_j^*$ are symmetric and idempotent if and only if $\boldsymbol{Q}_j\boldsymbol{T} = \boldsymbol{T}\boldsymbol{Q}_j, j = 1, \ldots, m$. We point out that, see [7], $pb(\mathcal{A}^*)$ is constituted by the nonnull matrices $\boldsymbol{T}\boldsymbol{Q}_j$ and $(\boldsymbol{I}_n - \boldsymbol{T})\boldsymbol{Q}_j, j = 1, \ldots, m$. □

Let the g_j row vectors of matrix $\boldsymbol{A}_j$ constitute an orthonormal basis for $\nabla_j = R(\boldsymbol{Q}_j)$. Now

$$\widetilde{\boldsymbol{\psi}} = \boldsymbol{U}\boldsymbol{Y}$$

is an LSE estimator of its mean vector

$$\boldsymbol{\psi} = \boldsymbol{U}\boldsymbol{\mu},$$

if and only if

$$\boldsymbol{U}\boldsymbol{T} = \boldsymbol{U}.$$

We now have

Theorem 1 *The OBS whose LSE are UBLUE are the COBS.*

Proof As for Proposition 2 we have only to establish the first part of the thesis. In COBS we have, whatever $\boldsymbol{\gamma}$, $\boldsymbol{T}\boldsymbol{V}(\boldsymbol{\gamma}) = \boldsymbol{V}(\boldsymbol{\gamma})\boldsymbol{T}$ as well as $\boldsymbol{T}^c\boldsymbol{V}(\boldsymbol{\gamma}) = \boldsymbol{V}(\boldsymbol{\gamma})\boldsymbol{T}^c$, with $\boldsymbol{T}^c = \boldsymbol{I}_n - \boldsymbol{T}$. Putting $\boldsymbol{U}_{\Omega} = \boldsymbol{U}\boldsymbol{T}$ and $\boldsymbol{U}_{\Omega^\perp} = \boldsymbol{U}\boldsymbol{T}^c$ we get

$$Cov(\boldsymbol{U}\boldsymbol{Y}) = \boldsymbol{U}\boldsymbol{V}(\boldsymbol{\gamma})\boldsymbol{U}^\top = (\boldsymbol{U}_{\Omega}\boldsymbol{U}_{\Omega^\perp})\boldsymbol{V}(\boldsymbol{\gamma})(\boldsymbol{U}_{\Omega}^\top\boldsymbol{U}_{\Omega^\perp}^\top) =$$

$$= \boldsymbol{U}_{\Omega}\boldsymbol{V}(\boldsymbol{\gamma})\boldsymbol{U}_{\Omega^\perp}^\top\boldsymbol{U}_{\Omega}\boldsymbol{V}(\boldsymbol{\gamma})\boldsymbol{U}_{\Omega^\perp}^\top,$$

since $\boldsymbol{U}_{\Omega}\boldsymbol{V}(\boldsymbol{\gamma})\boldsymbol{U}_{\Omega^\perp}^\top = \boldsymbol{U}\boldsymbol{T}\boldsymbol{V}(\boldsymbol{\gamma})\boldsymbol{T}^c\boldsymbol{U}^\top = \boldsymbol{U}\boldsymbol{V}(\boldsymbol{\gamma})\boldsymbol{T}\boldsymbol{T}^c\boldsymbol{U}^\top = \boldsymbol{0}_{n\times n}$ and, likewise $\boldsymbol{U}_{\Omega^\perp}\boldsymbol{V}(\boldsymbol{\gamma})\boldsymbol{U}_{\Omega}^\top = \boldsymbol{0}_{n\times n}$, considering Cov the covariance matrix.
Given another linear unbiased estimator $\boldsymbol{\psi}^* = \boldsymbol{L}\boldsymbol{Y}$ of $\boldsymbol{\psi}$ we have $\boldsymbol{L}\boldsymbol{\mu} = \boldsymbol{U}\boldsymbol{\mu}$, so $(\boldsymbol{L}_{\Omega} - \boldsymbol{U}_{\Omega})\boldsymbol{X}_0 = (\boldsymbol{L} - \boldsymbol{U})\boldsymbol{T}\boldsymbol{X}_0 = \boldsymbol{0}_{n\times k}$ since the row vectors of $(\boldsymbol{L} - \boldsymbol{U})\boldsymbol{T}$ belong to $\Omega = R(\boldsymbol{X}_0)$ and are orthogonal to Ω.

Thus $\boldsymbol{L}_{\Omega} = \boldsymbol{L}\boldsymbol{T} = \boldsymbol{U}\boldsymbol{T} = \boldsymbol{U}_{\Omega}$, so

$$Cov(\boldsymbol{L}\boldsymbol{Y}) \geq Cov(\boldsymbol{L}_{\Omega}\boldsymbol{Y}) = Cov(\boldsymbol{U}_{\Omega}\boldsymbol{Y}) = Cov(\widetilde{\boldsymbol{\psi}}),$$

and the proof is complete. □

We now look for an expression to $\widetilde{\boldsymbol{\psi}}$ which exhibits the algebraic structure of models with COBS. Let the g_j row vectors of A_j constitute an orthonormal basis for $R(\boldsymbol{Q}_j)$, so that we have

$$\boldsymbol{A}_j\boldsymbol{A}_j^\top = \boldsymbol{I}_{g_j}, \quad \boldsymbol{A}_j^\top\boldsymbol{A}_j = \boldsymbol{Q}_j, j = 1, \ldots, m,$$

we put $\boldsymbol{X}_{0,j} = \boldsymbol{A}_j\boldsymbol{X}_j$ and represent by $\boldsymbol{P}_j$ the orthogonal projection matrix on $\boldsymbol{\Omega}_j = R(\boldsymbol{X}_{0,j})$, $j = 1, \ldots, m$. If, with $p_j = rank(\boldsymbol{P}_j)$, the p_j row vectors of $\boldsymbol{W}_j$ constitute an orthonormal basis for Ω_j, we will have

$$\boldsymbol{W}_j\boldsymbol{W}_j^\top = \boldsymbol{I}_{p_j}, \quad \boldsymbol{W}_j^\top\boldsymbol{W}_j = \boldsymbol{P}_j, j = 1, \ldots, m.$$

When $p_j = 0$ we assume that $\boldsymbol{I}_0 = [0]$ and that $\boldsymbol{P}_j = \boldsymbol{0}_{n\times n}$.

We now establish

Proposition 3 *In models with COBS, the* $\dot{\boldsymbol{Q}}_j = \boldsymbol{Q}_j\boldsymbol{T}$ *and the* $\ddot{\boldsymbol{Q}}_j = \boldsymbol{A}_j^\top \boldsymbol{P}_j \boldsymbol{A}_j$ *are identical orthogonal projection matrices with rank* p_j, $j = 1, \ldots, m$.

Proof If $p_j = 0$ we have $\dot{\boldsymbol{Q}}_j = \ddot{\boldsymbol{Q}}_j = \boldsymbol{0}_{n\times n}$. We saw that in models with COBS the $\dot{\boldsymbol{Q}}_j$, $j = 1, \ldots, m$ are orthogonal projection matrices it being straightforward to show that the $\ddot{\boldsymbol{Q}}_j$, $j = 1, \ldots, m$, also are. Moreover

$R(\dot{\boldsymbol{Q}}_j) = R(\boldsymbol{Q}_j\boldsymbol{T}) = \boldsymbol{Q}_j R(\boldsymbol{T}) = \boldsymbol{Q}_j R(\boldsymbol{X}_0) = \boldsymbol{A}_j^\top \boldsymbol{A}_j R(\boldsymbol{X}_0) = \boldsymbol{A}_j^\top R(\boldsymbol{A}_j\boldsymbol{X}_0) = \boldsymbol{A}_j^\top R(\boldsymbol{X}_{0,j}) = \boldsymbol{A}_j^\top R(\boldsymbol{P}_j) = R(\boldsymbol{A}_j^\top \boldsymbol{P}_j) = R((\boldsymbol{A}_j^\top \boldsymbol{P}_j)(\boldsymbol{A}_j^\top \boldsymbol{P}_j)^\top) = R(\boldsymbol{A}_j^\top \boldsymbol{P}_j \boldsymbol{A}_j) = R(\ddot{\boldsymbol{Q}}_j)$, thus $\dot{\boldsymbol{Q}}_j = \ddot{\boldsymbol{Q}}_j$ and $rank(\ddot{\boldsymbol{Q}}_j) = rank(\dot{\boldsymbol{Q}}_j)$. Now $\boldsymbol{P}_j = \boldsymbol{A}_j \ddot{\boldsymbol{Q}}_j \boldsymbol{A}_j^\top$, so $p_j = rank(\boldsymbol{P}_j) = rank(\ddot{\boldsymbol{Q}}_j) = rank(\dot{\boldsymbol{Q}}_j)$ and the proof is complete. □

Corollary 2 *In models with COBS and matrix* $\boldsymbol{X}_0$ *with* k *linearly independent column vectors we have* $k = \sum_{j=1}^m p_j$.

Proof We have $k = rank(\boldsymbol{X}_0) = rank(\boldsymbol{T})$ so the thesis follows from

$$\boldsymbol{T} = \boldsymbol{I}_n\boldsymbol{T} = \left(\sum_{j=1}^m \boldsymbol{Q}_j\right)\boldsymbol{T} = \sum_{j=1}^m \dot{\boldsymbol{Q}}_j$$

and from the $\dot{\boldsymbol{Q}}_1, \ldots, \dot{\boldsymbol{Q}}_m$ being pairwise orthogonal so that $rank\left(\sum_{j=1}^m \dot{\boldsymbol{Q}}_j\right) = \left(\sum_{j=1}^m rank(\dot{\boldsymbol{Q}}_j)\right) = \sum_{j=1}^m p_j$. □

Let us have $p_j > 0$ if and only if $j \le l$, with $l \le m$, and put $\boldsymbol{Y}_j = \boldsymbol{A}_j\boldsymbol{Y}$ and $\boldsymbol{Z}_j = \boldsymbol{W}_j\boldsymbol{Y}_j$, $j = 1, \ldots, l$. Since $\dot{\boldsymbol{Q}}_j = \boldsymbol{0}_{n\times n}$, if $j > l$, whenever $l < m$, we have

$$\boldsymbol{T} = \sum_{j=1}^l \boldsymbol{Q}_j\boldsymbol{T} = \sum_{j=1}^l \dot{\boldsymbol{Q}}_j = \sum_{j=1}^l \ddot{\boldsymbol{Q}}_j = \sum_{j=1}^l \boldsymbol{A}_j^\top \boldsymbol{P}_j \boldsymbol{A}_j,$$

as well as, since $\boldsymbol{P}_j = \boldsymbol{W}_j^\top \boldsymbol{W}_j$, $j = 1, \ldots, l$

$$\widetilde{\boldsymbol{\mu}} = \boldsymbol{T}\boldsymbol{Y} = \sum_{j=1}^l \boldsymbol{A}_j^\top \boldsymbol{P}_j \boldsymbol{A}_j \boldsymbol{Y} = \sum_{j=1}^l \boldsymbol{A}_j^\top \boldsymbol{P}_j \boldsymbol{Y}_j =$$

$$= \sum_{j=1}^l \boldsymbol{A}_j^\top \boldsymbol{W}_j^\top \boldsymbol{W}_j \boldsymbol{Y}_j = \sum_{j=1}^l \boldsymbol{A}_j^\top \boldsymbol{W}_j^\top \boldsymbol{Z}_j$$

so that $\widetilde{\boldsymbol{\mu}} = \sum_{j=1}^l \boldsymbol{U}_j \boldsymbol{Z}_j$, with $\boldsymbol{U}_j = \boldsymbol{A}_j^\top \boldsymbol{W}_j^\top$, $j = 1, \ldots, l$.

3 Model Characterization

We now characterize models whose LSE are UBLUE. The estimable vectors of a model with mean vector $\boldsymbol{\mu} = \boldsymbol{X}_0\boldsymbol{\beta}_o$ are the

$$\boldsymbol{\psi} = \boldsymbol{U}\boldsymbol{\mu}.$$

The corresponding linear unbiased estimators are the $\boldsymbol{\psi}^* = \boldsymbol{L}\boldsymbol{Y}$ with

$$\boldsymbol{L} \in [\boldsymbol{\psi}] = \{\boldsymbol{L} : E(\boldsymbol{L}\boldsymbol{Y}) = \boldsymbol{\psi}\},$$

where $E(.)$ indicates mean vector. We now establish

Lemma 1 *We have* $E(\boldsymbol{L}_1\boldsymbol{Y}) = E(\boldsymbol{L}_2\boldsymbol{Y})$ *if and only if* $\boldsymbol{L}_1\boldsymbol{T} = \boldsymbol{L}_2\boldsymbol{T}$.

Proof Since $E(\boldsymbol{L}_l\boldsymbol{Y}) = \boldsymbol{L}_l\boldsymbol{\mu} = \boldsymbol{L}_l\boldsymbol{T}\boldsymbol{\mu}, l = 1, 2$, the sufficient condition is established. Inversely, if $E(\boldsymbol{L}_1\boldsymbol{Y}) = E(\boldsymbol{L}_2\boldsymbol{Y})$ we will have, whatever $\boldsymbol{\beta}_0$, $\boldsymbol{L}_1\boldsymbol{T}\boldsymbol{X}_0\boldsymbol{\beta}_0 = \boldsymbol{L}_2\boldsymbol{T}\boldsymbol{X}_0\boldsymbol{\beta}_0$ so that $\boldsymbol{L}_1\boldsymbol{T}\boldsymbol{X}_0 = \boldsymbol{L}_2\boldsymbol{T}\boldsymbol{X}_0$ and that $(\boldsymbol{L}_1\boldsymbol{T} - \boldsymbol{L}_2\boldsymbol{T})\boldsymbol{X}_0 = \boldsymbol{0}$, where $\boldsymbol{0}$ denotes a null matrix. Thus the row vectors of $\boldsymbol{W} = \boldsymbol{L}_1\boldsymbol{T} - \boldsymbol{L}_2\boldsymbol{T} = (\boldsymbol{L}_1 - \boldsymbol{L}_2)\boldsymbol{T}$ have to be orthogonal to $\boldsymbol{\Omega} = R(\boldsymbol{X}_0)$, but these vectors also belong to $\boldsymbol{\Omega}$ so they are null which gives $\boldsymbol{L}_1\boldsymbol{T} - \boldsymbol{L}_2\boldsymbol{T} = \boldsymbol{0}$ and so $\boldsymbol{L}_1\boldsymbol{T} = \boldsymbol{L}_2\boldsymbol{T}$ as we wanted to established. □

Now the LSE for $\boldsymbol{\psi} = \boldsymbol{U}\boldsymbol{\mu}$ is

$$\widetilde{\boldsymbol{\psi}} = \boldsymbol{L}(\boldsymbol{\psi})\boldsymbol{Y}$$

with $\boldsymbol{L}(\psi) = \boldsymbol{U}\boldsymbol{T}$ and $\widetilde{\boldsymbol{\mu}} = \boldsymbol{T}\boldsymbol{Y}$. We see that $\boldsymbol{L}(\boldsymbol{\psi}) \in [\boldsymbol{\psi}]$, since

$$E(\widetilde{\boldsymbol{\psi}}) = \boldsymbol{L}(\boldsymbol{\psi})\boldsymbol{\mu} = \boldsymbol{U}\boldsymbol{T}\boldsymbol{X}_0\boldsymbol{\beta}_0 = \boldsymbol{U}\boldsymbol{\mu} = \boldsymbol{\psi},$$

besides this, according to Lemma 1, $\boldsymbol{L} \in [\boldsymbol{\psi}]$ if and only if

$$\boldsymbol{L}\boldsymbol{T} = \boldsymbol{L}(\boldsymbol{\psi})\boldsymbol{T} = \boldsymbol{U}\boldsymbol{T}\boldsymbol{T} = \boldsymbol{U}\boldsymbol{T} = \boldsymbol{L}(\boldsymbol{\psi}).$$

Putting $\boldsymbol{T}^c = \boldsymbol{I}_n - \boldsymbol{T}$ we have, with $\boldsymbol{L} \in [\boldsymbol{\psi}]$,

$$\boldsymbol{L} = \boldsymbol{L}\boldsymbol{T} + \boldsymbol{L}\boldsymbol{T}^c = \boldsymbol{L}(\boldsymbol{\psi}) + r\boldsymbol{B},$$

with $-\infty < r < +\infty$ and $\boldsymbol{B} = \frac{1}{r}\boldsymbol{L}\boldsymbol{T}^c$. Thus,

$$Cov_\theta(\boldsymbol{L}\boldsymbol{Y}) = Cov_\theta(\boldsymbol{L}(\psi)\boldsymbol{Y}) + 2rCov_\theta(\boldsymbol{L}(\psi)\boldsymbol{Y}, \boldsymbol{B}\boldsymbol{Y}) + r^2Cov_\theta(\boldsymbol{B}\boldsymbol{Y})$$

it being easy to see that we have, whatever $r \in]-\infty; +\infty[$,

$$Cov_\theta(\widetilde{\boldsymbol{\psi}}) = Cov_\theta(\boldsymbol{L}(\psi)\boldsymbol{Y}) \leq Cov_\theta(\boldsymbol{L}\boldsymbol{Y})$$

if and only if $Cov_\theta(\boldsymbol{L}(\psi)\boldsymbol{Y}, \boldsymbol{BY}) = \boldsymbol{0}$. Since $\boldsymbol{B} = \frac{1}{r}\boldsymbol{L}\boldsymbol{T}^c$ we get

$$Cov_\theta(\boldsymbol{LTY}, \boldsymbol{LT}^c\boldsymbol{Y}) = \boldsymbol{0},$$

whenever

$$Cov_\theta(\boldsymbol{L}(\psi)\boldsymbol{Y}, \boldsymbol{BY}) = \boldsymbol{0}.$$

Now

$$Cov_\theta(\boldsymbol{LTY}, \boldsymbol{LT}^c\boldsymbol{Y}) = \boldsymbol{LTV}(\boldsymbol{\theta})\boldsymbol{T}^c\boldsymbol{L}^\top =$$

$$\boldsymbol{L}[\boldsymbol{TV}(\boldsymbol{\theta})(\boldsymbol{I}_n - \boldsymbol{T})]\boldsymbol{L}^\top = \boldsymbol{L}[\boldsymbol{TV}(\boldsymbol{\theta}) - \boldsymbol{TV}(\boldsymbol{\theta})\boldsymbol{T})]\boldsymbol{L}^\top,$$

so that to have

$$Cov_\theta(\widetilde{\boldsymbol{\psi}}) \leq Cov_\theta(\boldsymbol{LY})$$

for every $\boldsymbol{\theta}$, if and only if $\boldsymbol{TV}(\boldsymbol{\theta}) - \boldsymbol{TV}(\boldsymbol{\theta})\boldsymbol{T} = \boldsymbol{TV}(\boldsymbol{\theta})\boldsymbol{T}^c = \boldsymbol{0}$, which gives $\boldsymbol{TV}(\boldsymbol{\theta}) = \boldsymbol{TV}(\boldsymbol{\theta})T$ and

$$\boldsymbol{V}(\boldsymbol{\theta})\boldsymbol{T} = (\boldsymbol{TV}(\boldsymbol{\theta}))^\top = (\boldsymbol{TV}(\boldsymbol{\theta})\boldsymbol{T})^\top = \boldsymbol{TV}(\boldsymbol{\theta})\boldsymbol{T} = \boldsymbol{TV}(\boldsymbol{\theta}),$$

also for every $\boldsymbol{\theta}$.

We now establish

Theorem 2 *The LSE are UBLUE if and only if, for every* $\boldsymbol{\theta}$, $\boldsymbol{T}$ *commutes with* $\boldsymbol{V}(\boldsymbol{\theta})$,

Proof The preceding discussion establishes the necessary condition. To complete the proof we point out that, when $\boldsymbol{T}$ commutes with $\boldsymbol{V}(\boldsymbol{\theta})$ we have

$$Cov_\theta(\boldsymbol{LTY}, \boldsymbol{BY}) = rCov_\theta(\boldsymbol{LTY}, \frac{1}{r}\boldsymbol{LT}^c\boldsymbol{Y}) = \boldsymbol{LTV}(\boldsymbol{\theta})\boldsymbol{T}^c\boldsymbol{L}^\top = \boldsymbol{0}_{n\times n},$$

and so

$$Cov_\theta(\boldsymbol{LY}) = Cov_\theta(\boldsymbol{L}(\boldsymbol{\psi})\boldsymbol{Y}) + r^2Cov_\theta(\boldsymbol{BY}) \geq Cov_\theta\boldsymbol{L}(\boldsymbol{\psi}) = Cov_\theta(\widetilde{\boldsymbol{\psi}}).$$

□

Now the models with OBS where $\boldsymbol{T}$ commutes with the $\boldsymbol{M}_1, \ldots, \boldsymbol{M}_w$ and so with $\boldsymbol{V}(\boldsymbol{\theta})$, whatever $\boldsymbol{\theta}$, are those with COBS so these are the models with OBS whose LSE are UBLUE.

Corollary 3 *Models with OBS have LSE that are UBLUE if and only if they have COBS.*

In establishing Theorem 2, we did not require that

$$\boldsymbol{V}(\boldsymbol{\theta}) = \sum_{i=1}^{w} \theta_i \boldsymbol{M}_i$$

in order to widen the class of models to which our results applies. Moreover, as we stated in the introduction, when we restrict ourselves to OBS, assuming that

$$\boldsymbol{V}(\boldsymbol{\gamma}) = \sum_{j=1}^{m} \gamma_j \boldsymbol{Q}_j$$

with $\boldsymbol{\gamma} \in \nabla_{\geq}$, our result holds whatever the dimension ($\leq m$) of ∇.

4 Final Remarks

The models we considered have variance–covariance matrices $\boldsymbol{V}(\boldsymbol{\gamma}) = \sum_{j=1}^{m} \gamma_j \boldsymbol{Q}_j$ where the $\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_m$ are POOPM that add up to $\boldsymbol{I}_n$, and $\boldsymbol{\gamma} \in \nabla$ with $\dim(\nabla) = r \geq 1$. We discussed the role played by $\boldsymbol{T}$, the orthogonal projection matrix on the space spanned by the mean vector, commuting with the $\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_m$ in the LSE of estimable vectors being UBLUE, this is, being BLUE whatever $\boldsymbol{\gamma}$. Namely we showed that commutativity characterizes the models, in the class we consider, whose LSE are UBLUE. We point out that in our mixed models we had $\boldsymbol{\gamma} \in R(\boldsymbol{B}^{\top})_{\geq}$. To have, as required in [8, 9], the $\boldsymbol{\gamma} \in \mathbb{R}^m_{\geq}$, matrix $\boldsymbol{B}$ would have to have rank m and thus being invertible. This condition holds when $\boldsymbol{M}$ is a basis for $\boldsymbol{M}$, we then say, see [4], that the family $\boldsymbol{M}$ is perfect.

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Hadamard Matrices on Error Detection and Correction: Useful Links to BIBD

Carla Francisco, Teresa A. Oliveira, Amílcar Oliveira, and Francisco Carvalho

Abstract In the areas of Computer Science and Telecommunications there is a huge amount of applications in which error control, error detection and error correction are crucial tools to enable reliable delivery of digital data over unreliable communication, thus providing quality of service. Hadamard matrices can almost directly be used as an error-correcting code using an Hadamard code, generalized in Reed-Muller codes. Advances in algebraic design theory by using deep connections with algebra, finite geometry, number theory, combinatorics and optimization provided a substantial progress on exploring Hadamard matrices. Their construction and its use on combinatorics are crucial nowadays in diverse fields such as: quantum information, communications, networking, cryptography, biometry and security. Hadamard matrices give rise to a class of block designs named Hadamard configurations and different applications of it based on new technologies and codes of figures such as QR Codes are present almost everywhere. Some connections to Balanced Incomplete Block Designs are very well known as a tool to solve emerging problems in these areas. We will explore the use of Hadamard matrices on QR Codes error detection and correction. Some examples will be provided.

Keywords BIBD · Error-correcting code · Hadamard matrices · QR Codes

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1 Hadamard Matrices

An Hadamard[1] matrix is a square matrix $\mathbf{H}_n$ of order n with entries ± 1 and whose rows (or columns vice versa) are mutually orthogonal, see Seberry [24]. If $\mathbf{H}_n$ is Hadamard matrix, then $\mathbf{H}_n\mathbf{H}_n^\top = n\mathbf{I}_n$. An Hadamard matrix remains so when any row or column is multiplied by -1. Having this into consideration, one can always write an Hadamard matrix with its first row and first column having only $+1$'s, that it is the normal form of an Hadamard matrix, see Sylvester [26].

If $\mathbf{H}_n$ exists for $n = 1$, then $\mathbf{H}_2$ can be written like the one below:

$$\mathbf{H}_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

More examples of Hadamard matrices:

$$\mathbf{H}_4 = \left[\begin{array}{cc|cc} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ \hline 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{array}\right]; \quad \mathbf{H}_8 = \left[\begin{array}{cccc|cccc} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ \hline 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{array}\right]$$

4×4 Hadamard matrix $\qquad$ 8×8 Hadamard matrix

The necessary condition for the existence of an Hadamard matrix $\mathbf{H}_n$, $n > 2$ is that $n \equiv 0(mod 4)$; more about this can be found on Hall [8]. Hadamard matrices for all permissible values of $n \leq 100$, with the exception of $n = 92$ can be found on Plackett and Burman [18]. Only later on Baumert et al. [1] presented an Hadamard matrix of order 92.

According to Hedayat and Wallis [9] and to Sawade [23] Hadamard matrices have their existence confirmed for all permissible values of $n \leq 424$.

If $\mathbf{H}_m$ and $\mathbf{H}_n$ are Hadamard matrices of orders m and n, respectively, then their tensor product $\mathbf{H}_m \otimes \mathbf{H}_n$ is an Hadamard matrix of order mn, where $\otimes$ denotes the Kronecker matrix product. So, in particular, an Hadamard matrix $\mathbf{H}_n$ of order n where $n = 2s$ and $s \geq 2$ is an integer can be built by taking the s-fold tensor product

[1] Jacques Hadamard (1865–1963).

of $\mathbf{H}_2$ with itself, as it is given below:

$$\mathbf{H}_{2^s} = \underbrace{\mathbf{H}_2 \otimes \mathbf{H}_2 \otimes \cdots \otimes \mathbf{H}_2}_{s \text{ times}}.$$

Hadamard matrices are very well known because of the wide range of applications, not only in several areas of mathematics, but also in other sciences and mainly those connected with new technological advances, like cryptography Ogata et al. [15], image analysis, signal processing, coding theory and algorithm design, see e.g. Francisco [6]. In Statistics, Combinatorial Designs and Experimental design the Hadamard matrices play a key role in the block design construction. We refer to Din and Mavron [5] and to Koukouvinos [11] where one can see how these matrices are useful for the construction of BIBD (balanced incomplete block design)—see Sect. 2—, and for designs and secret sharing schemes, respectively.

2 Relationship Between Hadamard Matrices and BIBD

Consider now an Hadamard matrix $\mathbf{H}_{4u}$, which without loss of generality is assumed to be in its normal form. Delete from $\mathbf{H}_{4u}$, its first row and first column of all ones, thus obtaining a matrix $\mathbf{A}$ of order $(4u-1) \times (4u-1)$.

Taking $\mathbf{A}$ we can define $\mathbf{N} = \frac{1}{2}(\mathbf{A} + \mathbf{J}_{4u-1})$, where $\mathbf{J}_u = \mathbf{1}_u \mathbf{1}_u^\top$.

This means that $\mathbf{N}$ is obtained from $\mathbf{A}$, by replacing the -1's in $\mathbf{A}$ by zero and keeping $+1$'s unaltered. Then, it is easy to see that $\mathbf{N}$ is the incidence matrix of a balanced incomplete block design (BIBD) with parameters:

$$v = 4u - 1 = b \; ; \; r = 2u - 1 = k \; ; \; \lambda = u - 1 \tag{1}$$

as presented by Yates, see [28], in his agriculture experiments, where these parameters would stand for v varieties in b blocks of size k, so that each variety occurs exactly r times along the blocks and every pair of varieties concurs in exactly λ blocks, see Raghvarao [19].

Conversely, if $\mathbf{N}$ is the incidence matrix of a BIBD with parameters given by (1), then by replacing the 0's in $\mathbf{N}$ by -1 and bordering the resultant matrix by a row and column of all ones, one gets an Hadamard matrix of order $4u$.

We thus have the following theorem

Theorem 1 *The existence of an Hadamard matrix of order* $4u$ *is equivalent to the existence of a BIBD with parameters given by (1).*

Example 1 Consider an Hadamard matrix $\mathbf{H}_{16}$ which can be obtained by forming the tensor product $\mathbf{H}_4 \otimes \mathbf{H}_4$, where $\mathbf{H}_4$ is as below:

$$\mathbf{H}_4 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}$$

Following the construction method described above, we get a solution of a BIBD with parameters $v = 15 = b, r = 7 = k, \lambda = 3$.

A review of several construction methods to synthesize these matrices was presented by Oliveira [16, 17], namely Paley Matrices, Sylvester Matrices and Kronecker recursive product. We also refer to Stinson [25] and Cameron [4], as well as to the webpage

http://mathworld.wolfram.com/HadamardMatrix.html

for more examples of such matrices.

Now consider the BIBD (7,7,3,3,1) and the BIBD(13,13,4,4,1). If we add a row and a column of 1's, and if we replace all the null entrances in the matrix by (1), we obtain the following Hadamard matrices:

$$\mathbf{H}_7 = \begin{bmatrix} 1 & -1 & -1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 & -1 & 1 & -1 & 1 \\ -1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 \\ -1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

$$\mathbf{H}_{13} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 & -1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 \\ 1 & -1 & -1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 \end{bmatrix}$$

Fig. 1 BIBD (7,7,3,3,1)

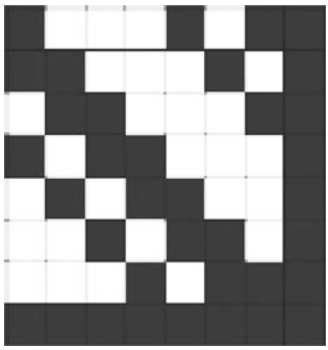
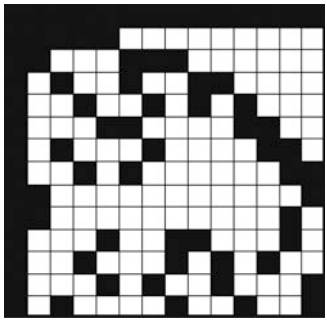


Fig. 2 BIBD (13,13,4,4,1)



Sometimes in the literature Hadamard matrices are represented by a square in black and white, as we can have for our examples. Using this form, in figures, see Figs. 1 and 2, we present Hadamard matrices corresponding to the BIBD(7,7,3,3,1) and BIBD (13,13,4,4,1), from [16, 17].

3 BIBD and R Project for Statistical Computing

As stated before, a BIBD is an arrangement of v treatments (varieties) in b blocks, each of size $k(< v)$, where each variety occurs exactly r times and every pair of varieties concurs in exactly λ blocks. The necessary, but not sufficient conditions for the existence of a BIBD are:

$$\begin{cases} v < b \\ vr = bk \\ \lambda(v-1) = r(k-1) \end{cases}$$

In order to generate BIBD with the aid of the computational statistical program 'R', we can use the extra 'package', 'crossdes'. This 'package' includes several functions that assist in building balanced designs. Each BIBD produced with the aid

of this 'package' has five parameters described above. To install the 'package' the command 'install.packages ("crossdes")' is used. To load the 'package' in order to be able to use the functions contained herein, the command 'library ("crossdes")' is used. The 'find.BIB' function is used to generate a block design with a specific number of treatments, blocks (which correspond to the lines of the generated design) and elements per block (corresponding to the columns of the generated design). It is also possible to use another function to test if the generated design meets the conditions to be a BIBD. For instance, to create a design with five treatments in four blocks of three elements the function is as follows (Fig. 3):

> find.BIB(5, 4, 3)

The corresponding *'R'* output is:

The resulting structure is not a BIBD because the treatments are not all repeated the same number of times. This observation can be confirmed by using the 'isGYD' function as follows: 'isGYD (find.BIB (5, 4, 3))'. The result of executing this function in 'R' is (Fig. 4):

Consider now another example, this time with seven treatments and seven blocks of three elements (Fig. 5):

It is confirmed through the use of the 'isGYD' function that this experimental design is indeed a BIBD:

Another useful 'package' to generate outlines designs for BIBDs is the 'dae'. As the one above, this package has several different functions targeted to aid in

	[,1]	[,2]	[,3]
[1,]	2	3	5
[2,]	1	2	4
[3,]	3	4	5
[4,]	1	3	5

Fig. 3 Output of instruction find.BIB(5,4,3)

```
> isGYD (find.BIB (5, 4, 3) )

[1] The design is neither balanced w. r. t. rows nor w. r. t. columns.
```

Fig. 4 Output of instruction isGYD(find.BIB(5,4,3))

```
> outro . plano = find. BIB (7, 7, 3)
> outro . plano
     [,1] [,2] [,3]
[1,]    1    2    6
[2,]    3    5    6
[3,]    4    6    7
[4,]    2    3    7
[5,]    1    3    4
[6,]    2    4    5
[7,]    1    5    7
```

Fig. 5 Output of instruction find.BIB(7,7,3)

```
> isGYD (find.BIB (7,7,3) )

[1] The design is a balanced incomplete block design w. r. t. rows.
```

Fig. 6 Output of instruction isGYD(find.BIB(7,7,3))

```
> BIBD.unit<-list(Blocks=4, Plots=3)
> BIBD.nest<-list(Plots="Blocks")
> Treats<-factor(c(1,2,3, 1,2,4, 1,3,4, 2,3,4), labels=c("A","B","C","D"))
> BIBD.lay<-fac.layout(unrandomized=BIBD.unit, nested.factors=BIBD.nest, randomized=Treats,  seed=987)
> BIBD.lay

   Units Permutation Blocks Plots Trats
1      1           2      1     1     C
2      2           3      1     2     A
3      3           1      1     3     B
4      4          10      2     1     B
5      5          12      2     2     C
6      6          11      2     3     D
7      7           9      3     1     C
8      8           7      3     2     D
9      9           8      3     3     A
10    10           4      4     1     A
11    11           5      4     2     D
12    12           6      4     3     B

> |
```

Fig. 7 Randomized factors BIBD with 3 treatments and 4 blocks

obtaining experimental designs. The following example illustrates the use of one of the features of "dae", the "fac.layout" to generate an experiment of BIBD consisting of randomized factors (Fig. 6):

A page from CRAN—The Comprehensive R Archive Network—aggregates all the existing information about the various 'packages' related to experimental design with the aid of the 'R'. This page can be found at the url: http://cran.r-project.org/web/views/ExperimentalDesign.html.

This page presents first the general-purpose packages and proceeds with those that perform more specific tasks such as the ones used in the design of experiments for agriculture, industry and clinical trials among others (Fig. 7).

4 Application of Hadamard Matrices to Error Correction

Reed–Muller codes, see Reed [20] and Muller [14], are a family of linear error-correcting codes that were first used in communications.

Special cases of Reed–Muller codes include the Hadamard code, the Walsh–Hadamard code and the Reed–Solomon code, see Wicker and Bhargava [27].

The Hadamard code is an error-correcting code that is used for error detection and correction when transmitting messages over very noisy or unreliable channels. A famous application of the Hadamard code was the NASA space probe Mariner 9 in 1971, where the code was used to transmit photos of Mars.

Generalized Hadamard codes are obtained from an $n \times n$ Hadamard matrix $\mathbf{H}$. In particular, the $2n$ codewords of the code are the rows of $\mathbf{H}$ and the rows of $\mathbf{H}$. To obtain a code over the alphabet $\{0, 1\}$, the mapping $1 \mapsto 1$, $1 \mapsto 0$, or, equivalently, $x \mapsto (1x)/2$, is applied to the matrix elements. That the minimum distance of the code is $n/2$ follows from the defining property of Hadamard matrices, namely that their rows are mutually orthogonal.

To get the punctured Hadamard code with $n = 2^{k-1}$ the chosen Hadamard matrix $\mathbf{H}$ has to be of Sylvester type, see [13], which gives rise to a message length of $\log_2(2n) = k$.

Quick response codes (QR-Codes) contain codewords that are 8 bits long and use the Reed–Solomon error correction algorithm with four different error correction levels. It is well known that higher the error correction level, the less the available storage capacity there is.

The Reed-Solomon algorithm was created by Irving Reed and Gustave Solomon, both engineers at MIT's Lincoln Labs, and their work, see Reed and Solomon [21], led to the extent of and later on used with the creation of the QR code in 1994 for the Japanese automotive industry by Denso Wave, a subsidiary that produces automatic identification products.

Since its debut a long way was overcome and the amount of information that a QR code may store is massive. The four levels of security, that include redundant information, may go up to 30%, allowing the retrieval of information even when the QR code is damaged and thus giving space for error correction.

Below some examples of the relation between QR codes and information capacity (Figs. 8, 9 and 10).

Crossing the level of information redundant and the number of characters, Version 1, will allow 41 characters at his lowest and 17 on its highest level. Version 40 allows 7089 numerical characters.

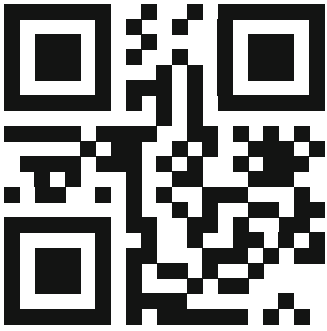


Fig. 8 Version 1, 21×21 blocks

Fig. 9 Version 1, 25 × 25 blocks

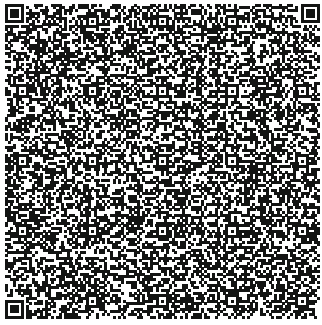


Fig. 10 Version 40, 117 × 117 blocks

Reed-Solomon codes are of the same family of error correcting codes as the Hadamard codes. The rows of a $k \times v$ generating matrix, for a generalized Reed-Solomon code $GR_k(c, 1)$, where $c = (1, c, \ldots, c^{v-1})$ for some $c \in GF(q)$, of order v, are rows of a cocyclic matrix. For $v = p$, an odd prime number, the resulting Reed-Solomon codes are cocyclic Hadamard codes. So Reed-Solomon codes are closely related to Hadamard matrices as well.

5 Biometry

In information technology, biometrics refers technologies to identify human body characteristics, such as fingerprints and iris, see Jain et al. [10]. However, there is a tremendous amount of research that demonstrates biometrics can be easily faked. There are several examples on the Internet on how to make false fingerprints or forge iris images, big companies like Facebook are making efforts to develop both hardware tokens and software-based authentication for their social network. Software code generation like QR Codes seem to offer a preferable solution, rather than biometric recognition, thanks to their mathematical properties, see Gonçalves [7].

Gregg Stefancik, a Facebook engineer has stated in an interview that he would like his company to eventually move away from using passwords, but opposes

Fig. 11 Damaged QR code

the use of biometrics. However biometrics security can be leveraged with a two-factor authentication solution, ensuring that alphanumeric passwords or generated codes enter the authentication steps, see Anongporn [22]. A combination of voice recognition based, for example, on a phrase, along with a generated QR Code is an extremely strong authentication solution, see Lakshmanaswamy et al. [12].

Lumidigm, an ATM manufacturer, is already using this principle on their machines. Their ATMs use biometrics and QR Codes for secure cash withdrawals.

6 Considerations and Remarks

The QR Codes are 2-dimensional bar codes that can be easily read by a device capable of image capture, as is the case of most existing mobile phones. These codes can represent text, an address for a web site (URL), a phone number, a geo-referenced location, an email, a contact or an SMS.

QR codes have, as the base of their error correcting structure, Hadamard matrices. The mathematical properties jointly with the new technological advances allow simple figures to contain and transmit a huge amount of information. The mathematical properties that are intrinsic to these structures will allow great advances for error detection and correction, in huge amounts of information. Potential developments using well-studied properties of randomized block designs, namely with Orthogonal Block Designs, see, e.g., Calinski and Kageyama [2] and Calinski and Kageyama [3], will create a vast spectrum of research (Fig. 11).

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Covariance Matrix Regularization for Banded Toeplitz Structure via Frobenius-Norm Discrepancy

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Abstract In many practical applications, the structure of covariance matrix is often blurred due to random errors, making the estimation of covariance matrix very difficult particularly for high-dimensional data. In this article, we propose a regularization method for finding a possible banded Toeplitz structure for a given covariance matrix A (e.g., sample covariance matrix), which is usually an estimator of the unknown population covariance matrix Σ. We aim to find a matrix, say B, which is of banded Toeplitz structure, such that the Frobenius-norm discrepancy between B and A achieves the smallest in the whole class of banded Toeplitz structure matrices. As a result, the obtained Toeplitz structured matrix B recoveries the underlying structure behind Σ. Our simulation studies show that B is also more accurate than the sample covariance matrix A when estimating the covariance matrix Σ that has a banded Toeplitz structure. The studies also show that the proposed method works very well in regularization of covariance structure.

Keywords Covariance matrix structure · Frobenius norm · Regularization · Toeplitz structure

1 Introduction

Estimation of covariance matrices is important in many application fields including spectroscopy, functional magnetic resonance imaging, text retrieval, gene array, climate study and imaging analysis. This problem has been widely researched in statistics. The traditional "Burg technique", which is to find the maximum likelihood

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estimator of a covariance matrix, needs to provide the sample covariance matrix and pre-specify the structure of the unknown population covariance matrix [3]. However, it is well known that the sample covariance matrix performs poorly for high-dimensional data, where the number of variables is bigger than the sample size [11]. Further, the underlying structure of the sample covariance matrix is usually blurred because of random noises from different sources.

For high-dimensional data, methods of covariance matrix regularization were developed in the literature, including hard-thresholding [2, 9], soft-thresholding and its various generalizations [18], and adaptive thresholding [4], among many others, but threshold estimators may have negative eigenvalues in finite samples. To overcome this difficulty, Rothman proposed a Lasso-type penalty based method to encourage sparsity and used a logarithmic barrier function to enforce the positive-definiteness [17]. Xue et al. [20] considered an alternating direction method to ensure the positive-definiteness of Lasso penalty covariance estimator. However, all such regularization approaches require a tuning parameter, and how to choose an appropriate tuning parameter remains a very challenging problem.

For covariance matrix estimation, it has recently attracted more attention on regularizing an estimated covariance matrix so that the underlying structure becomes clear [14, 16]. Recently, the technique based on entropy loss function aiming to avoid the selection of tuning parameter has been proposed to regularize an estimated covariance matrix into one of the structured covariance matrices: $MA(1)$, CS, $AR(1)$ and banded Toeplitz [12]. However, the technique cannot handle a high-dimensional data set, since the inverse of the sample covariance matrix does not exist. Very recently, the method of regularizing an estimated covariance matrix into the one with structures $MA(1)$, CS, $AR(1)$ and $ARMA(1, 1)$ via Frobenius-norm discrepancy was developed by [6, 7]. Although this method avoids the use of the inverse of the sample covariance matrix, it only considered the above four candidate covariance structures, that is, $MA(1)$, CS, $AR(1)$, $ARMA(1, 1)$. It is well known that banded Toeplitz covariance matrices are very common in practice, in particular, it is commonly used in time series. For example, in signal processes the covariance matrix of Gauss-Markov random process or cyclostationary process often displays a banded Toeplitz structure [5, 13, 19]. On the other hand, all the four structures, i.e., $MA(1)$, CS, $AR(1)$ and $ARMA(1, 1)$, are a special case of banded Toeplitz structures.

In order to study a more general structure, in this paper we consider the regularization problem for covariance matrix with banded Toeplitz structures. The

$m \times m$ covariance matrix is of the form

$$B(\sigma^2, c_1, \cdots, c_p) = \sigma^2 \begin{bmatrix} 1 & c_1 & c_2 & \cdots & c_p & 0 & \cdots & 0 \\ c_1 & 1 & c_1 & \ddots & \ddots & \ddots & \ddots & \vdots \\ c_2 & c_1 & 1 & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & c_p \\ c_p & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & \ddots & 1 & c_1 & c_2 \\ \vdots & \ddots & \ddots & \ddots & \ddots & c_1 & 1 & c_1 \\ 0 & \cdots & 0 & c_p & \cdots & c_2 & c_1 & 1 \end{bmatrix} \tag{1}$$

where $\sigma^2 > 0$, $c_1, c_2, \ldots, c_p$ $(m > p)$ are nonzero and all other off-diagonal elements are zero. Define $q(t) = 1 + 2\sum_{k=1}^{p} c_k \cos(kt)$, then B is positive-definite if and only if $q(t) \geq 0$, $q(t) \not\equiv 0$, for all $t \in R$ [15].

The outline of the paper is as follows. In Sect. 2, we transform the regularization problem into an optimization problem in numerical analysis and explore its general properties. In Sect. 3, we discuss the problem of finding the optimal structure from a class of banded Toeplitz structures, in the sense of minimizing the square of the Frobenius-norm discrepancy. In Sect. 4, we conduct simulation studies to measure the performance and effectiveness of the proposed approach. In Sect. 5, a brief discussion is provided.

2 Problem of Interest

In order to transform the regularization problem into an optimization problem, we suppose A is an available $m \times m$ estimator of a covariance matrix, for example, the sample covariance matrix. Note that it may also be one of those obtained by using SQRT-Lasso [1], matrix-logarithm transformation [8] and thresholding principal orthogonal complements [10] among many others. Let Ω be the set of all $m \times m$ positive definite covariance matrices with banded Toeplitz structure. A discrepancy between the given covariance matrix A and the set Ω is defined by

$$D(A, \Omega) := \min_{B \in \Omega} L(A, B), \tag{2}$$

where $L(A, B)$ is a measure of the distance between the two $m \times m$ matrices A and B, defined by the square of the Frobenius-norm. In other words,

$$L(A, B) := \mathrm{tr}((A - B)^T (A - B)). \tag{3}$$

Note that $f(B) := L(A, B) = \text{tr}((A-B)^T(A-B))$ is a strictly convex function of B [7]. Also, the set Ω is obviously convex. Since Ω is the set of all positive definite matrices having a banded Toeplitz structure, the optimization problem in (2) is convex and so it has a unique solution.

The idea is that, in this set Ω, the matrix B which satisfies the above equality can be considered as the regularized version of A. In other words, the matrix B with a banded Toeplitz structure is considered to have the underlying structure of Ω.

We remark that the matrix A does not require a non-singularity, meaning that it applies to the case when the matrix A is singular, for example, A is the sample covariance matrix for high-dimensional data. In other words, even if the given covariance matrix A is singular, we can find a covariance matrix B which has a nonsingular banded Toeplitz structure, such that the F-norm discrepancy function $L(A, B)$ achieves its smallest among the class of banded Toeplitz matrices.

3 Solution of Problem

The matrix B in (1) can be rewritten as

$$B(\sigma^2, c_1, \cdots, c_p) = \sigma^2(I + \sum_{i=1}^{p} c_i T_i),$$

where T_i is a symmetric matrix with ones on the ith superdiagonal and subdiagonal and zeros elsewhere.

The discrepancy function in (3) is now

$$f(\sigma^2, c_1, \cdots, c_p) = \text{tr}(AA^T) + \sigma^4(m + 2\sum_{i=1}^{p}(m-i)c_i^2) - 2\sigma^2(\text{tr}(A) + \sum_{i=1}^{p} c_i \text{tr}(AT_i)).$$

It follows that

$$\nabla f := \begin{bmatrix} \frac{\partial f}{\partial(\sigma^2)} \\ \frac{\partial f}{\partial c_1} \\ \vdots \\ \frac{\partial f}{\partial c_p} \end{bmatrix} = \begin{bmatrix} 2\sigma^2(m + 2\sum_{i=1}^{p}(m-i)c_i^2) - 2(\text{tr}(A) + \sum_{i=1}^{p} c_i \text{tr}(AT_i)) \\ 4\sigma^4(m-1)c_1 - 2\sigma^2 \text{tr}(AT_1) \\ \vdots \\ 4\sigma^4(m-p)c_p - 2\sigma^2 \text{tr}(AT_p) \end{bmatrix},$$

and

$$\nabla^2 f := \begin{bmatrix} \frac{\partial^2 f}{\partial(\sigma^2)^2} & \frac{\partial^2 f}{\partial(\sigma^2)\partial c_1} & \cdots & \frac{\partial^2 f}{\partial(\sigma^2)\partial c_p} \\ \frac{\partial^2 f}{\partial c_1 \partial(\sigma^2)} & \frac{\partial^2 f}{\partial c_1^2} & \cdots & \frac{\partial^2 f}{\partial c_1 \partial c_p} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{\partial^2 f}{\partial c_p \partial(\sigma^2)} & \frac{\partial^2 f}{\partial c_p \partial c_1} & \cdots & \frac{\partial^2 f}{\partial c_p^2} \end{bmatrix}$$

$$= \begin{bmatrix} 2m + 4\sum_{i=1}^{p}(m-i)c_i^2 & 8\sigma^2(m-1)c_1 - 2\mathrm{tr}(AT_1) & \cdots & 8\sigma^2(m-p)c_p - 2\mathrm{tr}(AT_p) \\ 8\sigma^2(m-1)c_1 - 2\mathrm{tr}(AT_1) & 4\sigma^4(m-1) & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 8\sigma^2(m-p)c_p - 2\mathrm{tr}(AT_p) & 0 & \cdots & 4\sigma^4(m-p) \end{bmatrix}.$$

Hence the stationary points $(\sigma^2, c_1, \cdots, c_p)$ must satisfy the following equations:

$$\begin{cases} m\sigma^2 + 2\sigma^2 \sum_{i=1}^{p}(m-i)c_i^2 - \mathrm{tr}(A) - \sum_{i=1}^{p} c_i \mathrm{tr}(AT_i) = 0 \\ 2\sigma^2(m-1)c_1 - \mathrm{tr}(AT_1) = 0 \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ 2\sigma^2(m-p)c_p - \mathrm{tr}(AT_p) = 0. \end{cases} \tag{4}$$

Thus a unique stationary point is

$$\begin{cases} \sigma^2 = \dfrac{\mathrm{tr}(A)}{m} \\ c_1 = \dfrac{m\mathrm{tr}(AT_1)}{2(m-1)\mathrm{tr}(A)} \\ \cdots\cdots\cdots\cdots\cdots \\ c_p = \dfrac{m\mathrm{tr}(AT_p)}{2(m-p)\mathrm{tr}(A)}. \end{cases} \tag{5}$$

Since

$$\nabla^2 f|_{(\sigma^2, c_1, \cdots, c_p)} := \begin{bmatrix} 2m + 4\sum_{i=1}^{p}(m-i)c_i^2 & 4\sigma^2(m-1)c_1 & \cdots & 4\sigma^2(m-p)c_p \\ 4\sigma^2(m-1)c_1 & 4\sigma^4(m-1) & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 4\sigma^2(m-p)c_p & 0 & \cdots & 4\sigma^4(m-p) \end{bmatrix},$$

the $k \times k$ leading principal minor of matrix $\nabla^2 f|_{(\sigma^2, c_1, \cdots, c_p)}$ is given by

$$W_k = \begin{cases} 2m + 4\sum_{i=1}^{p}(m-i)c_i^2 & k = 1 \\ (2m + 4\sum_{i=k}^{p}(m-i)c_i^2)\prod_{i=1}^{k-1} 4\sigma^4(m-i) & k = 2, \cdots, p \\ 2m\prod_{i=1}^{p} 4\sigma^4(m-i) & k = p+1. \end{cases}$$

Recalling that $\sigma^2 > 0$, $p \leq m-1$, $c_1, c_2, \ldots, c_p$ are nonzero, we have $W_k > 0$. The Hessian matrix $\nabla^2 f|_{(\sigma^2, c_1, \cdots, c_p)}$ is then positive definite, so that its stationary point is really a minimum point. This point, however, may be a local minima of $f(B)$. It is well-known that if the function is convex then the local minimum is actually the global minimum, but it is difficult to check if $f(B)$ is convex with respect to $(c_1, \cdots, c_p)$ here due to its complexity. We suggest to compare the function values at all the local minima so that the global minimum can be achieved.

We summarize the discussion above in the following theorem.

Theorem 1 *For a given estimator A of an $m \times m$ covariance matrix, define $f(B) := L(A, B)$ where B is a positive definite covariance matrix with a banded Toeplitz structure. Then the local or global minimum of $f(B)$ can be achieved as the solution of (5).*

4 Simulation Studies

To check the actual performance of the proposed regularization method, we carry out intensive simulation studies in this section. All the calculations are done using MATLAB R2012b, and we apply `fzero` and `fsolve` to find roots.

In the process of the simulation, we first generate an $m \times m$ covariance matrix Σ which has one of the following structures: order-1 moving average structure ($MA(1)$), compound symmetry structure (CS), order-1 autoregressive structure ($AR(1)$), order-1 autoregressive moving average structure ($ARMA(1, 1)$), cf. [6, 7], and a banded Toeplitz structure. We assume an m dimensional zero mean vector $\mu = \mathbf{0}$. We take a random sample of size n from multivariate normal distribution $N_m(\mathbf{0}, \Sigma)$ and then calculate the sample covariance matrix A. In the end, we find matrix B which has a banded Toeplitz structure mentioned above, achieving the minimum of the Frobenius-norm.

We need to state the following facts.

1. We only need to find the desired matrix among the ones which have the same structure as the correct covariance structure, because for the cases of $MA(1)$,

CS, $AR(1)$ or $ARMA(1, 1)$ [6, 7] already showed that the matrix B that has the minimum F-norm remains the same structure as the true covariance matrix.

2. Since the function $L(A, B)$ measures the absolute difference between matrices A and B, it can make the value of $L(A, B)$ too large. To reduce the influence of the dimension of covariance matrix and its elements on $L(A, B)$, we re-define the following function to replace $L(A, B)$

$$L^*(A, B) := \text{tr}((A - B)^T (A - B))/\text{tr}(A^T A), \tag{6}$$

which does not affect the finding of the optimal matrix B.

We will use the following notations:

- Σ: the true covariance matrix being tested;
- A: the covariance matrix obtained from sample;
- B: the matrix which minimizes $L^*(A, B)$ and has a structure of $MA(1)$, CS, $AR(1)$, $ARMA(1, 1)$ or banded Toeplitz;
- $L^*_{\Sigma,A}$, $L^*_{A,B}$ and $L^*_{\Sigma,B}$: the difference functions $L^*(\Sigma, A)$, $L^*(A, B)$ and $L^*(\Sigma, B)$, respectively.

For Σ having $MA(1)$, CS or $AR(1)$ structure, we set the sample size $n = 100$, matrix dimension $m = 10, 20, 50, 100, 200, 500, 1000$, $\sigma^2 = 0.5, 1, 2, 4$, parameter $c = 0.25, 0.5, 0.75$. For Σ having $ARMA(1, 1)$ structure, in addition to the above values, we set $r = 0.1, 0.35, 0.6$ when $c = 0.25$; $r = 0.2, 0.45, 0.75$ when $c = 0.5$; and $r = 0.25, 0.5, 0.8$ when $c = 0.75$.

We apply the method proposed in [6, 7] to find the matrix B which has $MA(1)$, CS, $AR(1)$ or $ARMA(1, 1)$ structure and has the minimum F-norm difference. We also apply the method proposed in this paper for the case when the matrix has a banded Toeplitz structure with $p = m - 1$.

Tables 1, 2, 3 and 4 give the average results for 100 run simulations. In each of those tables, the first column provides the structure of the true covariance matrix Σ, the second column presents the F-norm difference between the sample covariance matrix A and Σ; the third and fourth columns give the F-norm differences between B and A, Σ, respectively, where B is obtained by using the same structure as Σ; the fifth and sixth columns provide the F-norm differences between B and A, Σ, respectively, where B is obtained by assuming a banded Toeplitz structure.

To save space, in Tables 1, 2, 3 and 4 we only report simulation results for $m = 50, 100, 500$ and 1000 with $c = 0.5$. Other numerical results can be provided through contacting the corresponding author (J. Pan) but they are very similar to these reported here. From these tables, we can draw the following observations.

1. For the matrix B obtained by using either the same structure as Σ or a banded Toeplitz structure, the F-norm discrepancy between B and the real covariance matrix Σ is very small. It implies that the resulting covariance matrices have the same structure, and the minor difference is mainly due to random errors and computing errors.

Table 1 Simulation results with $m = 50$; $c = 0.5$

		B			
		Same structure		Toeplitz	
Σ	$L^*_{\Sigma,A}$	$L^*_{A,B}$	$L^*_{\Sigma,B}$	$L^*_{A,B}$	$L^*_{\Sigma,B}$
$\sigma^2 = 0.50$					
MA(1)	0.2584	0.2577	0.0006	0.2438	0.0146
CS	0.0500	0.0284	0.0216	0.0278	0.0222
AR(1)	0.2399	0.2383	0.0016	0.2247	0.0152
ARMA-r = 0.2	0.3184	0.3173	0.0012	0.3053	0.0131
ARMA-r = 0.45	0.2539	0.2524	0.0016	0.2397	0.0143
ARMA-r = 0.75	0.1772	0.1749	0.0023	0.1607	0.0165
$\sigma^2 = 1$					
MA(1)	0.2590	0.2582	0.0007	0.2436	0.0154
CS	0.0528	0.0284	0.0243	0.0278	0.0250
AR(1)	0.2406	0.2390	0.0016	0.2257	0.0149
ARMA-r = 0.2	0.3187	0.3176	0.0012	0.3056	0.0132
ARMA-r = 0.45	0.2553	0.2538	0.0016	0.2402	0.0151
ARMA-r = 0.75	0.1785	0.1765	0.0020	0.1628	0.0157
$\sigma^2 = 2$					
MA(1)	0.2591	0.2585	0.0006	0.2440	0.0151
CS	0.0430	0.0282	0.0148	0.0277	0.0153
AR(1)	0.2395	0.2375	0.0020	0.2242	0.0153
ARMA-r = 0.2	0.3185	0.3173	0.0012	0.3045	0.0140
ARMA-r = 0.45	0.2534	0.2512	0.0022	0.2386	0.0148
ARMA-r = 0.75	0.1772	0.1746	0.0026	0.1605	0.0167
$\sigma^2 = 4$					
MA(1)	0.2593	0.2587	0.0006	0.2449	0.0144
CS	0.0451	0.0284	0.0167	0.0278	0.0173
AR(1)	0.2426	0.2409	0.0017	0.2273	0.0153
ARMA-r = 0.2	0.3195	0.3182	0.0013	0.3053	0.0142
ARMA-r = 0.45	0.2544	0.2523	0.0020	0.2392	0.0151
ARMA-r = 0.75	0.1771	0.1744	0.0027	0.1607	0.0164

2. There is no doubt that the matrix B obtained using a banded Toeplitz structure has a smaller F-norm difference than those using $MA(1)$, CS, $AR(1)$ or $ARMA(1, 1)$ structures. This is because all those four cases are special cases of banded Toeplitz structures. The bigger the definition area, the smaller the optimal function value. However, the difference in their F-norms is rather small, implying that the identified Toeplitz structure actually reduces to one of the special structures.
3. The F-norm discrepancy between B obtained from our proposed method and the true covariance matrix Σ is smaller than the F-norm discrepancy between A and

Table 2 Simulation results with $m = 100$; $c = 0.5$

		B			
		Same structure		Toeplitz	
Σ	$L^*_{\Sigma,A}$	$L^*_{A,B}$	$L^*_{\Sigma,B}$	$L^*_{A,B}$	$L^*_{\Sigma,B}$
$\sigma^2 = 0.50$					
MA(1)	0.4069	0.4067	0.0002	0.3949	0.0120
CS	0.0521	0.0296	0.0225	0.0293	0.0229
AR(1)	0.3832	0.3825	0.0007	0.3711	0.0121
ARMA-r = 0.2	0.4793	0.4789	0.0004	0.4688	0.0105
ARMA-r = 0.45	0.4000	0.3993	0.0008	0.3882	0.0118
ARMA-r = 0.75	0.2945	0.2936	0.0009	0.2808	0.0136
$\sigma^2 = 1$					
MA(1)	0.4074	0.4072	0.0002	0.3960	0.0114
CS	0.0459	0.0297	0.0162	0.0293	0.0165
AR(1)	0.3825	0.3817	0.0007	0.3698	0.0127
ARMA-r = 0.2	0.4810	0.4805	0.0005	0.4705	0.0105
ARMA-r = 0.45	0.4003	0.3997	0.0006	0.3878	0.0125
ARMA-r = 0.75	0.2956	0.2945	0.0011	0.2814	0.0141
$\sigma^2 = 2$					
MA(1)	0.4067	0.4064	0.0002	0.3942	0.0125
CS	0.0512	0.0291	0.0221	0.0288	0.0224
AR(1)	0.3822	0.3816	0.0006	0.3699	0.0123
ARMA-r = 0.2	0.4804	0.4799	0.0005	0.4699	0.0105
ARMA-r = 0.45	0.4006	0.4000	0.0007	0.3887	0.0120
ARMA-r = 0.75	0.2937	0.2928	0.0009	0.2797	0.0139
$\sigma^2 = 4$					
MA(1)	0.4062	0.4059	0.0003	0.3946	0.0116
CS	0.0512	0.0284	0.0228	0.0281	0.0231
AR(1)	0.3823	0.3818	0.0005	0.3701	0.0122
ARMA-r = 0.2	0.4803	0.4798	0.0005	0.4695	0.0108
ARMA-r = 0.45	0.4011	0.4002	0.0009	0.3884	0.0126
ARMA-r = 0.75	0.2928	0.2919	0.0009	0.2792	0.0136

Σ. It implies that the proposed method reduces random noises, so that a better estimator of the covariance matrix is obtained.

Since the real covariance matrix Σ is unknown in practice, the F-norm discrepancy between B and the sample covariance matrix A becomes very important in finding the underlying structure of Σ.

For Σ having a banded Toeplitz structure, apart from the above values of n, m, σ^2 we actually randomly generate parameters $c_1, c_2, \cdots, c_p$ from uniform distribution $U(0, 1)$ but require the positive definiteness of covariance matrix Σ, where we choose $p = m - 1$. The results are presented in Table 5, where similarly each value is the average after repeating 100 times of simulations. The first column gives

Table 3 Simulation results with $m = 500$; $c = 0.5$

		B			
		Same structure		Toeplitz	
Σ	$L^*_{\Sigma,A}$	$L^*_{A,B}$	$L^*_{\Sigma,B}$	$L^*_{A,B}$	$L^*_{\Sigma,B}$
$\sigma^2 = 0.50$					
MA(1)	0.7716	0.7716	0.0000	0.7670	0.0047
CS	0.0493	0.0307	0.0186	0.0306	0.0187
AR(1)	0.7527	0.7526	0.0001	0.7476	0.0050
ARMA-r = 0.2	0.8206	0.8206	0.0000	0.8170	0.0036
ARMA-r = 0.45	0.7669	0.7668	0.0001	0.7622	0.0046
ARMA-r = 0.75	0.6702	0.6701	0.0001	0.6637	0.0065
$\sigma^2 = 1$					
MA(1)	0.7719	0.7719	0.0000	0.7674	0.0046
CS	0.0596	0.0303	0.0293	0.0302	0.0294
AR(1)	0.7523	0.7523	0.0000	0.7473	0.0050
ARMA-r = 0.2	0.8208	0.8208	0.0000	0.8172	0.0036
ARMA-r = 0.45	0.7673	0.7672	0.0001	0.7626	0.0047
ARMA-r = 0.75	0.6699	0.6699	0.0001	0.6633	0.0067
$\sigma^2 = 2$					
MA(1)	0.7716	0.7715	0.0000	0.7670	0.0045
CS	0.0543	0.0306	0.0237	0.0305	0.0238
AR(1)	0.7530	0.7529	0.0001	0.7480	0.0050
ARMA-r = 0.2	0.8204	0.8204	0.0000	0.8168	0.0036
ARMA-r = 0.45	0.7671	0.7670	0.0000	0.7624	0.0047
ARMA-r = 0.75	0.6705	0.6704	0.0001	0.6639	0.0066
$\sigma^2 = 4$					
MA(1)	0.7717	0.7717	0.0000	0.7671	0.0045
CS	0.0547	0.0304	0.0244	0.0303	0.0244
AR(1)	0.7529	0.7529	0.0001	0.7479	0.0050
ARMA-r = 0.2	0.8208	0.8207	0.0000	0.8171	0.0036
ARMA-r = 0.45	0.7669	0.7669	0.0000	0.7623	0.0047
ARMA-r = 0.75	0.6701	0.6700	0.0001	0.6635	0.0066

the dimension of the true covariance matrix Σ, the second column provides the F-norm discrepancy between the sample covariance matrix A and Σ, the rest columns present the F-norm discrepancy between A, Σ and the matrix B obtained using the specified structures indicated in the second line, respectively.

Form Table 5 we make conclusions below.

1. The matrix B having the minimum F-norm difference satisfies $L^*(\Sigma, B) < L^*(\Sigma, A)$, meaning that the estimator B obtained using the proposed regularization method removes the random noise in the sample covariance matrix A, so that a better estimator of the covariance matrix Σ is obtained.

Table 4 Simulation results with $m = 1000$; $c = 0.5$

		B			
		Same structure		Toeplitz	
Σ	$L^*_{\Sigma,A}$	$L^*_{A,B}$	$L^*_{\Sigma,B}$	$L^*_{A,B}$	$L^*_{\Sigma,B}$
$\sigma^2 = 0.50$					
MA(1)	0.8709	0.8709	0.0000	0.8683	0.0026
CS	0.0525	0.0308	0.0217	0.0308	0.0217
AR(1)	0.8587	0.8586	0.0000	0.8558	0.0028
ARMA-r = 0.2	0.9014	0.9014	0.0000	0.8994	0.0020
ARMA-r = 0.45	0.8678	0.8678	0.0000	0.8651	0.0027
ARMA-r = 0.75	0.8022	0.8022	0.0000	0.7983	0.0039
$\sigma^2 = 1$					
MA(1)	0.8709	0.8709	0.0000	0.8683	0.0026
CS	0.0550	0.0306	0.0244	0.0306	0.0245
AR(1)	0.8586	0.8586	0.0000	0.8558	0.0029
ARMA-r = 0.2	0.9014	0.9014	0.0000	0.8994	0.0020
ARMA-r = 0.45	0.8680	0.8680	0.0000	0.8654	0.0026
ARMA-r = 0.75	0.8020	0.8020	0.0000	0.7980	0.0040
$\sigma^2 = 2$					
MA(1)	0.8709	0.8709	0.0000	0.8683	0.0026
CS	0.0525	0.0302	0.0223	0.0301	0.0224
AR(1)	0.8586	0.8586	0.0000	0.8557	0.0029
ARMA-r = 0.2	0.9013	0.9013	0.0000	0.8993	0.0020
ARMA-r = 0.45	0.8678	0.8678	0.0000	0.8652	0.0026
ARMA-r = 0.75	0.8018	0.8018	0.0000	0.7978	0.0040
$\sigma^2 = 4$					
MA(1)	0.8709	0.8709	0.0000	0.8683	0.0026
CS	0.0555	0.0309	0.0245	0.0309	0.0245
AR(1)	0.8585	0.8585	0.0000	0.8557	0.0028
ARMA-r = 0.2	0.9013	0.9013	0.0000	0.8993	0.0020
ARMA-r = 0.45	0.8679	0.8679	0.0000	0.8652	0.0027
ARMA-r = 0.75	0.8021	0.8020	0.0000	0.7981	0.0040

2. The matrix B having the minimum F-norm difference and obtained by using a banded Toeplitz structure has a small value of $L^*(\Sigma, B)$. Hence, we can really find the structure of the true covariance matrix Σ through B which uses the information of the sample covariance matrix A.

It is worth noting that conclusions made in this section are valid for all the studied structures of Σ and all the settings of parameters $n, m, \sigma^2, c, r, c_1, c_2, \cdots, c_p$. Thus, the proposed method is reliable in this sense. Especially, the proposed regularization method works very well even for high-dimensional covariance matrix, where we considered the cases for the sample size $n = 100$ and the dimension of the covariance matrix $m = 100, 200, 500$ and 1000, respectively.

Table 5 Simulation results with Toeplitz structure

		B									
		MA(1)		CS		AR(1)		ARMA(1,1)		Toeplitz	
	$L^*_{\Sigma,A}$	$L^*_{A,B}$	$L^*_{\Sigma,B}$	$L^*_{A,B}$	$L^*_{\Sigma,B}$	$L^*_{A,B}$	$L^*_{\Sigma,B}$	$L^*_{A,B}$	$L^*_{\Sigma,B}$	$L^*_{A,B}$	$L^*_{\Sigma,B}$
$\sigma^2 = 0.50$											
$m = 10$	0.0775	0.2049	0.1431	0.1262	0.0695	0.1202	0.0624	0.0820	0.0281	0.0581	0.0194
$m = 20$	0.1329	0.2685	0.1523	0.2177	0.0990	0.1837	0.0691	0.1336	0.0181	0.1154	0.0175
$m = 50$	0.2693	0.3637	0.0960	0.3856	0.1248	0.3192	0.0533	0.2871	0.0271	0.2541	0.0152
$m = 100$	0.4876	0.5106	0.0237	0.5015	0.0166	0.5087	0.0218	0.5128	0.0251	0.4774	0.0102
$m = 200$	0.6569	0.6703	0.0136	0.6668	0.0108	0.6695	0.0129	0.6722	0.0155	0.6500	0.0069
$m = 500$	0.8319	0.8352	0.0034	0.8336	0.0019	0.8352	0.0033	0.8355	0.0037	0.8305	0.0014
$m = 1000$	0.9091	0.9100	0.0009	0.9095	0.0005	0.9100	0.0009	0.9101	0.0009	0.9090	0.0001
$\sigma^2 = 1$											
$m = 10$	0.0852	0.1848	0.1169	0.1011	0.0413	0.1365	0.0768	0.1246	0.0711	0.0635	0.0218
$m = 20$	0.1564	0.2366	0.0827	0.1801	0.0323	0.2253	0.0741	0.2622	0.1067	0.1400	0.0164
$m = 50$	0.3097	0.3684	0.0618	0.3398	0.0338	0.3611	0.0553	0.3852	0.0780	0.2959	0.0138
$m = 100$	0.4943	0.5120	0.0176	0.5122	0.0194	0.5115	0.0171	0.5152	0.0209	0.4843	0.0100
$m = 200$	0.6598	0.6701	0.0102	0.6672	0.0077	0.6696	0.0098	0.6715	0.0115	0.6528	0.0069
$m = 500$	0.8320	0.8346	0.0027	0.8338	0.0020	0.8345	0.0026	0.8352	0.0033	0.8306	0.0014
$m = 1000$	0.9089	0.9099	0.0010	0.9096	0.0007	0.9099	0.0010	0.9101	0.0012	0.9087	0.0002
$\sigma^2 = 2$											
$m = 10$	0.0908	0.1445	0.0683	0.0956	0.0230	0.1282	0.0557	0.1563	0.0817	0.0714	0.0194
$m = 20$	0.1488	0.2081	0.0651	0.2195	0.0818	0.1741	0.0333	0.1522	0.0153	0.1418	0.0070
$m = 50$	0.3208	0.3557	0.0375	0.3399	0.0235	0.3521	0.0342	0.3622	0.0427	0.3068	0.0140
$m = 100$	0.4923	0.5115	0.0193	0.5094	0.0189	0.5110	0.0188	0.5152	0.0229	0.4820	0.0103
$m = 200$	0.6631	0.6727	0.0096	0.6759	0.0135	0.6726	0.0096	0.6733	0.0103	0.6563	0.0068
$m = 500$	0.8310	0.8352	0.0043	0.8337	0.0029	0.8351	0.0043	0.8357	0.0049	0.8296	0.0014
$m = 1000$	0.9088	0.9099	0.0010	0.9095	0.0008	0.9099	0.0010	0.9101	0.0012	0.9084	0.0004

$\sigma^2 = 4$											
$m = 10$	0.0664	0.2742	0.2150	0.1093	0.0656	0.1233	0.0828	0.0684	0.0268	0.0492	0.0172
$m = 20$	0.1540	0.2462	0.0960	0.1886	0.0462	0.2239	0.0765	0.2807	0.1302	0.1368	0.0172
$m = 50$	0.3098	0.3743	0.0653	0.3392	0.0346	0.3686	0.0599	0.3915	0.0831	0.2962	0.0137
$m = 100$	0.4889	0.5151	0.0291	0.4994	0.0122	0.5144	0.0284	0.5189	0.0329	0.4783	0.0107
$m = 200$	0.6636	0.6728	0.0095	0.6764	0.0133	0.6728	0.0095	0.6734	0.0102	0.6569	0.0067
$m = 500$	0.8319	0.8350	0.0032	0.8339	0.0021	0.8350	0.0031	0.8354	0.0036	0.8305	0.0014
$m = 1000$	0.9089	0.9100	0.0011	0.9095	0.0007	0.9100	0.0011	0.9101	0.0012	0.9085	0.0004

5 Discussion

For an estimator A of the covariance matrix Σ, we propose a new regularization method to find the matrix B that has a banded Toeplitz structure. By doing so, we not only find the structure of Σ but also a better estimator B in the sense of F-norm difference function. The method reveals the underlying covariance/correlation structure of the random process, and also reduces random noises.

We choose the sample covariance matrix A as the estimator of Σ in the simulations. Actually, we do not always have to choose the sample covariance matrix. Theoretically, the matrix A can be taken as any other reasonable estimators obtained using certain statistical method. Once matrix A is obtained, we can always do the regularization using the proposed method, so that the estimation can be improved in the sense of F-norm difference. Note that there is no strict condition imposed to the symmetric matrix A, which may be singular and/or high-dimensional. Also, the distribution of data which formulates the estimator A might be unknown. Hence the proposed method is more flexible in this sense.

Our simulation studies only considered the data having Gaussian distribution and the paper only studied the F-norm discrepancy. In practice, there are other distributions and other loss functions such as quadratic loss function. The study of such issues may be challenging but important. We will investigate this in our follow-up work.

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Penalized Relative Error Estimation of a Partially Functional Linear Multiplicative Model

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Abstract Functional data become increasingly popular with the rapid technological development in data collection and storage. In this study, we consider both scalar and functional predictors for a positive scalar response under the partially linear multiplicative model. A loss function based on the relative errors is adopted, which provides a useful alternative to the classic methods such as the least squares. Penalization is used to detect the true structure of the model. The proposed method can not only identify the significant scalar variables but also select the basis functions (on which the functional variable is projected) that contribute the response. Both estimation and selection consistency properties are rigorously established. Simulation is conducted to investigate the finite sample performance of the proposed method. We analyze the Tecator data to demonstrate application of the proposed method.

Keywords Functional data · Partially linear · Multiplicative model · Penalized strategies · Prediction · Simulation

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1 Introduction

With rapid technological development in data collection and storage, functional data are commonly encountered with a dense sampling of observations over time and space. Recently popularized wearable devices generate functional data where tracking data are collected in continuous time. In signal processing and spectral analysis, data that take the form of curves and images are of a functional nature. In classical longitudinal studies, data that are measured at a dense grid can be considered as functional. Regression models with functional explanatory variables have been extensively studied over the past two decades. The most popular one is the functional linear model. Later extensions include the generalized functional linear model, functional quadratic model, single-index functional regression model, and others. We refer to [13] and references therein for a more comprehensive review of the field.

In many applications, the response variable is positive, such as life time data which are particularly common in economic and biomedical studies. Zhang et al. [17] proposed a functional multiplicative model to study the scalar response with functional predictors. As also noted by many researches concerning scalar predictors [2, 3, 16], the multiplicative model is useful and more flexible in analyzing data with positive responses. In practice, a response is related to not only functional variables but also scalar variables. Therefore, a model that considers both types of predictors is more general and more widely applicable.

Let $Y \in \mathbb{R}^+$ be the positive scalar response of interest, $Z \in \mathbb{R}^q$ be the q-dimensional scalar variables, and X be a non-stationary smooth random function in $L_2(T)$ on a finite domain T with a smooth mean function $\mu_X(s) = \mathrm{E}X(s)$. In this study, we consider the partially functional linear multiplicative model

$$Y = \exp\left(Z^\top \theta + \int_T \gamma(t) X^c(t) dt\right) \varepsilon, \tag{1}$$

where $X^c(s) = X(s) - \mu_X(s)$, $\theta \in \mathbb{R}^q$ is the regression parameter vector, $\gamma(t)$ is the smooth and square integrable regression function, and ε is the random error with $P(\varepsilon > 0) = 1$. By taking a logarithmic transformation, model (1) reduces to the partially functional linear model, which has been studied by [7, 12] and others.

For estimation, absolute errors are the most popular choices for defining loss functions, such as the least squares. In some scenarios, loss functions based on relative errors may be more appropriate and provide a useful alternative to the absolute error-based criteria in general [14, 17]. Relative errors have been proposed and studied in literature. There are two types of relative errors, relative to target Y and relative to the prediction of Y. Narula and Wellington [10] and Park and Stefanski [11] developed the relative error criteria with respect to target for statistical inference in linear models and non-linear models. Chen et al. [2] showed that this relative error could be inappropriate in some cases and proposed the least absolute relative errors criterion (LARE) using both types of relative errors for the linear

multiplicative model. Consistency and asymptotic normality of the LARE estimator have been well established. In addition, the LARE criterion is scale free, which plays a particularly important role in applying this criterion to certain types of data. We refer to [3, 16] for its extensions.

In the analysis of functional data, variable selection has been commonly conducted. Inclusion of many irrelevant variables in the regression model may compromise estimation and prediction accuracy, as well as model interpretability. Variable selection identifies variables that are truly associated with the response and usually leads to a sparser model. Penalization is a popular technique for variable selection. A penalization approach considers the objective function

$$Q(\beta; \lambda) = L(\beta) + \lambda\rho(\beta), \tag{2}$$

where $L(\beta)$ is the loss function, $\rho(\beta)$ is the penalty function, and $\lambda(>0)$ is a data-dependent tuning parameter that controls the amount of penalization. A large number of penalty functions have been developed, including Lasso (and its variants such as adaptive Lasso), MCP, SCAD, and many others. We refer to [1] and others for detailed discussions on penalization methods.

In this study, we consider the modeling of a positive scalar response variable with both scalar and functional predictors under the partially linear multiplicative model. Working with both types of predictors makes the proposed method more general and more widely applicable in practice. The multiplicative model can be more flexible for a positive response variable. We propose a penalized relative errors criterion based on LARE to estimate the parametric vector θ and regression function $\gamma(t)$ in model (1). The relative error approach offers a useful alternative to the classic methods such as the least squares. The built-in variable selection functionality allows the proposed method to handle a relatively high dimensional scenario and identify variables that contribute to the response variable. To the best of our knowledge, there is a lack of study simultaneously examining the relative error-based criterion and variable selection under the functional data settings. The proposed method is theoretically grounded. Both estimation and selection consistency properties are rigorously established. It is notable that the proposed method can not only identify the significant scalar covariates but also select the basis functions that contribute to the response.

The rest of this article is organized as follows. In Sect. 2, we propose the penalization method for estimation and establish the theoretical properties, following a presentation of data and model. In Sect. 3, we conduct simulation to evaluate the finite sample performance of the proposed method. In Sect. 4, we apply the proposed method to the Tecator data. The article concludes with discussion in Sect. 5. Proofs are provided in Appendix.

2 Method

2.1 Model

Suppose that we have n independent and identically distributed observations $\{(X_1, Z_1, Y_1), \ldots, (X_n, Z_n, Y_n)\}$. For $s_1, s_2 \in T$, let $G_X(s_1, s_2) = \mathrm{Cov}(X_i(s_1), X_i(s_2))$ be the covariance function. With the Karhunen-Loève expansion,

$$X_i(s) = \mu_X(s) + \sum_{j=1}^{\infty} \eta_{ij}\phi_j(s),$$

where $\{\phi_j(s), j = 1, 2, \cdots\}$ are orthogonal eigenfunctions of $G_X(s_1, s_2)$ with corresponding non-increasing eigenvalues $\{\nu_j, j = 1, 2, \cdots\}$, and scores η_{ij} are uncorrelated random variables with mean $\mathrm{E}(\eta_{ij}) = 0$ and variance $\mathrm{Var}(\eta_{ij}) = \nu_j$. Since $\{\phi_j(s), j = 1, 2, \cdots\}$ defines a complete basis, $\gamma(t)$ can be represented as

$$\gamma(t) = \sum_{j=1}^{\infty} \beta_j\phi_j(t),$$

with $\sum_j \beta_j < \infty$. Applying the orthogonality property of eigenfunctions, we have that model (1) can be alternatively expressed as

$$Y_i = \exp(Z_i^\top\theta + \sum_{j=1}^{\infty} \eta_{ij}\beta_j)\varepsilon_i. \tag{3}$$

Truncating with a positive number K, we obtain a truncated basis representation of the functional predictor as

$$\beta = (\beta_1, \beta_2, \cdots, \beta_K)^\top, \quad U_i = (\eta_{i1}, \eta_{i2} \cdots, \eta_{iK})^\top.$$

Then model (3) reduces to

$$Y_i = \exp(Z_i^\top\theta + U_i^\top\beta)\tilde{\varepsilon}_i, \tag{4}$$

where $\tilde{\varepsilon}_i = \exp\left(\sum_{j=K+1}^{\infty} b_j\eta_{ij}\right)\varepsilon_i$. Scores η_{ij} and eigenfunctions $\phi_j(t)$ are usually unknown and need to be estimated. The most common technique is the functional principal component analysis (FPCA). We refer to [15] for a detailed description. Following [15], we can obtain $\hat{\phi}_j(t)$ and $\hat{U}_i = (\hat{\eta}_{i1}, \cdots, \hat{\eta}_{iK})^\top$.

2.2 Estimation

For estimating model (3), we propose the following objective function

$$Q_n(\beta,\theta)=\frac{1}{n}\sum_{i=1}^{n}\left\{\left|\frac{Y_i-\exp(Z_i^\top\theta+\hat{U}_i^\top\beta)}{Y_i}\right|+\left|\frac{Y_i-\exp(Z_i^\top\theta+\hat{U}_i^\top\beta)}{\exp(Z_i^\top\theta+\hat{U}_i^\top\beta)}\right|\right\}$$
$$+\sum_{k=1}^{q}\xi_k|\theta_k|+\sum_{j=1}^{K}\lambda_j|\beta_j|, \tag{5}$$

where ξ_k and λ_j ($k=1,\cdots,q$ and $j=1,\cdots,K$) are tuning parameters that control the degree of penalization. Estimators $\hat{\beta}_j$ and $\hat{\theta}_k$ can be obtained by minimizing $Q_n(\beta,\theta)$, and estimator $\hat{\gamma}(t)$ can be obtained by $\hat{\gamma}(t)=\sum_{j=1}^{K}\hat{\beta}_j\hat{\phi}_j(t)$.

The first part of $Q_n(\beta,\theta)$ is LARE, which uses relative errors with respect to both the target and predictor, i.e.,

$$\frac{Y_i-\exp(Z_i^\top\theta+\hat{U}_i^\top\beta)}{Y_i}\quad\text{and}\quad\frac{Y_i-\exp(Z_i^\top\theta+\hat{U}_i^\top\beta)}{\exp(Z_i^\top\theta+\hat{U}_i^\top\beta)}.$$

As pointed out in [2], using only one of the two is inadequate and may lead to biased estimation. The rest of $Q_n(\beta,\theta)$ consists of two penalty terms such that selection is conducted on both scalar variables and the basis functions for the functional variable. Variable selection on scalar variables is commonly used in practice. We also consider variable selection for the functional data part with the consideration that K is determined for a better approximation of X, without considering the association between X and the response. For practical use, it is desirable to use a large K and conduct variable selection to retain the ones that are the most relevant to the response. In this study, we use the adaptive Lasso penalty which is representative of the Lasso family and enjoys good properties [18]. With the adaptive Lasso,

$$\lambda_j=\lambda/|\tilde{\beta}_j|\quad\text{and}\quad\xi_k=\xi/|\tilde{\theta}_k|,$$

where $\tilde{\beta}=(\tilde{\beta}_1,\cdots,\tilde{\beta}_K)^\top$ and $\tilde{\theta}=(\tilde{\theta}_1,\cdots,\tilde{\theta}_q)$ are the unpenalized estimators.

Tuning Parameters Tuning parameters λ and ξ can be obtained by minimizing BIC. Let df be the number of non-zero coefficients $\{\hat{\beta},\hat{\theta}\}$. We consider

$$BIC=\log\hat{\sigma}_n^2+\frac{\log(n)}{n}df,$$

where

$$\hat{\sigma}_n^2 = \frac{1}{n}\sum_{i=1}^{n}\left\{\left|\frac{Y_i - \exp(Z_i^\top\hat{\theta} + \hat{U}_i^\top\hat{\beta})}{Y_i}\right| + \left|\frac{Y_i - \exp(Z_i^\top\hat{\theta} + \hat{U}_i^\top\hat{\beta})}{exp(Z_i^\top\hat{\theta} + \hat{U}_i^\top\hat{\beta})}\right|\right\}.$$

In simulation, we provide two estimators based on the proposed method. The first one, P_{BIC1}, sets both tuning parameters equal and uses BIC to determine the value. The second one, P_{BIC2}, chooses λ and ξ on a two-dimensional grid.

2.3 Statistical Properties

Let $A = \{j : |\beta_j| \neq 0\}$ and $B = \{k : |\theta_k| \neq 0\}$. To derive the asymptotic properties of the estimators, we make the following assumptions:

(C1) X_i has a finite fourth order moment.
(C2) There exist positive constants C and $\alpha > 1$ such that

$$\nu_k - \nu_{k+1} \geq C^{-1}K^{-\alpha-1}, k = 1, 2, \ldots.$$

(C3) There exist positive constants c and $b > 1$ such that $|\beta_j| \leq cj^{-b}$.
(C4) $n^{-1}K^{2\alpha+3} \to 0$.
(C5) Let $W_i = (Z_i^\top, U_i^\top)^\top$. Define matrices $V_1 = E(\frac{W_i W_i^\top}{\varepsilon_i^2})$ and $V_2 = E(W_i W_i^\top \varepsilon_i^2)$. There exist constants c_1, c_2, c_3, and c_4, such that $0 < c_1 < \rho_{\min}(V_1) \leq \rho_{\max}(V_1) < c_2 < \infty$ and $0 < c_3 < \rho_{\min}(V_2) \leq \rho_{\max}(V_2) < c_4 < \infty$, where $\rho_{\min}(\cdot)$ and $\rho_{\max}(\cdot)$ are the minimum and maximum eigenvalues.
(C6) The matrices $D_1 = E\{WW^\top\varepsilon\}$ and $D_2 = E\{WW^\top\frac{1}{\varepsilon}\}$ are positive definite.
(C7) Denote $\lambda_n = \max\{\lambda_j, j \in A\}$ and $\xi_n = \max\{\xi_k, k \in B\}$, $\sqrt{n}K\lambda_n \to 0$ and $\sqrt{n}K\xi_n \to 0$.
(C8) Denote $\lambda_n^* = \min\{\lambda_j, j \in A^c\}$ and $\xi_n^* = \min\{\xi_k, k \in B^c\}$, $\sqrt{n}K\lambda_n^* \to \infty$ and $\sqrt{n}K\xi_n^* \to \infty$.

Remark (C1) is a regular condition in functional data analysis. (C2) requires that the spacings between eigenvalues are not too small. It implies that each ν_k is greater than a constant multiple of $k^{-\alpha}$. This condition is needed to obtain the bound of $\hat{\phi}_j(t) - \phi_j(t)$ and $\hat{\eta}_j - \eta_j$, $j = 1, \cdots, K$. (C3) prevents the coefficients β_j from decreasing too slowly. This condition is imposed to control the tail behavior for a large K and so is not as restrictive as it appears. (C4) is the sparsity assumption that requires the number of functional principal components cannot be too large. (C7) is imposed for estimation consistency, and (C8) is imposed for selection consistency.

Theorem 1 establishes the consistency of estimators $\beta_j, j = 1, \cdots, K$ and $\theta_k, k = 1, \cdots q$. Let $\hat{A}_n = \{j : |\hat{\beta}_j| \neq 0\}$ and $\hat{B}_n = \{k : |\hat{\theta}_k| \neq 0\}$. Theorem 2 establishes selection consistency. Proofs of these theorems are provided in Appendix.

Theorem 1 *Under (C1)–(C7), we have*

$$\|\hat{\gamma} - \gamma\| = o_p(1), \hat{\theta}_k - \theta_k = o_p(1), k \in \{1, 2, \ldots, q\}$$

where $\|\hat{\gamma} - \gamma\| = (\int_T (\hat{\gamma} - \gamma)^2 dt)^{1/2}$.

Theorem 2 *Under (C1)–(C8) , we have*

$$P(\hat{A}_n = A) \to 1, \quad P(\hat{B}_n = B) \to 1.$$

3 Simulation

In this section, we conduct simulation to evaluate the finite sample performance of the proposed method. We consider two examples. In both examples, the response variables are randomly generated from $Y_i = \exp(Z_i^\top \theta + U_i^\top \beta + e_i)$, where $e_i \sim N(0, \sigma^2)$ and $\sigma^2 \in \{0.1, 1\}$, with sample size $n \in \{50, 100, 200\}$. The scalar variable Z_i is a q-dimensional vector generated from a multivariate normal distribution with mean 0 and auto-regressive covariance where $\text{cov}(Z_{ij_1}, Z_{ij_2}) = 0.5^{|j_1 - j_2|}$ for $1 \le j_1, j_2 \le q$. Functional data are generated from the process $X_i(s) = \sum_{j=1}^{L} \eta_{ij} \phi_j(s)$, where $\phi_{2l-1}(s) = -\sqrt{2}\cos\{(2l-1)\pi s\}$ and $\phi_{2l}(s) = -\sqrt{2}\sin\{(2l)\pi s\}$ with $s \in [0, 1]$ for $l = 1, \cdots, (L/2)$. η_{ij} are independent and identically distributed as $N(0, \nu_j)$. Other specifications and evaluation criteria are further introduced below in each example.

In Example 1, we design a relatively low-dimensional setup for which we compare the variable selection and prediction performance. In Example 2, we use a higher dimension for which we compare the variable selection and estimation performance. We compare the proposed estimators with the alternative penalization estimators, L_{BIC1} and L_{BIC2}, which are adaptive Lasso estimators based on the partially functional linear model $\log Y_i = Z_i^\top \theta + U_i^\top \beta + e_i$. L_{BIC1} corresponds to P_{BIC1} and sets the two tuning parameters equal. L_{BIC2} corresponds to P_{BIC2} and determines the two tuning parameters separately. For prediction, we additionally consider the oracle estimator (based on the true model, denote as "OE") and unpenalized estimator (based on the full model, denote as "UE"). All results are based on 500 replicates.

Example 1 For the scalar variable part, $q = 4$, and $\theta = (2, 1, 0, 0, 0, 0, 0)$. For the functional variable part, $L = 4$, and the corresponding eigenvalues are $\nu_1 = 2$, $\nu_2 = 1$, $\nu_3 = 0.5$, and $\nu_4 = 0.1$. $U_i = (\eta_{i1}, \cdots, \eta_{i4})$, and $\beta = (2, 1.5, 0, 0)$.

To assess variable selection performance, we report the percentage of correctly identified models ("C"), the percentage of over-fitted models ("O") in which all the significant scalar variables and basis functions are identified with at least one spurious scalar variable or basis function included, and average model size ("M") which counts the number of non-zero coefficients. To evaluate prediction, a testing

Table 1 Summary of variable selection and prediction performance for Example 1

n	Method	$\sigma^2 = 0.1$				$\sigma^2 = 1$			
		C	O	M	RPE	C	O	M	RPE
50	OE	–	–	–	0.511	–	–	–	0.500
	UE	–	–	–	0.495	–	–	–	0.498
	P_{BIC1}	0.664	0.168	5.384	0.497	0.450	0.378	5.692	0.496
	P_{BIC2}	0.704	0.128	5.332	0.499	0.472	0.356	5.642	0.508
	L_{BIC1}	0.624	0.376	5.522	0.619	0.402	0.594	5.946	0.642
	L_{BIC2}	0.582	0.418	5.568	0.641	0.410	0.586	5.916	0.645
100	OE	–	–	–	0.338	–	–	–	0.354
	UE	–	–	–	0.342	–	–	–	0.361
	P_{BIC1}	0.824	0.058	5.190	0.337	0.584	0.298	5.478	0.352
	P_{BIC2}	0.838	0.044	5.174	0.336	0.624	0.258	5.424	0.350
	L_{BIC1}	0.720	0.280	5.332	0.396	0.578	0.422	5.554	0.395
	L_{BIC2}	0.682	0.318	5.364	0.397	0.592	0.408	5.528	0.397
200	OE	–	–	–	0.364	–	–	–	0.334
	UE	–	–	–	0.375	–	–	–	0.344
	P_{BIC1}	0.976	0.004	5.024	0.372	0.838	0.146	5.180	0.333
	P_{BIC2}	0.978	0.002	5.022	0.372	0.858	0.126	5.158	0.333
	L_{BIC1}	0.702	0.298	5.316	0.490	0.708	0.292	5.338	0.334
	L_{BIC2}	0.684	0.316	5.332	0.490	0.710	0.290	5.332	0.335

"C","O", "M", and "RPE" are the percentage of correctly identified models, percentage of over-fitted models, average model size, and average median relative prediction errors, respectively, based on 500 replicates. "–" if not applicable

sample of size 100 is generated on which the median relative prediction error ("RPE") is calculated as median$\{(Y_i - \hat{Y}_i)^2/Y_i^2\}_{i=1}^{100}$.

Table 1 presents the summary evaluation of variable selection and prediction performance. In terms of variable selection, the proposed method outperforms the alternative penalization method with a higher percentage of correctly identified models, a smaller percentage of over-fitted models, and an overall smaller model size. For example, when $n = 50$ and $\sigma^2 = 1$, the percentages of correctly identified and over-fitted models are 0.472 and 0.356 for P_{BIC2}, compared to 0.410 and 0.586 for L_{BIC2}, respectively. In this case, the average model sizes for P_{BIC2} and L_{BIC2} are 5.642 and 5.916, respectively. In terms of prediction, performance of the proposed method is the closest to the oracle. Such satisfactory performance demonstrates advantages of the proposed method over the alternative penalization method. Compared with the unpenalized method under the full model, the proposed method improves prediction by reducing model complexity, indicating the importance of variable selection.

Example 2 For the scalar variable part, $q = 15$, and $\theta = (2_5^\top, 0_{10}^\top)$. For the functional variable part, $L = 10$, and the corresponding eigenvalues are $\nu_j = 9j^{-2}$, $j = 1, \cdots, 10$. $U_i = (\eta_{i1}, \cdots, \eta_{i10})$, and $\beta = (2_5^\top, 0_5^\top)$.

Table 2 Summary of variable selection and prediction performance for Example 2

n	Method	FN_s	FP_s	FN_f	FP_f	MSE_s	MSE_f
$\sigma^2 = 0.1$							
50	P_{BIC1}	0.050	1.772	0.476	0.602	0.023	0.422
	P_{BIC2}	0.018	1.408	0.456	0.640	0.024	0.422
	L_{BIC1}	0.040	0.516	0.132	4.406	0.000	211.7
	L_{BIC2}	0.040	0.540	0.142	4.208	0.000	201.7
100	P_{BIC1}	0.006	0.936	0.180	0.098	0.006	0.052
	P_{BIC2}	0.004	0.774	0.178	0.110	0.006	0.048
	L_{BIC1}	0.000	0.360	0.084	4.568	0.000	249.3
	L_{BIC2}	0.000	0.370	0.090	4.384	0.000	245.1
200	P_{BIC1}	0.000	0.298	0.082	0.012	0.003	0.020
	P_{BIC2}	0.000	0.252	0.078	0.008	0.003	0.020
	L_{BIC1}	0.000	0.188	0.104	4.582	0.000	528.7
	L_{BIC2}	0.000	0.196	0.104	4.436	0.000	505.6
$\sigma^2 = 1$							
50	P_{BIC1}	0.056	2.166	0.540	0.734	0.040	0.454
	P_{BIC2}	0.028	1.796	0.514	0.752	0.045	0.451
	L_{BIC1}	0.012	1.752	0.274	3.420	0.028	153.1
	L_{BIC2}	0.010	1.940	0.268	3.424	0.029	132.3
100	P_{BIC1}	0.000	1.690	0.130	0.236	0.012	0.070
	P_{BIC2}	0.000	1.446	0.144	0.238	0.013	0.066
	L_{BIC1}	0.000	1.056	0.132	3.454	0.009	255.7
	L_{BIC2}	0.000	1.180	0.132	3.464	0.010	237.5
200	P_{BIC1}	0.000	0.966	0.016	0.042	0.005	0.024
	P_{BIC2}	0.000	0.838	0.012	0.046	0.004	0.023
	L_{BIC1}	0.000	0.574	0.098	3.510	0.004	415.1
	L_{BIC2}	0.000	0.636	0.100	3.526	0.004	361.4

"FN", "FP", and "MSE" are average number of false negatives, average number of false positives, and average mean square errors of estimated coefficients, respectively. The results are reported separately for the scalar variable part and functional variable part, based on 500 replicates

Under this higher dimensional setup, we evaluate the performance of variable selection and estimation by examining the scalar variable part and functional variable part separately. For each part, we report the average number of false negatives ("FN") and average number of false positives ("FP") for assessing variable selection. For evaluating estimation accuracy, we consider the mean squared errors $MSE_s = \frac{1}{15}\sum_{j=1}^{15}(\hat{\theta}_j - \theta_j)^2$ and $MSE_f = \frac{1}{10}\sum_{j=1}^{10}(\hat{\beta}_j - \beta_j)^2$. Summary results are reported in Table 2.

For the scalar variable part, the alternative penalization method has slightly better performance in both selection and estimation. However, the advantage diminishes with increasing sample sizes. In general, the proposed method is quite competitive. For example, we examine P_{BIC2} and L_{BIC2} under $n = 50$ and $\sigma^2 = 1$. In this case, the average number of false negatives, false positives, and mean square errors are

0.028, 1.796, and 0.045 for P_{BIC2}, compared to 0.010, 1.940, and 0.029 for L_{BIC2}. Still with $\sigma^2 = 1$, when n increases to 200, the average number of false negatives and mean square errors of both P_{BIC2} and L_{BIC2} reduce to 0 and 0.004.

For the functional variable part, the proposed method significantly outperforms the alternative penalization method with a smaller number of false positives and smaller mean square errors. Performance of the proposed method improves with increasing sample sizes, resulting in more obvious advantages in both selection and estimation. We note that the number of false positives and the mean square errors stay almost the same for the alternative method with increasing sample sizes. For example, when $\sigma^2 = 1$, the numbers of false positives stay roughly around 3.5. We suspect that this poor performance may be caused by the measurement errors in functional principal scores under the high-dimensional setup. The proposed method survives in this case by taking advantages of relative errors.

4 Application

In this section, we demonstrate application of the proposed method to the Tecator data which is available at http://lib.stat.cmu.edu/datasets/tecator. The data contain 215 meat samples. For each sample, the contents of fat, moisture, and protein are measured. In addition, the data consists of a 100-channel spectrum of absorbances recorded on a Tecator Infratec Food and Feed Analyzer working in the wavelength range 850–1050 nm. More detailed information is available at the aforementioned website. The goal is to estimate the fat content given moisture, protein, and spectrometric curve.

The 100-channel spectrum measured over the wavelength range 850–1050 nm provides a dense measurement spaced 2 nm apart that can be considered as functional data. We denote it as $\{x_1, \ldots, x_{100}\}$. Figure 1 plots 30 randomly selected spectrometric curves. For the functional data part, we select the first four estimated eigenfunctions which explain more than 95% of the total variation. We plot the four selected eigenfunctions in Fig. 2. The contents of moisture and protein are scalar variables. Inspired by the work of [5], we also consider x_{45}, x_{49}, and x_{53} as scalar variables, which are the most predictive design covariates to optimize the prediction. Additionally, we include x_{92}, x_{96}, and x_{100}, which are near the border of range and may have some useful information. Totally, we have an 8-dimensional scale vector: content of moisture, content of protein, x_{45}, x_{49}, x_{53}, x_{92}, x_{96}, and x_{100}.

We randomly generate a training sample of size 160 and a testing sample of size 55. We apply the proposed and an alternative penalization methods as described in simulation to the training data. Table 3 presents the estimated coefficients of both scalar variable part and functional data part. For P_{BIC1} and P_{BIC2}, x_{49} is a significant variable as suggested in [5]. x_{92}, x_{96}, and x_{100} are not selected, which is consistent with [8] where only the most informative part of the spectra with wavelengths ranging from 902 to 1028 nm is considered. For selection with the basis functions, P_{BIC2} selects only the first one, the same as the result of [8].

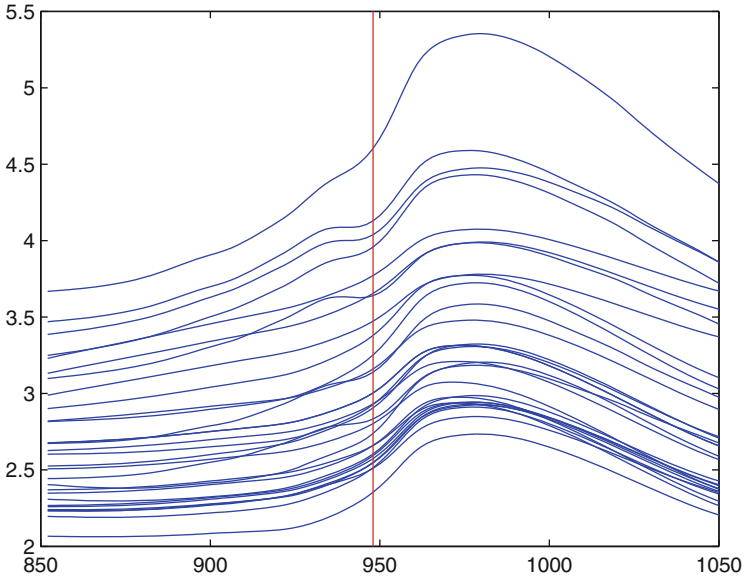

Fig. 1 Functional predictor trajectories of 30 randomly selected meat specimens. The red line denotes the location of x_{49}

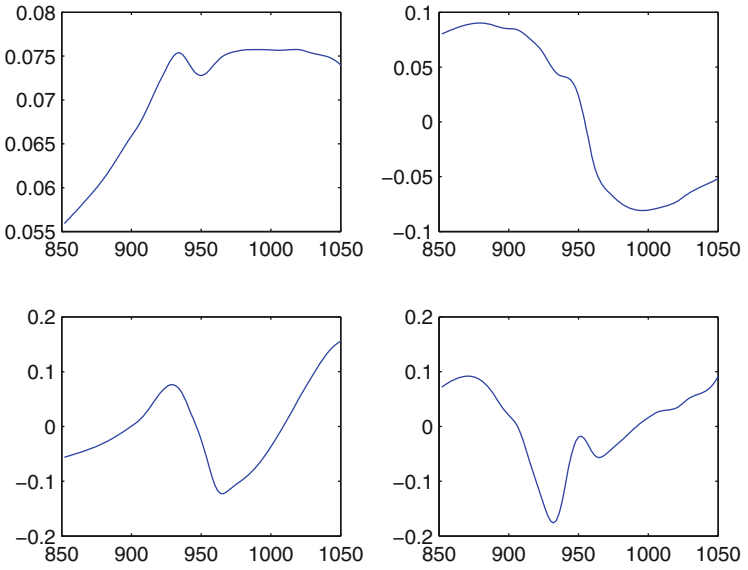

Fig. 2 Plots of the first four eigenfunctions

Table 3 Analysis of the Tecator data: estimated regression coefficients with the training data

	Moisture	Protein	x_{45}	x_{49}	x_{53}	x_{92}	x_{96}	x_{100}
P_{BIC1}	−0.057	−0.022	0.001	2.046	0	0	0	0
P_{BIC2}	−0.062	0	0	1.992	0	0	0	0
L_{BIC1}	−0.097	−0.066	0	0	2.295	39.562	−67.349	28.158
L_{BIC2}	−0.101	−0.077	0	−5.211	4.446	72.745	−125.472	56.174
	η_1	η_2	η_3	η_4				
P_{BIC1}	−0.135	−0.002	0	0				
P_{BIC2}	−0.135	0	0	0				
L_{BIC1}	−0.205	0.186	0	1.166				
L_{BIC2}	−0.204	0.592	0	0				

L_{BIC1} and L_{BIC2} in general select more variables. For example, in the scalar variable part, x_{92}, x_{96}, and x_{100} are selected by L_{BIC1} and L_{BIC2}. To evaluate prediction performance, we apply the estimated coefficients to the testing sample and obtain the median relative prediction errors. For both the proposed and alternative penalization methods, we consider the corresponding unpenalized counterparts as well. The values for P_{BIC1}, P_{BIC2}, and the unpenalized counterpart are 0.032, 0.021, and 0.094, respectively. The values for L_{BIC1}, L_{BIC2}, and the unpenalized counterpart are 0.015, 0.011, and 0.149, respectively. Prediction of the proposed method is comparable to the alternative penalization method and both outperform the unpenalized counterparts.

5 Discussion

As functional data become more commonly encountered, there is an increasing interest in modeling this type of data. Regression models with functional explanatory variables have been extensively studied. In this study, we consider a special case with a positive response for which we use the partially functional linear multiplicative model, an alternative to the popular linear models. For estimation, a relative error-based loss function is proposed with penalization to conduct variable selection. The purpose is not to challenge the absolute error-based criteria, but to provide an alternative perspective to examine data. In practice, whether or not to use the relative error-based loss functions may also depend on the purpose of studies. One contribution of the proposed method is conducting variable selection that can not only identify significant scalar covariates but also select the basis functions that contribute to the response. We note that this is extremely helpful under the functional data setup due to the truncated basis representation. With variable selection functionality, a larger number of basis functions can be retained among which the informative ones are kept during estimation. The proposed method still requires that the number of scalar variables and the number of basis functions to

be estimated is less than the sample size, which excludes the high-dimensional variables such as"-omics" measurements. Extension to those high-dimensional scenarios will be examined in the future.

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Appendix

Denote $\delta = (\theta^\top, \beta^\top)^\top$ and $\hat{\delta} = (\hat{\theta}^\top, \hat{\beta}^\top)^\top$. To facilitate proof of the theorems, we introduce Lemmas 1–3 where proof of Lemmas 1 and 2 can be found in [7] and proof of Lemma 3 can be found in [9].

Lemma 1 *Under (C1), (C2), and (C5), we have*

$$n^{-1}\sum_{i=1}^{n}(\hat{\eta}_{ij}\hat{\eta}_{ik} - \eta_{ij}\eta_{ik}) = O_p(j^{\alpha/2+1}n^{-1/2} + k^{\alpha/2}n^{-1/2}),$$
$$n^{-1}\sum_{i=1}^{n}(\hat{\eta}_{ij} - \eta_{ij})z_{ik} = O_p(j^{\alpha/2+1}n^{-1/2}).$$

Lemma 2 *Under (C1)–(C5), we have*

$$n^{-1}\sum_{i=1}^{n}\sum_{j=K+1}^{\infty}\eta_{ij}\beta_j z_{il} = O_p(n^{-1/2}).$$

Lemma 3 *Under (C1) and (C2), we have*

$$|\hat{\eta}_{ij} - \eta_{ij}| = O_p(K^{\alpha+1}/\sqrt{n}),$$
$$\|\hat{\phi}_j - \phi_j\| = O_p(K^{2\alpha+2}/n).$$

Proof of Theorem 1 Let $\alpha_n = \sqrt{K/n}$. We first show that $\|\hat{\delta} - \delta\| = O_p(\alpha_n)$. Following [4], it is sufficient to show that, for any given $\varepsilon > 0$, there exists a large constant C, such that

$$P\{\inf_{\|u\|=C} Q_n(\delta + \alpha_n u)) > Q_n(\delta))\} = 1 - \varepsilon,$$

where $\delta_C = \{\delta^* = \delta + \alpha_n u, \|u\| = C\}$ for $C > 0$. This implies that, with probability $1 - \varepsilon$, there exists a minimum in the ball δ_C. Hence, the consistency of δ is established.

By some simplifications, we have

$$\begin{aligned}\psi_n(u) &= Q_n(\delta+\alpha_n u)) - Q_n(\delta)) \\ &= \sum_{i=1}^{n}\{|1-Y_i^{-1}\exp\{\hat{W}_i^\top(\delta+\alpha_n u)\}| - |1-Y_i^{-1}\exp(\hat{W}_i^\top\delta)|\} \\ &\quad + \sum_{i=1}^{n}\{|1-Y_i\exp\{-\hat{W}_i^\top(\delta+\alpha_n u)\}|] - |1-Y_i\exp\{-\hat{W}_i^\top\delta\}|\} \\ &\quad + n\sum_{l=1}^{q}\{\xi_l|\theta_l+u_l\alpha_n| - \xi_l|\theta_l|\} + n\sum_{j=1}^{K}\{\lambda_j|\beta_j+u_{j+q}\alpha_n| - \lambda_j|\beta_j|\} \\ &\equiv I_1+I_2+I_3+I_4. \end{aligned} \tag{6}$$

For I_1, by applying the identity in [6],

$$|x-y|-|x| = -y[I(x>0)-I(x<0)] + 2\int_0^y [I(x\le s)-I(x\le 0)]ds,$$

which is valid for $x\neq 0$, we have

$$\begin{aligned} I_1 &= -\sum_{i=1}^{n} w_{1i}[I(1-Y_i^{-1}\exp(\hat{W}_i^\top\delta)>0) - I(1-Y_i^{-1}\exp(\hat{W}_i^\top\delta)<0)] \\ &\quad + 2\sum_{i=1}^{n}\int_0^{w_{1i}} [I(1-Y_i^{-1}\exp(\hat{W}_i^\top\delta)\le s) - I(1-Y_i^{-1}\exp(\hat{W}_i^\top\delta)\le 0)]ds \\ &\equiv I_{11}+I_{12}, \end{aligned}$$

where

$$w_{1i} = Y_i^{-1}\{\exp(\hat{W}_i^\top(\delta+\alpha_n u)) - \exp(\hat{W}_i^\top\delta)\}.$$

By Taylor expansion, we have

$$\begin{aligned} I_{11} &= \sum_{i=1}^{n}\alpha_n u\hat{W}_i^\top Y_i^{-1}\exp(\hat{W}_i^\top\delta)sgn(1-Y_i^{-1}\exp(\hat{W}_i^\top\delta)) \\ &\quad + \alpha_n^2 u^\top\{\sum_{i=1}^{n}\hat{W}_i^\top\hat{W}_i Y_i^{-1}\exp(\xi_i^{[1]})sgn(1-Y_i^{-1}\exp(\hat{W}_i^\top\delta))\}u/2 \\ &\equiv I_{111}+I_{112}, \end{aligned}$$

where $\xi_i^{[1]}$ lies between $\hat{W}_i^\top(\delta+\alpha_n u)$ and $\hat{W}_i^\top\delta$.

For I_{111}, by Lemma 2, we have

$$\begin{aligned} I_{111} &= \sum_{i=1}^{n} \alpha_n u \hat{W}_i^\top \frac{1}{\varepsilon_i} sgn(1 - Y_i^{-1} \exp(\hat{W}_i^\top \delta)) \\ &\quad + \sum_{i=1}^{n} \alpha_n^2 u^\top \frac{1}{\varepsilon_i} \hat{W}_i^\top \hat{W}_i u sgn(1 - Y_i^{-1} \exp(\hat{W}_i^\top \delta)) + o_p(1) \\ &\equiv I_{1111} + I_{1112} + o_p(1). \end{aligned}$$

It follows directly from Lemma 1 and (C5) that $I_{1111} = O_p(1)\|\alpha_n u\|$. Moreover, under (C5), $I_{1112} = \alpha_n^2 u^\top D_2 u/2$ and $I_{112} = \alpha_n^2 u^\top D_2 u/2 + o_p(1)\|\alpha_n u\|^2$.

Hence,

$$I_{11} = O_p(1)\|\alpha_n u\| + \alpha_n^2 u^\top D u/2 + o_p(1)\|u\|.$$

For I_{12}, denote $c_{1i} = \exp(\hat{W}_i^\top \hat{\delta} - W_i^\top \delta - H)$, $c_{2i} = \exp(\hat{W}_i^\top \delta - W_i^\top \delta - H)$ and $\tau = s\varepsilon_i$, then

$$\begin{aligned} I_{12} &= 2\sum_{i=1}^{n} \int_0^{w_{1i}} [I(1 - \varepsilon_i^{-1} c_{2i} \le s) - I(1 - \varepsilon_i^{-1} c_{2i} \le 0)] ds \\ &= 2\sum_{i=1}^{n} \int_0^{c_{1i} - c_{2i}} \varepsilon_i^{-1} [I(\varepsilon_i \le c_{2i} + \delta) - I(\varepsilon_i \le c_{2i})] d\delta \\ &= 2\sum_{i=1}^{n} \int_0^{c_{1i} - c_{2i}} E_{\varepsilon|X}\{\varepsilon_i^{-1} [I(\varepsilon_i \le c_{2i} + \tau) - I(\varepsilon_i \le c_{2i})]\} d\tau + o_p(1) \\ &= 2\sum_{i=1}^{n} \int_0^{c_{1i} - c_{2i}} E_{\varepsilon|X}\{[I(\varepsilon_i \le c_{2i} + \tau) - I(\varepsilon_i \le c_{2i})]\} d\delta \\ &\quad + 2\sum_{i=1}^{n} \int_0^{c_{1i} - c_{2i}} E_{\varepsilon|X}\{(\varepsilon_i^{-1} - 1)[I(\varepsilon_i \le c_{2i} + \tau) - I(\varepsilon_i \le c_{2i})]\} d\delta + o_p(1) \\ &= \alpha_n^2 u^\top \sum_{i=1}^{n} \hat{W}_i \hat{W}_i^\top u [1 + o_p(1)] \\ &= \alpha_n^2 u^\top D_2 u + o_p(1)\|\alpha_n u\|^2. \end{aligned}$$

Therefore, we have

$$I_1 = O_p(1)\|\alpha_n u\| + \alpha_n^2 u^\top D_2 u/2 + o_p(1)\|u\|. \tag{7}$$

Similarly, it can be shown that

$$I_2 = O_p(1)\|\alpha_n u\| + \alpha_n^2 u^\top D_1 u/2 + o_p(1)\|u\|. \tag{8}$$

Adopting the approach in [6], we have

$$|\theta_l + u_l\alpha_n| - |\theta_l| \to \alpha_n\{u_l sgn(\theta_l)I(\theta_l \neq 0) + |u_l|I(\theta_l = 0)\},$$
$$|\beta_j + u_{j+q}\alpha_n| - |\beta_j| \to \alpha_n\{u_{j+q} sgn(\beta_j)I(\beta_j \neq 0) + |u_{j+q}|I(\beta_j = 0)\}.$$

According to (C7), we have

$$I_3 > O(1)\|u\| \tag{9}$$

and

$$I_4 > O(1)\|u\|. \tag{10}$$

Combining (6)–(10), for a sufficiently large C, we have $\psi_n(u) > 0$. Therefore, $\|\hat{\delta} - \delta\| = O_p(\sqrt{K/n})$.

Next we show $\|\hat{\gamma}(t) - \gamma(t)\| = o_p(1)$. In fact,

$$\|\hat{\gamma}_1(t) - \gamma_1(t)\| \leq \sum_{j=1}^{K} \|\hat{\beta}_j\hat{\phi}_j(t) - \beta_j\phi_j(t)\| + \|\sum_{j>K} \beta_j\phi_j(t)\|$$

$$\leq \sum_{j=1}^{K}[|\hat{\beta}_j - \beta_j|\|\phi_j(s)\| + |\hat{\beta}_j - \beta_j|\|\hat{\phi}_j(s) - \phi_j(s)\| + |\beta_j|\|\hat{\phi}_j(s) - \phi_j(s)\|]$$

$$+\|\sum_{j>K} \beta_j\phi_j(s)\|$$

$$\equiv F_1 + F_2.$$

By result of the first part and Lemma 3, we can obtain

$$F_1 = O_p(\frac{K^{2\alpha+3}}{n}).$$

By the square integrable property of $\gamma(t)$, we have $F_2 = o_p(1)$. From the above results and condition (C4), we obtain

$$\|\hat{\gamma}(t) - \gamma(t)\| = o_p(1).$$

This completes the proof of Theorem 1. □

Proof of Theorem 2 For $j \in A$ and $k \in B$, the consistency result in Theorem 1 indicates that $\hat{\theta} \to \theta$ and $\hat{\beta} \to \beta$ in probability. Therefore, $P(j \in \hat{A}_n) \to 1$ and $P(k \in \hat{B}_n) \to 1$. Then it suffices to show that $P(j \in \hat{A}_n) \to 0$ for $\forall j \notin A$ and $P(k \in \hat{B}_n) \to 0$ for $\forall k \notin B$.

For $\forall j \in \hat{A}_n$ and $\forall k \in \hat{B}_n$, we have

$$\begin{aligned}
0 = \frac{\partial \psi_n(u)}{\partial u} &= \sum_{i=1}^{n} \{|1 - Y_i^{-1} \exp\{\hat{W}_i^\top(\delta)\}| - |1 - Y_i^{-1} \exp(\hat{W}_i^\top \delta)|\} \hat{W}_{ijk} \\
&\quad + \sum_{i=1}^{n} \{|1 - Y_i \exp\{-\hat{W}_i^\top(\delta)\}|] - |1 - Y_i \exp\{-\hat{W}_i^\top \delta\}|\} \hat{W}_{ijk} \\
&\quad + \sum_{i=1}^{n} \{|1 - Y_i^{-1} \exp\{\hat{W}_i^\top(\delta)\}| - |1 - Y_i^{-1} \exp(\hat{W}_i^\top \delta)|\} \hat{W}_{ijk} \hat{W}_i^\top u \\
&\quad + \sum_{i=1}^{n} \{|1 - Y_i \exp\{-\hat{W}_i^\top(\delta)\}|] - |1 - Y_i \exp\{-\hat{W}_i^\top \delta\}|\} \hat{W}_{ijk} \hat{W}_i^\top u \\
&\quad + n\alpha_n \xi_j sgn(\theta_j) + n\alpha_n \lambda_k sgn(\beta_k) \\
&\equiv N_1 + N_2 + N_3 + N_4 + N_5 + N_6.
\end{aligned}$$

By similar arguments with Theorem 1, we have

$$N_k = O_p(1), k = 1, \cdots, 4.$$

According to (C8), we have

$$N_k \to \infty, k = 5, 6.$$

Consequently, we must have $P(j \in \hat{A}_n) \to 0$ and $P(k \in \hat{B}_n) \to 0$ for $\forall j \notin A$ and $\forall k \notin B$. This completes the proof Theorem 2. □

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High-Dimensional Regression Under Correlated Design: An Extensive Simulation Study

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Abstract Regression problems where the number of predictors, p, exceeds the number of responses, n, have become increasingly important in many diverse fields in the last couple of decades. In the classical case of "small p and large n," the least squares estimator is a practical and effective tool for estimating the model parameters. However, in this so-called Big Data era, models have the characteristic that p is much larger than n. Statisticians have developed a number of regression techniques for dealing with such problems, such as the Lasso by Tibshirani (J R Stat Soc Ser B Stat Methodol 58:267–288, 1996), the SCAD by Fan and Li (J Am Stat Assoc 96(456):1348–1360, 2001), the LARS algorithm by Efron et al. (Ann Stat 32(2):407–499, 2004), the MCP estimator by Zhang (Ann Stat. 38:894–942, 2010), and a tuning-free regression algorithm by Chatterjee (High dimensional regression and matrix estimation without tuning parameters, 2015, https://arxiv.org/abs/1510.07294). In this paper, we investigate the relative performances of some of these methods for parameter estimation and variable selection through analyzing real and synthetic data sets. By an extensive Monte Carlo simulation study, we also compare the relative performance of proposed methods under correlated design matrix.

Keywords Correlated design · Penalized and non-penalized methods · High-dimensional data · Monte Carlo

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1 Introduction

There are a host of buzzwords in today's data-centric world. We encounter data in all walks of life, and for analytically- and objectively-minded people, data is crucial to their goals. However, making sense of the data and extracting meaningful information from it may not be an easy task. The rapid growth in the size and scope of data sets in a variety of disciplines have naturally led to the usage of the term, Big Data. The word Big Data is nebulously defined. Generally speaking, it is often used to denote a dataset containing a large number of sample observations with factors that could induce significant problems when analyzing it. Due to these barriers when analyzing data, statisticians could play a vital role in the data world. A variety of statistical and computational tools are needed to reveal the story that is contained in the data and statisticians should fulfill expectations on a need for innovative statistical strategies for understanding and analyzing them.

Among many problems arisen from Big Data, in the realm of statistics, many people worked on the so-called high dimensional data (HDD), which are data sets containing larger number of predictors than the number of observations. The analysis of HDD is important in multiple research fields such as engineering, social media networks, bioinformatics and medical, environmental, and financial studies among others. There is an increasing demand for efficient prediction strategies and variable selection procedures for analyzing HDD. Some examples of HDD that have prompted demand are gene expression arrays, social network modeling and clinical, genetic, and phenotypic data. Developing innovative statistical learning algorithms and data analytic techniques play a fundamental role for the future of research in these fields. More public and private sectors are now acknowledging the importance of statistical tools and its critical role in analyzing HDD.

The challenges are to find novel statistical methods to extract meaningful conclusions and interpretable results from HDD. The classical statistical strategies do not provide solutions to such problems. Traditionally, statisticians used best-subset selection or other variable selection procedures to choose predictors that are highly correlated with the response variable. Based on the selected predictors, statisticians employed classical statistical methods to analyze HDD. However, with a huge number of predictors, implementing a best-subset selection is already computationally burdensome. On top of that, these variable selection techniques suffer from high variability due to their nature. To resolve such issues, a class of penalized estimation methods have been proposed. They are referred to as penalized estimation methods since they share the idea to estimate parameters in a model using classical least squares approach with an additional penalty term. Some of these methods not only perform variable selection and parameter estimation simultaneously, but also are extremely computationally efficient.

There are two main objectives of this paper. First is to give an idea how existing HDD methods perform on datasets when the correlations among response variables are present. Many statisticians studied HDD methods under the assumption that response variables are independent. This assumption certainly allowed statisticians

to develop more complex estimation methods and provided practitioners with cautionary aspects when dealing with datasets containing non-independent variables. However, the assumption is not realistic, which necessitates statistical methods not relying on independence assumption. By examining how existing HDD method works on non-independent setting, we expect to gain some insights on developing novel estimation strategies and variable selection procedures for the datasets with non-independent variables. In addition to that many existing HDD analysis methods rely on a tuning parameter, which is burdensome to calibrate. It makes harder for non-technical scientists to analyze HDD and further, even for technical scientists, tuning parameter brings difficulty in reproducing research outcomes. Recently original methods that don't require tuning parameter when analyzing HDD were introduced. In this paper, we also compare the performance of these new methods with the ones using tuning parameters in a variety of different settings.

The rest of the paper is organized as follows: In Sect. 2, we review the definitions and basic properties of the regression methods which we will mainly focus on. In Sect. 3, we explain our simulation set-up for synthetic data and present the simulation results. Sect. 4 shows an application of the methods to two real data sets, prostate data and riboflavin production in *Bacillus subtilis* data. We finish the paper by Sect. 5 with some concluding remarks and future research directions.

2 Penalized Regression Methods

Consider the following linear model

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}, \tag{1}$$

where $\mathbf{Y} = (y_1, y_2, \ldots, y_n)'$ is a vector of responses, $\mathbf{X} = [x_{ij}]$ is an $n \times p$ fixed design matrix, $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_p)'$ is an unknown vector of parameters, and $\boldsymbol{\varepsilon} = (\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n)'$ is the vector of unobserved random errors. We assume that coordinates of the error vector $\boldsymbol{\varepsilon}$ are i.i.d. normally distributed with mean zero and variance σ^2. For the rest of the paper, without loss of generality, we assume that the predictors and responses in (1) are standardized so that $\sum_{i=1}^n y_i = 0$ and $\sum_{i=1}^n x_{ij} = 0$, $\sum_{i=1}^n x_{ij}^2 = 1$, for all j.

For a given model as in (1), there are three main tasks that need to be performed by a practitioner:

1. Parameter estimation: Finding an estimator $\widehat{\boldsymbol{\beta}}$ for $\boldsymbol{\beta}$.
2. Variable selection or model selection: Selecting the non-zero entries of $\boldsymbol{\beta}$ accurately.
3. Prediction: Estimating $\mathbf{X}\boldsymbol{\beta}$.

For the case $n > p$, the classical estimator of $\boldsymbol{\beta}$ is the ordinary least square estimator (OLS), which is obtained by minimizing the residual sum of squares. It is given by

$$\widehat{\boldsymbol{\beta}}^{\text{OLS}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}.$$

However, in the high-dimensional setting, where $p > n$, the inverse of the Gram matrix, $(\mathbf{X}'\mathbf{X})^{-1}$, does not exist. More precisely, there will be infinitely many solutions for the least squares minimization, hence there is no well-defined solution. In fact, even in the case $p \leq n$ and p close to n, the OLS estimator is not considered very useful because standard deviations of estimators are usually very high. In many regression models, in particular for the high dimensional case, only some of the predictors have a direct significant effect on the response variables. Therefore it is convenient to assume that the underlying true model is sparse; that is, the true model has only a relatively small number of non-zero predictors. The sparsity induced methods also play an important role in high dimensional statistics because they induce interpretable models. It is well-known that the least squares estimation procedure is unlikely to yield zero estimates for many of the model coefficients. There are many alternatives to the least square estimation such as subset selection, dimension reduction, and penalization methods. Each of them has its own advantages and disadvantages. For a thorough exposition, see [1, 14].

In this paper, we consider the penalized least square regression methods to obtain estimators for the model parameters in (1). The key idea in penalized regression methods is minimizing an objection function $L_{\rho,\lambda}$ in the form of

$$L_{\rho,\lambda}(\boldsymbol{\beta}) = (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) + \lambda\rho(\boldsymbol{\beta}) \tag{2}$$

to obtain an estimate for the model parameter $\boldsymbol{\beta}$. The first term in the objective function is the sum of the squared error loss, the second term ρ is a penalty function, and λ is a tuning parameter which controls the trade-off between two components of $L_{\rho,\lambda}$.

The penalty function is usually chosen as a norm on $\mathbb{R}^p$, in most cases an l_q-norm, which can be written as

$$\rho_q(\boldsymbol{\beta}) = \sum_{j=1}^{p} |\beta_j|^q, \ q > 0. \tag{3}$$

The class of estimators employing the above type of penalties are called the bridge estimators, proposed by Frank and Friedman [11].

The ridge regression [11, 17] minimizes the residual sum of squares subject to an l_2-penalty, that is,

$$\widehat{\boldsymbol{\beta}}^{\text{Ridge}} = \arg\min_{\boldsymbol{\beta}} \left\{ \sum_{i=1}^{n} (y_i - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 \right\}, \tag{4}$$

where λ is a tuning parameter. Although the ridge estimator is a continuous shrinkage method and has a better prediction performance than OLS through bias-variance trade-off, it does not set any OLS estimates to zero, so obtaining a sparse model is not possible. However, in the case of l_q-penalty with $q \leq 1$, some coefficients are set exactly to zero. And the optimization problem for (2) becomes a convex optimization problem, which can be easily solved, for the case $q \geq 1$. Therefore, l_1-penalty is special for both reasons.

There are other penalized regression methods with more sophisticated penalty functions which not only shrink all the coefficients toward zero, but also set some of them exactly to zero. As a result, this class of estimators usually produce biased estimates for the parameters due to the shrinkage, but have some advantages such as producing more interpretable submodels and reducing the variance of the estimator.

Several penalty estimators have been proposed in the literature for linear and generalized linear models. In this paper, we only consider the *least absolute shrinkage and selection operator* (Lasso) [26], the *smoothly clipped absolute deviation* (SCAD) [9], *the adaptive Lasso* (aLasso) [30], and the *minimax concave penalty* (MCP) method [29]. These methods perform parameter estimation and model selection simultaneously. In addition to these penalty estimators, we also consider the *tuning-free regression method* (CTFR) which has been recently proposed by Chatterjee in [6].

It is known that as the prediction performance of Ridge, Bridge, and Lasso are compared, none of them uniformly dominates others [12]. But the Lasso has a significant advantage over ridge and bridge estimators in terms of variable selection performance, see [12] and [26]. Another important advantage of penalized regression techniques is that they can be used when the number of predictors, p, is much larger than the number of observations, n. However, in an effort to achieve meaningful estimation and selection properties, most penalized regression methods make some important assumptions on both the true model and the designed matrix. We refer to [5] and [14] for more insights.

2.1 Lasso

The Lasso was proposed by Tibshirani [26], which performs variable selection and parameter estimation simultaneously, thanks to the l_1-penalty. The Lasso estimator is defined by

$$\widehat{\boldsymbol{\beta}}_n^{\text{Lasso}} = \arg\min_{\boldsymbol{\beta}} \left\{ \sum_{i=1}^{n} (y_i - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right\}. \tag{5}$$

Note that for the high-dimensional case, $p > n$, there might be multiple solutions of (5); nevertheless for any two solutions $\widehat{\boldsymbol{\beta}}_n^1$, $\widehat{\boldsymbol{\beta}}_n^2$, we have $\mathbf{X}\widehat{\boldsymbol{\beta}}_n^1 = \mathbf{X}\widehat{\boldsymbol{\beta}}_n^2$ which implies that all solutions have the same prediction performance [27].

In order to understand the role of the penalty function in shrinkage, it is instructive to consider the orthogonal design, that is, $n = p$ and the design matrix $\mathbf{X} = \boldsymbol{I}_n$ is the identity matrix [19]. In this case, the OLS solution minimizes

$$\sum_{i=1}^{p}(y_i - \beta_i)^2$$

and the estimates are given by

$$\widehat{\beta}_i^{\text{OLS}} = y_i \quad \text{for all} \quad 1 \le i \le p.$$

The ridge regression solution minimizes

$$\sum_{i=1}^{p}(y_i - \beta_i)^2 + \lambda \sum_{i=1}^{p} \beta_i^2$$

and hence the estimates are given by

$$\widehat{\beta}_i^{\text{Ridge}} = y_i/(1+\lambda) \quad \text{for all} \quad 1 \le i \le p.$$

Similarly, the Lasso solution minimizes

$$\sum_{i=1}^{p}(y_i - \beta_i)^2 + \lambda \sum_{i=1}^{p} |\beta_i|$$

and the estimates take the form

$$\widehat{\beta}_i^{\text{Lasso}} = \begin{cases} y_i - \lambda/2 & \text{if} \quad y_i > \lambda/2; \\ y_i + \lambda/2 & \text{if} \quad y_i < -\lambda/2; \\ 0 & \text{if} \quad |y_i| \le \lambda/2. \end{cases}$$

We see that the shrinkage applied by Ridge and Lasso affect the estimated parameters differently. In the Lasso solution, the least square coefficients with absolute value less than $\lambda/2$ are set exactly equal to zero, and other least squares coefficients are shrunken towards zero by a constant amount, $\lambda/2$. As a result, sufficiently small coefficients are all estimated as zero. On the other hand, the ridge regression shrinks each least squares estimate towards zero by multiplying each one by a constant proportional to $1/\lambda$. For more general design matrix, we do not have explicit solutions for the estimates, but the effect of the shrinkage is similar as in orthogonal design case, see [14, 15] and [19] for more on this topic.

Originally, the Lasso solutions were obtained via quadratic programming by Tibshirani [26]. Later, Efron et al. proposed Least Angle Regression (LARS) algorithm, which is a homotopy method that constructs a piece-wise linear solution path in an effective way [8] . Coordinate descent algorithms, which use the sparsity assumption, are also simple and very fast to compute for the Lasso estimator [10]. The popular *glmnet* package of R language implements coordinate descent for the Lasso solution [10]. Further, the Lasso estimator remains numerically feasible for dimensions of p that are much higher than the sample size n.

Tuning parameter plays a very crucial role for the performance of the Lasso as well. Meinshausen and Bühlmann [23] showed that if the penalty parameter λ is tuned to obtain optimal prediction, then consistent variable selection cannot hold: the Lasso solution includes many noise variables besides the true signals. Leng et al. [22] proved this fact in a short argument by considering a model with orthogonal design. Thus, we can say that variable selection and parameter estimation are closely related but different problems.

There has been significant progress on the theoretical properties of Lasso's performance for parameter estimation and prediction in the last two decades. It was first proved by Knight and Fu [20] that the estimator $\widehat{\boldsymbol{\beta}}$ is consistent when p is fixed and n tends to infinity provided that the tuning parameter satisfies a growth condition. Under the assumption that

$$\frac{1}{n}\mathbf{X}'\mathbf{X} \to \boldsymbol{C}$$

where $\boldsymbol{C}$ is a positive definite matrix, Knight and Fu also [20] proved that the Lasso solution has the following properties depending on how the tuning parameter is chosen. Consider

$$\widehat{\boldsymbol{\beta}}_n = \arg\min_{\boldsymbol{\beta}} \left\{ \sum_{i=1}^{n} (y_i - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda_n \sum_{j=1}^{p} |\beta_j| \right\}. \tag{6}$$

Then

(a) If $\lambda_n/n \to \lambda_0 \geq 0$, then $\hat{\boldsymbol{\beta}}_n \xrightarrow{p} \arg\min V_1$ where

$$V_1(u) = (u - \boldsymbol{\beta})'\boldsymbol{C}(u - \boldsymbol{\beta}) + \lambda_0 \sum_{i=1}^{p} |u_i|.$$

(b) If $\lambda_n/\sqrt{n} \to \lambda_0 \geq 0$, then $\sqrt{n}(\widehat{\boldsymbol{\beta}}_n - \boldsymbol{\beta}) \xrightarrow{d} \arg\min V_2$ where

$$V_2(u) = -2u^T\boldsymbol{W} + u^T\boldsymbol{C}u + \lambda_0 \sum_{i=1}^{p} [u_i \operatorname{sgn}(\beta_i) I_{\beta_i \neq 0} + |u_i| I_{\beta_i = 0}].$$

The results above imply that when $\lambda_n = O(\sqrt{n})$, the Lasso estimator cannot recover the true signals with a positive probability, and $\lambda_n = o(n)$ is sufficient for consistency.

It is well-known that with non-singular $\boldsymbol{C}$, the OLS estimator is consistent when p is fixed and n tends to infinity, and

$$\sqrt{n}(\widehat{\boldsymbol{\beta}}_n^{\text{OLS}} - \boldsymbol{\beta}) \to_d N(\mathbf{0}, \sigma^2 \boldsymbol{C}^{-1}).$$

In the regime where both n and p tend to infinity, the standard consistency definition is not valid for any estimator $\widehat{\boldsymbol{\beta}}$. Greenshtein and Ritov [13] introduced the "persistency" concept in this setting as an analogue of consistency of an estimator, and proved that the Lasso estimator is persistent under some assumptions on the design matrix. Since the Lasso automatically sets some components of $\widehat{\boldsymbol{\beta}}$ to zero, model selection consistency for the Lasso estimator is a crucial problem. In the case that the tuning parameter is chosen by a deterministic rule, under a couple of assumptions on the design matrix and sparsity of $\boldsymbol{\beta}$, it is known that the Lasso estimator recovers the true parameter set, see [3, 5]. Even though these theoretical results are satisfactory, the assumption that the tuning parameter is to be chosen deterministically does not shed light on practical applications of the Lasso, because in most applications the tuning parameter is chosen using some data-driven methods such as cross-validation. There are only few theoretical results on the Lasso when the tuning parameter is chosen in a data-dependent way, see the recent result of [7] and the references therein. For an in-depth study of Lasso, see two recent excellent books [5] and [15].

In many diverse applications of regression, it is not realistic to assume that the predictors are independent. Therefore the influence of correlations among predictors on parameter estimation and prediction is an important problem. In general, it was believed that there would be large prediction errors when the predictors are correlated. However, recent results in [16] show that this is not necessarily true, and they argue that for correlated designs, small tuning parameters can be chosen so that some satisfactory error bounds on the prediction error can be achieved. Their theoretical arguments and simulation results show that Lasso performs well under any degree of correlations if the tuning parameter is chosen suitably. Besides this fact, they show that choosing λ proportional to $\sqrt{n \log p}$ and ignoring the correlations in the design is not favorable. In the next section, we present our simulation results on the cross-validated Lasso's prediction performance under correlated design.

2.2 aLasso

Zhou [30] introduced the adaptive Lasso (aLasso) by modifying the Lasso penalty by using adaptive weights on the l_1-penalty. In the same paper, it has been shown theoretically that the adaptive Lasso estimator is able to identify the true model

consistently, and has the so-called oracle property. An estimator is said to have oracle property if asymptotically the method performs as well as if the statistician had known which coefficients were non-zero and which were zero in advance.

The aLasso $\widehat{\beta}^{\text{aLasso}}$ is obtained by

$$\widehat{\boldsymbol{\beta}}^{\text{aLasso}} = \arg\min_{\boldsymbol{\beta}} \left\{ \sum_{i=1}^{n} (y_i - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} \widehat{w}_j |\beta_j| \right\}, \tag{7}$$

where the weight function is

$$\widehat{w}_j = \frac{1}{|\widehat{\beta}_j^*|^\gamma}; \quad \gamma > 0,$$

and $\widehat{\beta}_j^*$ is a root-n-consistent estimator of β. The minimization procedure for the aLasso solution does not induce any computational difficulty and can be solved very efficiently, for the details see section 3.5 in [30], see and [18]. Zhou [30] also proved that if $\lambda_n/\sqrt{n} \to 0$ and $\lambda_n n^{(\gamma-1)/2} \to \infty$, the aLasso estimates have the following properties:

1. aLasso has variable selection consistency with probability one as n tends to infinity.
2. $$\sqrt{n}(\widehat{\boldsymbol{\beta}}_n^{\text{aLasso}} - \boldsymbol{\beta}) \to_d N(\mathbf{0}, \sigma^2 \boldsymbol{C}_{11}^{-1})$$

   where $\boldsymbol{C}_{11}^{-1}$ is the submatrix of $\boldsymbol{C}$ which corresponds to the non-zero entries of $\boldsymbol{\beta}$.

2.3 SCAD

Although the Lasso method does both shrinkage and variable selection due to the nature of the l_1-penalty by setting many coefficients identically to zero, it does not possess oracle properties, as discussed in [9]. To overcome the inefficiency of traditional variable selection procedures, Fan and Li [9] proposed SCAD to select variables and estimate the coefficients of variables automatically and simultaneously. In the same paper, they proved that SCAD has oracle property as well. This method not only retains the good features of both subset selection and ridge regression, but also produces sparse solutions, ensures continuity of the selected models (for the stability of model selection), and has unbiased estimates

for large coefficients. The estimator is obtained by

$$\widehat{\boldsymbol{\beta}}^{\text{SCAD}} = \arg\min_{\boldsymbol{\beta}} \left\{ \sum_{i=1}^{n} (y_i - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \sum_{j=1}^{p} p_{\gamma,\lambda}(|\beta_j|) \right\}. \tag{8}$$

Here $p_{\gamma,\lambda}(\cdot)$ is the smoothly clipped absolute deviation penalty which is defined on $[0, \infty)$ by

$$p_{\gamma,\lambda}(x) = \begin{cases} \lambda x, & \text{if } x \leq \lambda, \\ \frac{\gamma\lambda x - 0.5(x^2+\lambda^2)}{\gamma-1} & \text{if } \lambda < x \leq \gamma\lambda, \\ \frac{\lambda^2(\gamma^2-1)}{2(\gamma-1)} & \text{if } x > \gamma\lambda \end{cases}$$

where $\lambda \geq 0$ and $\gamma > 2$. Note that SCAD is identical with the Lasso for $|x| \leq \lambda$, then continuously changes to a quadratic function until $|x| = \gamma\lambda$, and then it remains constant for all $|x| > \gamma\lambda$. The lower values of γ produce more variable but less biased estimates. For $\gamma = \infty$, the SCAD penalty is equivalent to the l_1-penalty.

2.4 MCP

Zhang [28] introduced a new penalization method for variable selection, which is given by

$$\widehat{\boldsymbol{\beta}}^{\text{MCP}} = \arg\min_{\boldsymbol{\beta}} \left\{ \sum_{i=1}^{n} (y_i - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \sum_{j=1}^{p} p_{\gamma,\lambda}(|\beta_j|) \right\},$$

where the MCP penalty $p_{\gamma,\lambda}(\cdot)$ is given by

$$p_{\gamma,\lambda}(x) = \begin{cases} \lambda|x| - \frac{x^2}{2\gamma}, & \text{if } |x| \leq \gamma\lambda, \\ \frac{1}{2}\gamma\lambda^2 & \text{if } |x| > \gamma\lambda, \end{cases}$$

where $\gamma > 1$ and λ are regularization parameters. The MCP has the threshold value $\gamma\lambda$. The penalty is a quadratic function for values less than the threshold and is constant for values greater than it. The parameter $\gamma > 0$ controls the convexity and therefore the bias of the estimators. The lower values of γ give us more variable but less biased estimates. By controlling the parameter γ, under less restricted assumptions than those required by the Lasso, one can reduce almost all the bias

of the estimators and obtain consistent variables. The MCP solution path converges to Lasso path as $\gamma \to \infty$. Zhang [29] proves that the estimator possesses selection consistency at the universal penalty level $\lambda = \sigma\sqrt{2/n \log p}$ under the sparse Riesz condition on the design matrix $\mathbf{X}$. It has been proven that the MCP has oracle property, for more on the properties of the estimator, see [28, 29].

2.5 CTFR

Chatterjee [6] introduced a general theory for Gaussian mean estimation that, when applied to the linear regression problem, only requires the design matrix and the response vector as input and hence no tuning parameter is required. In [6], Chatterjee showed that the proposed estimator is adaptively minimax rate-optimal in high-dimensional regression case. We call this estimator Chatterjee's tuning-free regression, CTFR in short, in this paper. The estimator $\widehat{\boldsymbol{\beta}}$ is obtained by

$$\widehat{\boldsymbol{\beta}}^{\text{CTFR}} = \underset{\boldsymbol{\beta}\in\mathbb{R}^p}{\arg\min}\{|\boldsymbol{\beta}|_1 : ||\mathbf{Y}' - \mathbf{X}\boldsymbol{\beta}||_2^2 \le k\hat{\sigma}^2\}$$

where k is the rank of $\mathbf{X}$, $\mathbf{Y}'$ is the projection of $\mathbf{Y}$ onto the column space of $\mathbf{X}$, and $\hat{\sigma}$ is a randomized estimator of σ introduced in the same paper. For the details, see the paper [6]. The following result from the same paper gives an upper bound on the expected mean squared prediction error of $\hat{\boldsymbol{\beta}}$:

$$\frac{\mathbb{E}||\mathbf{X}\widehat{\boldsymbol{\beta}} - \mathbf{X}\boldsymbol{\beta}||_2^2}{n\sigma^2} \le C\left(r + r^2 + \sqrt{\frac{\log(p+n)}{n}} + \frac{\log(p+n)}{n}\right)$$

where $r = \frac{|\boldsymbol{\beta}|_1\gamma}{\sigma}\sqrt{\frac{\log(p+n)}{n}}$, $\gamma = \max_{1\le j\le p}||\mathbf{X}_j||/\sqrt{n}$, and C is a universal constant.

Chatterjee [6] compared his proposed estimator's performance with the 10-fold cross validated Lasso. The proposed estimator has generally higher prediction error than the 10-fold cross-validated Lasso. On the other hand, the proposed estimator has better performance at model selection: the number of false positives returned by the proposed estimator is significantly less than that of the 10-fold cross-validated Lasso. See the next section, for more simulation results.

2.6 TREX

Lederer and Muller [21] introduced another tuning-free regression method, TREX, which is obtained by a careful analysis of Square-Root Lasso [2]. They showed that TREX can outperform a cross-validated Lasso in terms of variable selection

and computational efficiency through a detailed numeric study. The estimator is defined as

$$\widehat{\boldsymbol{\beta}}^{\text{TREX}} \in \arg\min_{\boldsymbol{\beta}\in\mathbb{R}^p}\{\frac{||\mathbf{Y}-\mathbf{X}\boldsymbol{\beta}||_2^2}{\frac{1}{2}||\mathbf{X}'(\mathbf{Y}-\mathbf{X}\boldsymbol{\beta})||_\infty}+|\boldsymbol{\beta}|_1\}.$$

For some numerical results on the variable selection performance of the estimator, see [21].

3 Experimental Study

3.1 Simulation Setup

We consider the model

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon} \tag{9}$$

where $\mathbf{X}$ is $n \times p$ dimensional predictor matrix, $\mathbf{Y}$ is the n-dimensional response vector, and $\boldsymbol{\epsilon}$ is the n-dimensional unobserved error vector. $\boldsymbol{\beta}$ is a p-dimensional vector of coefficients. Each component of $\boldsymbol{\epsilon}$ is generated from standard normal distribution.

In our simulation study, we basically follow the simulation set-up of [24]. All simulations were based on a sample size of $n = 100$. We considered two different values for the number of predictor variables: $p = 500$ and $p = 1000$. Entries of the predictor matrix $\mathbf{X}$ were randomly sampled from the standard normal distribution. Correlation between columns of $\mathbf{X}$ is set to ρ, where $\rho \in \{0, 0.2, 0.4, 0.6, 0.8\}$.

The number of non-zero elements of $\boldsymbol{\beta}$ was set to $\lceil n^\alpha \rceil$, where α controls the sparsity of $\boldsymbol{\beta}$. We chose $\alpha \in \{0.1, 0.3, 0.5, 0.7, 0.9\}$. We picked $\lceil n^\alpha \rceil$ number of indices randomly. For these indices, the coordinates of $\boldsymbol{\beta}$ were sampled from a $Laplace(1)$ distribution while the rest of the coordinates of $\boldsymbol{\beta}$ were set to zero. The resulting $\boldsymbol{\beta}$ vector was rescaled according to the pre-specified signal-to-noise ratio, snr, defined as $\frac{\boldsymbol{\beta}'\boldsymbol{\Sigma}\boldsymbol{\beta}}{\sigma^2}$, where $snr \in \{0.5, 1, 2, 5, 10, 20\}$. Here $\boldsymbol{\Sigma}$ is the covariance matrix of the predictors. We assumed homoscedasticity condition where σ^2 is the error variance of each predictor variables. We assume that $\sigma = 1$ in all our simulations.

We investigate the relative performance of the following five estimators:

1. Lasso
2. aLasso
3. CTFR
4. SCAD
5. MCP

Tuning parameters for the above methods, except for CTFR, were chosen to minimize 10-fold cross validation error. For aLasso, we used the obtained Lasso estimate as the weight for the penalty term. In the simulation tables, we summarize our simulation results by comparing the performance of estimator CTFR, SCAD, MCP, and aLasso with relative to Lasso. The performance was measured based on the following metrics, respectively:

(a) TP = the number of true positives
(b) FP = the number of false positives
(c) PE = the prediction error

We define the relative number of true positives of listed methods to Lasso as:

$$RTP = \frac{\text{number of true positives of any method in the list}}{\text{number of true positives of Lasso}}.$$

Clearly the value greater than one, which is shown as bold in Tables 1–10, will indicate the superiority of the suggested method over Lasso in selecting true positives, otherwise Lasso is relatively performing well. For instance, in Table 1, for $p = 500$ and parameters $(\rho, \alpha, \text{snr}) = (0, 0.1, 0.5)$, the value 0.712 in RTP of CTFR is computed by

$$\frac{\text{number of true positives of CTFR}}{\text{number of true positives of Lasso}} = 0.712.$$

Similarly two other relative measures RFP and RPE are, respectively, defined as:

$$RFP = \frac{\text{number of false positives of any method in the list}}{\text{number of false positives of Lasso}}.$$

$$RPE = \frac{\text{prediction error of any method in the list}}{\text{prediction error of Lasso}}.$$

For our simulations, we used a *cv.glmnet* function in the *glmnet* package in R language for Lasso and aLasso, and a *cv.ncvreg* function in the *ncvreg* package for SCAD and MCP methods. The implementation of CTFR is done in R language, and it can be provided upon request.

3.2 Simulation Results

In this section, we present our simulation results (Tables 2, 3, 4, 5, 6, 7, 8, 9, 10).

Table 1 Simulation results for $p = 500$ and $\rho = 0$

	α	0.1	0.3	0.5	0.7	0.9	0.1	0.3	0.5	0.7	0.9
		snr = 0.5					snr = 1				
RTP	CTFR	0.712	0.227	0.679	0.475	0.907	0.926	0.220	0.193	**1.155**	**1.089**
	MCP	0.619	**1.258**	0.450	0.530	0.608	0.473	**1.981**	0.197	0.572	**1.680**
	SCAD	0.443	1.000	**2.364**	0.434	**1.291**	0.577	**1.045**	**2.056**	0.658	0.971
	aLasso	0.500	0.608	**1.711**	**1.970**	**1.079**	0.176	**1.155**	0.911	**5.630**	**1.023**
RFP	CTFR	0.105	0.108	0.225	0.130	0.170	0.027	0.038	0.029	0.164	0.158
	MCP	0.233	0.320	0.268	0.205	0.135	0.155	0.414	0.142	0.232	0.357
	SCAD	0.500	0.872	0.903	0.500	0.738	0.572	0.820	0.849	0.633	0.498
	aLasso	**1.200**	0.625	**1.416**	0.742	**1.198**	0.497	**1.731**	0.551	**1.666**	**1.012**
RPE	CTFR	**1.587**	0.837	0.936	**1.283**	**1.979**	**2.542**	0.843	0.902	**3.439**	**3.212**
	MCP	0.496	0.900	0.795	**1.017**	**1.020**	0.312	**1.003**	0.302	1.149	**2.813**
	SCAD	0.309	0.812	**1.596**	**1.117**	0.856	0.288	0.630	**1.276**	0.925	**1.166**
	aLasso	**1.114**	**1.323**	**2.868**	**3.250**	**1.619**	0.759	**2.234**	**1.623**	**4.947**	**1.313**
		snr = 2					snr = 5				
RTP	CTFR	0.970	0.171	0.312	0.628	**1.109**	0.820	0.199	0.320	0.717	**1.115**
	MCP	0.781	**1.140**	0.235	0.673	**1.500**	0.500	**2.000**	0.367	0.744	**1.280**
	SCAD	0.556	0.945	**1.750**	0.486	**1.394**	0.301	**1.000**	**3.260**	0.706	0.954
	aLasso	0.306	0.711	**1.391**	**3.150**	0.986	0.149	0.602	**1.640**	**6.450**	0.936
RFP	CTFR	0.001	0.002	0.006	0.031	0.102	0.002	0.001	0.008	0.043	0.059
	MCP	0.156	0.165	0.109	0.170	0.342	0.084	0.189	0.157	0.163	0.171
	SCAD	0.620	0.451	0.577	0.541	0.547	0.229	0.423	**1.042**	0.575	0.378
	aLasso	0.604	**1.047**	0.921	**1.411**	0.934	0.430	0.849	0.967	**1.967**	0.842
RPE	CTFR	**3.712**	**1.040**	**1.954**	**3.231**	**6.045**	**5.945**	**1.745**	**3.441**	**7.927**	**12.286**
	MCP	0.284	0.469	0.295	0.811	**2.743**	0.185	0.418	0.161	**1.179**	4.221
	SCAD	0.289	0.437	0.984	0.501	**1.611**	0.139	0.351	0.977	0.597	**2.011**
	aLasso	**1.108**	**1.606**	**2.169**	**3.538**	**1.148**	0.731	**1.551**	**2.164**	**3.674**	0.831
		snr = 10					snr = 20				
RTP	CTFR	0.520	0.102	0.222	0.429	**1.140**	**1.000**	0.084	0.307	0.574	**1.437**
	MCP	0.667	**1.470**	0.399	0.713	**1.135**	0.508	**1.930**	0.347	0.857	**1.157**
	SCAD	0.241	**1.007**	**4.130**	0.662	0.957	0.228	0.995	**4.450**	0.635	0.930
	aLasso	0.140	0.361	**2.767**	**6.930**	0.946	0.127	0.449	**2.213**	**7.74**	0.955
RFP	CTFR	0.000	0.000	0.002	0.013	0.029	0.000	0.000	0.001	0.011	0.071
	MCP	0.098	0.274	0.139	0.150	0.176	0.067	0.279	0.090	0.113	0.160
	SCAD	0.305	0.487	**1.389**	0.402	0.403	0.176	0.637	0.989	0.412	0.303
	aLasso	0.323	0.639	**1.316**	**2.645**	0.862	0.256	0.641	**1.374**	**3.304**	0.881
RPE	CTFR	**8.631**	**2.160**	**3.318**	**10.859**	**22.52**	**17.507**	**2.128**	**9.489**	**19.077**	**48.814**
	MCP	0.208	0.521	0.289	**1.231**	**3.826**	0.127	0.726	0.164	0.775	**10.836**
	SCAD	0.168	0.497	**1.665**	**1.009**	**1.454**	0.118	0.529	**1.701**	0.268	**6.561**
	aLasso	0.411	**1.078**	**2.678**	**4.806**	0.874	0.631	**1.122**	**2.446**	**4.640**	0.598

Table 2 Simulation results for $p = 500$ and $\rho = 0.2$

	α	0.1	0.3	0.5	0.7	0.9	0.1	0.3	0.5	0.7	0.9
		snr = 0.5					snr = 1				
RTP	CTFR	0.658	**0.190**	0.425	0.441	0.873	0.697	0.389	0.210	0.846	0.589
	MCP	0.944	0.816	0.463	0.438	0.294	0.678	**1.414**	0.341	0.476	0.669
	SCAD	0.574	**1.042**	**1.737**	0.546	0.781	0.728	**1.027**	**1.212**	0.845	0.72
	aLasso	0.500	0.544	**2.028**	**2.237**	**1.083**	0.350	**1.081**	0.993	3.01	**1.21**
RFP	CTFR	0.141	0.064	0.145	0.158	0.309	0.024	0.123	0.045	0.173	0.097
	MCP	0.281	0.16	0.287	0.179	0.143	0.124	0.262	0.177	0.161	0.112
	SCAD	0.696	0.951	0.621	0.539	0.511	0.615	0.625	0.497	0.838	0.353
	aLasso	**1.511**	0.758	**1.974**	0.985	**1.068**	0.857	**1.286**	0.812	**1.376**	**1.387**
RPE	CTFR	**1.436**	0.653	**1.016**	**1.553**	**2.837**	**2.496**	0.793	0.918	**2.585**	**2.74**
	MCP	0.666	0.460	0.571	**1.029**	**1.656**	0.292	0.84	0.316	**1.127**	**2.565**
	SCAD	0.453	0.666	**1.314**	0.804	**1.136**	0.371	0.632	**1.070**	0.757	**1.314**
	aLasso	**1.232**	**1.420**	**3.455**	**2.746**	**1.397**	**1.026**	**1.981**	**1.780**	**3.287**	**1.086**
		snr = 2					snr = 5				
RTP	CTFR	0.970	0.232	0.469	0.720	0.725	0.670	0.062	0.280	0.569	**2.367**
	MCP	0.529	**1.730**	0.389	0.650	**1.081**	1.000	0.740	0.336	0.723	0.963
	SCAD	0.474	0.995	**2.100**	0.635	**1.071**	0.283	0.796	**3.230**	0.624	0.958
	aLasso	0.282	0.886	**1.095**	**3.470**	0.967	0.181	0.283	3.643	**5.410**	0.968
RFP	CTFR	0.036	0.036	0.122	0.121	0.087	0.002	0.000	0.056	0.029	0.213
	MCP	0.052	0.316	0.209	0.224	0.139	0.169	0.120	0.141	0.126	0.160
	SCAD	0.248	0.592	**1.213**	0.840	0.385	0.291	0.386	0.947	0.413	0.375
	aLasso	0.673	0.985	**1.185**	**2.15**	0.933	0.510	0.608	**2.307**	**2.117**	0.903
RPE	CTFR	**4.165**	**1.074**	**1.611**	**3.687**	**5.036**	**5.894**	**1.105**	**2.275**	**6.683**	**13.925**
	MCP	0.165	**1.107**	0.226	0.972	**3.298**	0.410	0.851	0.444	0.891	**3.595**
	SCAD	0.176	0.631	**1.290**	0.486	**1.943**	0.252	0.731	**2.233**	0.513	**2.038**
	aLasso	0.833	**1.993**	**1.657**	**4.283**	**1.069**	0.599	0.944	**2.748**	**4.194**	0.926
		snr = 10					snr = 20				
RTP	CTFR	0.980	0.128	0.266	0.603	**2.257**	1.000	0.153	0.206	0.759	**1.420**
	MCP	0.329	**2.941**	0.303	0.677	**1.256**	0.500	**2.000**	0.266	0.762	**1.405**
	SCAD	0.159	0.993	**6.118**	0.779	0.756	0.316	1.000	**3.040**	0.610	0.895
	aLasso	0.064	0.475	**2.105**	**15.412**	0.949	0.130	0.633	**1.575**	**7.540**	0.963
RFP	CTFR	0.000	0.001	0.046	0.032	0.371	0.000	0.001	0.001	0.068	0.103
	MCP	0.073	0.144	0.096	0.094	0.279	0.067	0.064	0.070	0.100	0.140
	SCAD	0.147	0.190	1.220	0.390	0.322	0.147	0.154	0.582	0.344	0.271
	aLasso	0.259	0.780	**1.326**	**3.922**	0.893	0.300	0.794	**1.204**	**2.866**	0.898
RPE	CTFR	**11.352**	**2.611**	**2.308**	**18.033**	**15.039**	**21.037**	**2.078**	**6.812**	**18.013**	**46.238**
	MCP	0.125	0.442	0.310	**1.403**	**4.361**	0.134	0.249	0.069	**1.176**	**13.914**
	SCAD	0.091	0.192	**2.381**	**1.139**	**1.655**	0.100	0.175	0.830	0.471	**4.997**
	aLasso	0.398	1.509	**2.044**	**7.357**	0.994	0.506	**1.363**	**2.264**	**5.146**	0.619

Table 3 Simulation results for $p = 500$ and $\rho = 0.4$

	α	0.1	0.3	0.5	0.7	0.9	0.1	0.3	0.5	0.7	0.9
		snr = 0.5					snr = 1				
RTP	CTFR	0.838	0.268	0.421	0.598	0.761	0.904	0.357	0.323	0.736	0.673
	MCP	0.540	**1.368**	0.369	0.443	0.472	0.354	**2.654**	0.333	0.423	0.557
	SCAD	0.504	0.973	**1.574**	0.556	0.793	0.393	0.98	**2.365**	0.813	0.517
	aLasso	0.479	0.882	**1.310**	**2.559**	**1.293**	0.187	**1.050**	0.98	**5.846**	**1.365**
RFP	CTFR	0.184	0.155	0.201	0.263	0.224	0.041	0.104	0.250	0.099	0.153
	MCP	0.145	0.189	0.204	0.176	0.098	0.072	0.225	0.341	0.094	0.091
	SCAD	0.466	0.573	0.606	0.735	0.371	0.245	0.528	**1.140**	0.734	0.252
	aLasso	**1.531**	**1.126**	**1.468**	**1.550**	**1.294**	0.575	0.955	**1.696**	**2.014**	**1.533**
RPE	CTFR	**1.678**	0.992	**1.657**	**1.120**	**1.686**	**2.367**	**1.006**	0.764	**3.500**	**3.079**
	MCP	0.358	**1.442**	0.729	**1.095**	**1.522**	0.291	0.930	0.363	**1.097**	**3.059**
	SCAD	0.346	0.846	**1.801**	0.559	**1.793**	0.334	0.576	**1.269**	0.860	**1.197**
	aLasso	**1.769**	**1.837**	**2.115**	**3.028**	**1.460**	0.676	**2.440**	**2.037**	**4.562**	**1.091**
		snr = 2					snr = 5				
RTP	CTFR	1.000	0.187	0.351	0.769	0.900	0.554	0.206	0.255	0.621	**1.188**
	MCP	0.550	**1.560**	0.283	0.488	0.726	0.466	**1.913**	0.417	0.472	0.592
	SCAD	0.427	0.978	**1.930**	0.422	0.997	0.277	0.984	**3.685**	0.558	0.689
	aLasso	0.298	0.786	**1.267**	**3.490**	0.987	0.173	0.551	**1.806**	**5.511**	**1.049**
RFP	CTFR	0.098	0.045	0.024	0.211	0.153	0.000	0.022	0.002	0.255	0.151
	MCP	0.080	0.136	0.059	0.146	0.101	0.054	0.106	0.088	0.129	0.086
	SCAD	0.247	0.470	0.426	0.415	0.364	0.216	0.254	0.700	0.611	0.240
	aLasso	**1.152**	0.999	**1.097**	**1.570**	0.970	0.380	0.854	**1.045**	**2.307**	**1.157**
RPE	CTFR	**2.591**	**1.006**	**2.454**	**2.395**	**5.005**	**5.673**	**1.737**	**4.061**	**4.630**	**8.596**
	MCP	0.212	**1.201**	0.335	**1.243**	**2.896**	0.296	0.626	0.360	**1.363**	**3.855**
	SCAD	0.153	0.759	**1.379**	0.666	**2.156**	0.222	0.353	**1.882**	0.636	**2.792**
	aLasso	**1.072**	**1.460**	**2.278**	**3.410**	**1.045**	0.735	**1.223**	**2.203**	**4.195**	0.798
		snr = 10					snr = 20				
RTP	CTFR	1.000	0.130	0.249	0.586	**1.240**	1.000	0.118	0.310	0.338	**1.096**
	MCP	0.649	**1.480**	0.282	0.633	0.703	0.532	**1.930**	0.297	0.637	0.960
	SCAD	0.283	0.961	**3.390**	0.584	0.569	0.266	**1.043**	**3.620**	0.516	0.720
	aLasso	0.127	0.433	**2.273**	**7.650**	0.967	0.131	0.519	**1.989**	**7.380**	0.918
RFP	CTFR	0.006	0.019	0.012	0.018	0.070	0.001	0.002	0.049	0.007	0.065
	MCP	0.038	0.093	0.044	0.076	0.088	0.053	0.053	0.038	0.066	0.082
	SCAD	0.109	0.316	0.478	0.242	0.150	0.103	0.296	0.386	0.223	0.167
	aLasso	0.508	0.957	1.311	**2.270**	0.904	0.559	0.657	**1.365**	**2.000**	0.830
RPE	CTFR	**7.373**	0.999	**4.014**	**14.454**	**30.866**	**11.127**	**1.383**	**6.855**	**22.267**	**50.654**
	MCP	0.145	0.533	0.175	**1.623**	**10.358**	0.158	0.562	0.106	**1.583**	**15.923**
	SCAD	0.114	0.429	**1.305**	0.746	**5.527**	0.109	0.396	**1.064**	0.681	**7.130**
	aLasso	0.566	**1.092**	**2.844**	**4.668**	0.718	0.546	**1.199**	**2.298**	**4.481**	0.652

Table 4 Simulation results for $p = 500$ and $\rho = 0.6$

	α	0.1	0.3	0.5	0.7	0.9	0.1	0.3	0.5	0.7	0.9
		snr = 0.5					snr = 1				
RTP	CTFR	0.627	0.287	0.296	0.537	0.841	0.897	0.256	0.348	0.521	0.816
	MCP	**1.111**	0.72	0.336	0.211	0.317	0.816	0.586	0.189	0.247	0.326
	SCAD	0.988	0.952	0.773	0.510	0.634	0.549	0.855	**1.161**	0.469	0.511
	aLasso	0.620	0.805	**1.524**	**2.227**	**1.65**	0.374	0.514	**1.974**	**2.874**	**1.142**
RFP	CTFR	0.077	0.099	0.151	0.166	0.346	0.211	0.330	0.302	0.178	0.101
	MCP	0.058	0.069	0.058	0.087	0.119	0.085	0.075	0.144	0.071	0.048
	SCAD	0.358	0.272	0.310	0.342	0.620	0.304	0.367	0.452	0.384	0.177
	aLasso	**1.356**	**1.254**	**1.647**	**1.336**	**1.766**	**1.531**	**1.354**	**1.774**	**1.136**	**1.202**
RPE	CTFR	**1.587**	**1.649**	0.908	**2.012**	**1.636**	**1.729**	0.497	0.879	**2.911**	**5.476**
	MCP	0.767	0.517	0.993	**1.208**	**1.172**	0.999	0.820	0.524	**1.247**	**3.192**
	SCAD	0.528	0.601	0.824	**2.327**	0.476	0.562	0.868	**1.435**	0.854	**1.517**
	aLasso	**1.190**	**1.901**	**2.819**	**2.828**	**2.869**	**1.028**	**1.669**	**3.480**	**3.521**	**1.190**
		snr = 2					snr = 5				
RTP	CTFR	0.788	0.238	0.260	0.602	**1.648**	0.682	0.080	0.324	0.748	0.993
	MCP	0.615	0.750	0.289	0.402	0.388	0.449	**1.261**	0.176	0.453	0.458
	SCAD	0.347	0.780	**1.700**	0.810	0.443	0.307	0.913	**2.080**	0.367	0.481
	aLasso	0.188	0.454	**2.308**	**5.012**	**1.283**	0.165	0.605	**1.681**	**5.852**	0.947
RFP	CTFR	0.192	0.174	0.144	0.064	0.316	0.033	0.003	0.195	0.054	0.103
	MCP	0.040	0.073	0.054	0.035	0.060	0.033	0.035	0.032	0.031	0.031
	SCAD	0.127	0.265	0.394	0.291	0.271	0.126	0.277	0.273	0.115	0.118
	aLasso	0.866	**1.121**	**1.753**	**1.703**	**1.599**	0.959	0.837	**1.701**	**1.407**	0.906
RPE	CTFR	**3.057**	**1.029**	**1.198**	**4.154**	**4.341**	**3.621**	0.957	**1.399**	**6.32**	**15.521**
	MCP	0.609	0.998	0.952	**1.473**	**1.617**	0.504	0.851	0.337	**1.413**	**7.398**
	SCAD	0.278	0.642	**2.473**	**1.827**	0.839	0.278	0.746	**1.738**	0.895	**3.342**
	aLasso	0.731	**1.362**	**3.509**	**5.013**	**1.509**	0.753	**1.445**	**2.473**	**3.838**	0.888
		snr = 10					snr = 20				
RTP	CTFR	0.515	0.196	0.233	0.578	**1.686**	1.000	0.139	0.252	0.409	0.930
	MCP	0.635	**1.515**	0.37	0.669	0.537	0.500	**2.000**	0.398	0.715	0.631
	SCAD	0.311	0.962	**2.949**	0.710	0.436	0.225	1.000	**4.290**	0.665	0.555
	aLasso	0.140	0.478	**2.051**	**7.000**	0.957	0.120	0.449	**2.215**	**8.080**	0.958
RFP	CTFR	0.000	0.120	0.009	0.039	0.328	0.017	0.011	0.011	0.014	0.070
	MCP	0.029	0.025	0.015	0.039	0.075	0.016	0.019	0.013	0.027	0.038
	SCAD	0.089	0.094	0.149	0.156	0.175	0.037	0.057	0.172	0.147	0.098
	aLasso	0.359	0.908	**1.576**	**2.354**	0.919	0.533	0.734	**1.401**	**2.641**	0.890
RPE	CTFR	**8.243**	**1.327**	**6.267**	**13.243**	**14.622**	**9.918**	**2.532**	**12.086**	**27.137**	**39.189**
	MCP	0.267	0.269	0.193	**1.420**	**3.765**	0.160	0.287	0.122	**1.539**	**9.805**
	SCAD	0.118	0.297	0.930	**1.110**	**2.468**	0.090	0.152	**1.187**	0.430	**4.786**
	aLasso	0.732	**1.070**	**3.361**	**4.406**	**1.028**	0.518	**1.208**	**2.533**	**5.022**	0.655

Table 5 Simulation results for $p = 500$ and $\rho = 0.8$

	α	0.1	0.3	0.5	0.7	0.9	0.1	0.3	0.5	0.7	0.9
		snr = 0.5					snr = 1				
RTP	CTFR	0.727	0.364	0.580	0.276	0.926	0.891	0.191	0.218	0.752	1.737
	MCP	0.185	0.818	0.227	0.140	0.161	0.860	0.855	0.093	0.183	0.381
	SCAD	0.230	0.796	**1.212**	0.227	**1.040**	0.476	0.842	**1.055**	0.350	0.341
	aLasso	0.600	0.678	**1.852**	**2.424**	**2.173**	0.234	0.590	**2.035**	**5.509**	**1.191**
RFP	CTFR	0.390	0.322	0.268	0.340	0.483	0.195	0.155	0.275	0.124	0.290
	MCP	0.110	0.068	0.092	0.067	0.068	0.024	0.036	0.065	0.042	0.021
	SCAD	0.265	0.306	0.396	0.412	0.416	0.047	0.146	0.483	0.171	0.123
	aLasso	**1.896**	**1.330**	**2.135**	**2.038**	**2.113**	**1.181**	0.976	**2.789**	**2.391**	**1.333**
RPE	CTFR	**1.826**	**1.741**	**3.041**	0.686	**1.304**	**2.472**	**1.015**	0.809	**2.897**	**3.735**
	MCP	**1.401**	**1.317**	**2.374**	**1.323**	0.844	0.409	0.613	0.994	**1.269**	**1.407**
	SCAD	0.674	**1.177**	**2.083**	0.889	**1.224**	0.253	0.572	**1.896**	**2.012**	0.639
	aLasso	**4.137**	**1.879**	**4.102**	**3.505**	**4.485**	0.843	**1.471**	**4.418**	**5.314**	**1.850**
		snr = 2					snr = 5				
RTP	CTFR	0.850	0.249	0.163	0.213	0.688	0.515	0.289	0.185	0.629	**1.619**
	MCP	0.351	**1.633**	0.588	0.332	0.130	0.730	0.598	0.263	0.402	0.404
	SCAD	0.217	0.786	3.033	0.763	0.215	0.636	0.659	**1.134**	0.735	0.290
	aLasso	0.148	0.542	**1.799**	**7.500**	**1.163**	0.155	0.768	**1.452**	**6.216**	**1.237**
RFP	CTFR	0.057	0.022	0.007	0.013	0.314	0.000	0.456	0.025	0.033	0.460
	MCP	0.015	0.088	0.052	0.035	0.046	0.035	0.098	0.028	0.028	0.120
	SCAD	0.048	0.141	0.185	0.138	0.184	0.085	0.278	0.081	0.107	0.165
	aLasso	0.516	0.763	**1.174**	**2.276**	**1.425**	0.336	**2.441**	**1.227**	**2.419**	**1.512**
RPE	CTFR	**2.954**	**3.133**	**1.966**	**4.271**	**2.185**	**5.646**	**1.478**	**1.187**	**13.083**	**5.675**
	MCP	0.388	**1.844**	**1.661**	**1.701**	**1.042**	0.621	**1.530**	0.627	**1.834**	**2.417**
	SCAD	0.224	0.983	**3.186**	**3.348**	0.668	0.272	**1.467**	**1.351**	**3.054**	0.942
	aLasso	0.574	**1.201**	**2.521**	**5.198**	**1.854**	0.579	**1.684**	**2.702**	**4.246**	**1.425**
		snr = 10					snr = 20				
RTP	CTFR	0.825	0.151	0.160	0.323	0.986	0.725	0.092	0.146	0.367	0.699
	MCP	0.392	**1.587**	0.247	0.554	0.695	0.355	**1.912**	0.184	0.547	**1.097**
	SCAD	0.176	0.937	**3.062**	0.538	0.386	0.227	0.928	**2.712**	0.478	0.442
	aLasso	0.100	0.416	**2.350**	**9.600**	0.938	0.094	0.601	**1.633**	**10.325**	0.965
RFP	CTFR	0.108	0.167	0.001	0.005	0.121	0.052	0.001	0.037	0.003	0.037
	MCP	0.018	0.068	0.017	0.064	0.067	0.024	0.023	0.029	0.030	0.056
	SCAD	0.028	0.094	0.118	0.078	0.070	0.050	0.029	0.138	0.060	0.053
	aLasso	0.581	0.843	**1.314**	**3.154**	0.866	0.586	0.594	**1.272**	**2.431**	0.857
RPE	CTFR	**7.220**	0.955	**6.125**	**19.082**	**27.456**	**8.939**	**1.910**	**3.453**	**38.43**	**62.878**
	MCP	0.515	**1.482**	0.389	**2.041**	**4.982**	0.474	0.630	0.158	**1.997**	**17.944**
	SCAD	0.233	0.795	**3.028**	**1.335**	**2.709**	0.312	0.347	**1.947**	0.684	**7.063**
	aLasso	0.550	**1.183**	**2.885**	**6.099**	0.971	0.574	**1.406**	**2.095**	**5.125**	0.607

Table 6 Simulation results for $p = 1000$ and $\rho = 0$

	α	0.1	0.3	0.5	0.7	0.9	0.1	0.3	0.5	0.7	0.9
		snr = 0.5					snr = 1				
RTP	CTFR	0.759	0.626	0.556	0.459	0.368	0.735	0.331	0.299	0.770	**1.039**
	MCP	0.481	**1.379**	0.929	0.563	0.215	**1.197**	0.704	0.669	0.692	0.587
	SCAD	0.452	**1.009**	**2.086**	**1.091**	0.476	0.778	**1.013**	**1.276**	**1.364**	0.564
	aLasso	0.468	0.807	**1.292**	**2.103**	**1.081**	0.419	0.595	**1.645**	**2.378**	**1.214**
RFP	CTFR	0.057	0.204	0.244	0.118	0.196	0.033	0.022	0.030	0.128	0.192
	MCP	0.174	0.342	0.446	0.304	0.058	0.206	0.192	0.361	0.233	0.188
	SCAD	0.453	0.896	0.935	0.945	0.439	0.687	0.734	0.836	**1.327**	0.337
	aLasso	**1.175**	0.675	**1.416**	0.806	0.998	0.724	0.843	**1.166**	**1.262**	**1.229**
RPE	CTFR	**1.491**	0.888	0.900	**1.231**	**1.387**	**2.105**	0.648	**1.109**	**2.353**	**4.058**
	MCP	0.335	**1.591**	0.660	**1.008**	**1.225**	0.480	0.518	0.316	0.983	**2.523**
	SCAD	0.337	0.975	**1.514**	0.938	**1.018**	0.415	0.630	**1.048**	0.642	**1.475**
	aLasso	**1.035**	**1.555**	**1.870**	**3.003**	**1.320**	**1.022**	**1.755**	**2.943**	**3.191**	**1.094**
		snr = 2					snr = 5				
RTP	CTFR	0.735	0.213	0.326	0.582	0.662	0.530	0.085	0.257	0.503	**2.944**
	MCP	0.444	**1.809**	0.671	0.620	0.470	**1.796**	0.510	0.566	0.772	0.746
	SCAD	0.259	0.985	**3.912**	0.914	0.685	0.287	0.944	**3.590**	0.776	0.866
	aLasso	0.183	0.526	**1.902**	**5.603**	0.931	0.196	0.158	**6.278**	**4.970**	0.952
RFP	CTFR	0	0.001	0.011	0.130	0.120	0.000	0.000	0.005	0.030	0.239
	MCP	0.053	0.392	0.242	0.162	0.177	0.351	0.122	0.213	0.157	0.117
	SCAD	0.121	0.692	**2.271**	0.580	0.438	0.248	0.585	**1.423**	0.636	0.383
	aLasso	0.326	0.837	**1.078**	**2.730**	0.933	0.418	0.319	**3.034**	**2.428**	0.914
RPE	CTFR	**4.262**	0.837	**1.353**	**3.693**	**5.560**	**5.893**	0.768	**2.886**	**5.751**	**28.943**
	MCP	0.226	**1.057**	0.269	**1.239**	**3.184**	0.763	0.292	0.263	**1.152**	**4.738**
	SCAD	0.146	0.627	**1.982**	0.951	**1.324**	0.226	0.55	**1.904**	0.619	**2.354**
	aLasso	0.431	**1.336**	**2.230**	**5.961**	**1.046**	0.546	0.748	**5.573**	**4.379**	0.809
		snr = 10					snr = 20				
RTP	CTFR	0.980	0.143	0.243	0.625	**1.079**	1.000	0.200	0.375	0.289	0.965
	MCP	0.329	**2.922**	0.441	0.886	**1.262**	0.505	**1.990**	0.599	0.802	0.923
	SCAD	0.156	0.987	**6.314**	0.914	0.956	0.220	**1.005**	**4.640**	0.768	**1.045**
	aLasso	0.083	0.472	**2.099**	**11.941**	0.964	0.168	0.436	**2.268**	**5.840**	0.947
RFP	CTFR	0.000	0.000	0.000	0.032	0.051	0.000	0.000	0.002	0.002	0.044
	MCP	0.091	0.166	0.170	0.129	0.170	0.108	0.176	0.116	0.134	0.141
	SCAD	0.098	0.484	**1.683**	0.571	0.375	0.109	0.509	0.947	0.446	0.416
	aLasso	0.253	0.615	**1.487**	**3.27**	0.873	0.432	0.576	**1.400**	**2.026**	0.890
RPE	CTFR	**9.020**	**1.403**	**3.391**	**13.554**	**28.543**	**15.614**	**2.076**	**9.076**	**13.473**	**41.154**
	MCP	0.164	0.438	0.132	**1.117**	**6.171**	0.143	0.443	0.115	**1.044**	**7.410**
	SCAD	0.073	0.440	**1.498**	0.519	**2.170**	0.067	0.404	**1.362**	0.308	**3.708**
	aLasso	0.361	**1.159**	**2.822**	**5.423**	0.691	0.653	**1.039**	**2.358**	**3.825**	0.540

Table 7 Simulation results for $p = 1000$ and $\rho = 0.2$

	α	0.1	0.3	0.5	0.7	0.9	0.1	0.3	0.5	0.7	0.9
		snr = 0.5					snr = 1				
RTP	CTFR	0.885	0.447	0.604	0.566	0.581	0.926	0.447	0.411	0.462	0.579
	MCP	0.581	**1.500**	0.582	0.414	0.475	0.376	**2.370**	0.941	0.598	0.401
	SCAD	0.515	0.965	**2.038**	0.589	**1.072**	0.274	**1.023**	**3.796**	**1.082**	0.548
	aLasso	0.468	0.970	**1.337**	**2.404**	**1.326**	0.247	0.675	**1.534**	**4.593**	**1.165**
RFP	CTFR	0.213	0.106	0.268	0.267	0.330	0.028	0.075	0.085	0.158	0.170
	MCP	0.213	0.428	0.186	0.143	0.339	0.079	0.327	0.322	0.214	0.122
	SCAD	0.641	0.804	**1.324**	0.416	**1.010**	0.407	0.670	**1.114**	**1.070**	0.291
	aLasso	0.940	**2.095**	**1.501**	**1.963**	**1.524**	0.784	**1.124**	0.986	**2.347**	**1.296**
RPE	CTFR	**1.983**	**1.033**	0.914	**1.327**	**1.822**	**2.179**	**1.011**	**1.564**	**1.797**	**2.534**
	MCP	0.348	**1.478**	0.939	0.988	**1.043**	0.171	**1.007**	0.564	**1.090**	**1.741**
	SCAD	0.291	0.903	**2.507**	**1.283**	0.693	0.201	0.671	**1.998**	0.700	**1.506**
	aLasso	0.897	**1.536**	**2.567**	**4.958**	**1.983**	0.984	**1.510**	**1.950**	**3.868**	**1.115**
		snr = 2					snr = 5				
RTP	CTFR	0.820	0.299	0.474	0.612	0.944	0.505	0.095	0.210	0.879	0.955
	MCP	0.794	**1.06**	0.761	0.678	0.616	0.752	**1.232**	0.283	0.730	**1.226**
	SCAD	0.380	0.937	**2.710**	0.855	0.941	0.503	0.962	**1.899**	0.842	0.759
	aLasso	0.329	0.456	**2.063**	**3.240**	**1.186**	0.191	0.693	**1.617**	**5.152**	**1.005**
RFP	CTFR	0.008	0.066	0.049	0.128	0.143	0.000	0.000	0.006	0.106	0.112
	MCP	0.122	0.191	0.305	0.182	0.151	0.157	0.245	0.086	0.143	0.207
	SCAD	0.358	0.552	**1.109**	0.757	0.589	0.405	0.624	0.680	0.548	0.358
	aLasso	0.825	**1.207**	**1.252**	**1.763**	**1.450**	0.496	**1.002**	**1.860**	**2.350**	0.959
RPE	CTFR	**3.771**	**1.030**	**2.273**	**2.335**	**4.520**	**5.604**	0.933	**1.905**	**8.132**	**14.42**
	MCP	0.239	0.653	0.537	**1.138**	**1.636**	0.276	0.841	0.216	**1.069**	**5.701**
	SCAD	0.174	0.545	**1.648**	0.870	**1.190**	0.268	0.765	**1.376**	0.586	**2.383**
	aLasso	**1.034**	**1.239**	**2.743**	**3.355**	**1.140**	0.657	**1.357**	**2.453**	**3.867**	0.762
		snr = 10					snr = 20				
RTP	CTFR	1.000	0.165	0.403	0.579	**1.224**	0.500	0.133	0.289	0.525	0.780
	MCP	0.641	**1.460**	0.569	0.803	0.449	0.524	**1.870**	0.480	0.829	0.796
	SCAD	0.255	0.949	**3.950**	0.707	0.771	0.268	**1.010**	**3.780**	0.767	0.836
	aLasso	0.212	0.408	**2.487**	**4.770**	0.994	0.169	0.512	**1.932**	**5.88**	0.969
RFP	CTFR	0.001	0.001	0.027	0.061	0.156	0.000	0.000	0.004	0.042	0.067
	MCP	0.055	0.180	0.115	0.147	0.072	0.110	0.176	0.097	0.116	0.101
	SCAD	0.129	0.429	0.890	0.453	0.368	0.258	0.587	0.786	0.404	0.333
	aLasso	0.783	**1.119**	**1.452**	**2.005**	0.966	0.842	0.631	**1.492**	**1.922**	0.904
RPE	CTFR	**8.882**	0.78	**4.895**	**6.526**	**24.055**	**10.489**	**1.118**	**6.953**	**14.263**	**49.102**
	MCP	0.115	0.729	0.127	**1.010**	**11.007**	0.285	0.612	0.05	**1.025**	**17.04**
	SCAD	0.089	0.628	**1.562**	0.265	**5.789**	0.195	0.483	0.843	0.227	**6.902**
	aLasso	0.618	**1.139**	**2.416**	**3.732**	0.591	0.559	**1.243**	**2.278**	**3.743**	0.524

Table 8 Simulation results for $p = 1000$ and $\rho = 0.4$

	α	0.1	0.3	0.5	0.7	0.9	0.1	0.3	0.5	0.7	0.9
		snr = 0.5					snr = 1				
RTP	CTFR	0.804	0.600	0.413	0.693	0.288	0.839	0.377	0.534	0.662	**1.049**
	MCP	0.538	**1.625**	0.678	0.433	0.307	0.505	**1.500**	0.503	0.437	0.531
	SCAD	0.853	0.952	**1.393**	**1.033**	0.673	0.438	**1.039**	**1.887**	0.814	0.908
	aLasso	0.606	**1.413**	0.740	**2.339**	**1.678**	0.362	0.908	**1.379**	**3.161**	**1.344**
RFP	CTFR	0.096	0.184	0.115	0.168	0.175	0.084	0.141	0.138	0.355	0.340
	MCP	0.122	0.226	0.257	0.169	0.196	0.056	0.133	0.137	0.209	0.225
	SCAD	0.631	0.562	0.833	0.668	0.711	0.308	0.468	0.647	0.748	0.724
	aLasso	**1.351**	**1.388**	**1.011**	**1.380**	**2.037**	**1.612**	**1.971**	**1.744**	**2.607**	**1.898**
RPE	CTFR	**1.721**	**1.083**	0.922	**1.685**	**1.478**	**1.923**	**1.727**	**1.795**	**1.785**	**1.637**
	MCP	0.335	**1.201**	0.644	0.992	**1.436**	0.193	**1.078**	0.935	**1.193**	**1.268**
	SCAD	0.389	0.712	**1.309**	**1.115**	0.846	0.198	0.661	**1.539**	0.931	**1.092**
	aLasso	**1.256**	**2.169**	**1.840**	**3.910**	**1.692**	**1.965**	**1.958**	**2.004**	**4.032**	**2.062**
		snr = 2					snr = 5				
RTP	CTFR	0.610	0.369	0.235	0.600	0.538	0.797	0.179	0.431	0.627	0.948
	MCP	0.503	**1.86**	0.439	0.477	0.432	0.273	**2.922**	0.487	0.636	0.448
	SCAD	0.526	0.959	**1.810**	0.833	0.514	0.204	0.995	**4.031**	0.571	0.911
	aLasso	0.310	**1.037**	0.954	**3.290**	**1.167**	0.208	0.699	**1.418**	**5.328**	**1.157**
RFP	CTFR	0.012	0.019	0.010	0.111	0.065	0.004	0.003	0.009	0.083	0.212
	MCP	0.045	0.126	0.117	0.104	0.063	0.019	0.169	0.073	0.09	0.085
	SCAD	0.386	0.315	0.488	0.624	0.252	0.064	0.418	0.791	0.336	0.434
	aLasso	0.826	**1.576**	0.613	**1.155**	**1.224**	**1.234**	0.776	**1.235**	**2.666**	**1.446**
RPE	CTFR	**3.331**	0.968	**1.354**	**4.099**	**3.961**	**5.762**	**1.190**	**4.086**	**3.541**	**8.023**
	MCP	0.164	0.737	0.300	**1.300**	**4.057**	0.177	**1.029**	0.212	**1.137**	**4.446**
	SCAD	0.200	0.448	**1.241**	0.795	**1.746**	0.124	0.457	**2.027**	0.449	**3.143**
	aLasso	0.766	**2.062**	**1.619**	**3.412**	0.879	0.784	**1.297**	**1.976**	**5.084**	0.659
		snr = 10					snr = 20				
RTP	CTFR	0.760	0.266	0.295	0.449	**1.234**	1.000	0.218	0.199	0.819	0.625
	MCP	0.543	**1.670**	0.668	0.776	0.598	0.500	**2.000**	0.403	0.699	0.734
	SCAD	0.245	0.946	**4.070**	0.963	0.669	0.292	1.000	**3.190**	0.544	0.984
	aLasso	0.169	0.453	**2.196**	**5.750**	**1.105**	0.223	0.585	**1.695**	**4.740**	0.964
RFP	CTFR	0.000	0.001	0.011	0.013	0.136	0.000	0.000	0.004	0.219	0.042
	MCP	0.027	0.063	0.080	0.053	0.052	0.043	0.032	0.073	0.069	0.065
	SCAD	0.067	0.147	0.638	0.337	0.238	0.094	0.150	0.567	0.282	0.261
	aLasso	0.358	0.630	**1.369**	**2.511**	**1.330**	0.534	0.739	**1.377**	**2.538**	0.929
RPE	CTFR	**9.362**	**2.832**	**5.703**	**10.875**	**10.578**	**17.463**	**1.954**	**5.972**	**6.616**	**43.547**
	MCP	0.089	0.599	0.287	0.996	**3.081**	0.142	0.211	0.127	**1.025**	**14.857**
	SCAD	0.084	0.348	**1.510**	0.552	**1.855**	0.080	0.190	**1.500**	0.212	**8.766**
	aLasso	0.550	**1.100**	**2.085**	**3.886**	0.702	0.779	**1.208**	**2.117**	**3.327**	0.533

Table 9 Simulation results for $p = 1000$ and $\rho = 0.6$

	α	0.1	0.3	0.5	0.7	0.9	0.1	0.3	0.5	0.7	0.9
		snr = 0.5					snr = 1				
RTP	CTFR	0.640	0.234	0.606	0.333	**1.111**	0.942	0.295	0.560	0.489	**1.172**
	MCP	**2.167**	0.135	0.449	0.212	0.158	0.781	**1.058**	0.337	0.213	0.259
	SCAD	0.754	0.861	0.978	0.505	0.485	0.370	0.984	**1.788**	0.554	0.716
	aLasso	0.929	0.316	**3.556**	**1.697**	**1.140**	0.369	0.526	**2.438**	**4.000**	1.488
RFP	CTFR	0.084	0.651	0.113	0.274	0.186	0.071	0.030	0.322	0.231	0.289
	MCP	0.063	0.116	0.098	0.079	0.039	0.037	0.033	0.117	0.093	0.052
	SCAD	0.353	0.668	0.278	0.745	0.150	0.141	0.285	0.471	0.613	0.345
	aLasso	0.935	**2.771**	**1.444**	**2.399**	**1.363**	**1.779**	**1.265**	**3.143**	**2.200**	**1.985**
RPE	CTFR	**1.491**	0.556	**1.456**	0.984	**4.102**	**1.850**	0.752	**1.252**	**2.103**	**4.051**
	MCP	**1.19**	0.815	0.841	**1.145**	**1.405**	0.253	0.546	0.661	**1.382**	**2.295**
	SCAD	0.344	**1.148**	**1.430**	0.555	**1.706**	0.185	0.484	**1.821**	0.815	**1.574**
	aLasso	**1.847**	**1.598**	**4.677**	**2.539**	**1.432**	**1.353**	**1.716**	**3.678**	**3.777**	**1.204**
		snr = 2					snr = 5				
RTP	CTFR	0.840	0.158	0.320	0.610	**1.821**	1.000	0.300	0.315	0.403	0.540
	MCP	**1.071**	0.667	0.441	0.270	0.300	0.495	**1.970**	0.612	0.525	0.332
	SCAD	0.340	0.893	**2.240**	0.450	0.504	0.270	0.995	**3.510**	0.614	0.483
	aLasso	0.273	0.280	**3.750**	**3.840**	**1.196**	0.202	0.541	**1.830**	**4.910**	0.958
RFP	CTFR	0.181	0.062	0.024	0.280	0.223	0.093	0.066	0.014	0.020	0.053
	MCP	0.026	0.029	0.047	0.067	0.058	0.024	0.010	0.031	0.033	0.028
	SCAD	0.197	0.138	0.343	0.393	0.215	0.084	0.073	0.245	0.209	0.145
	aLasso	**1.687**	**1.710**	**1.550**	**2.162**	**1.528**	0.947	0.756	**1.308**	**1.632**	0.998
RPE	CTFR	**2.758**	0.522	**2.149**	**2.399**	**8.809**	**3.585**	**1.405**	**3.76**	**6.616**	**11.561**
	MCP	0.581	0.310	0.385	**1.558**	**3.064**	0.167	0.316	0.209	**1.587**	**4.892**
	SCAD	0.249	0.287	**1.802**	0.783	**2.235**	0.105	0.220	**1.320**	0.821	**2.827**
	aLasso	**1.189**	**1.446**	**4.137**	**4.281**	0.963	0.706	**1.135**	**2.268**	**4.001**	0.759
		snr = 10					snr = 20				
RTP	CTFR	1.000	0.293	0.245	0.473	**1.411**	1.000	0.167	0.284	0.404	**2.381**
	MCP	0.613	**1.510**	0.415	0.570	0.566	0.952	1.000	0.547	0.563	0.406
	SCAD	0.388	0.939	**2.31**	0.846	0.421	0.257	0.962	**3.610**	0.896	0.393
	aLasso	0.166	0.624	**1.571**	**5.810**	**1.118**	0.138	0.270	**3.676**	**7.130**	**1.080**
RFP	CTFR	0.000	0.180	0.043	0.020	0.282	0.008	0.022	0.048	0.017	0.191
	MCP	0.021	0.018	0.029	0.027	0.055	0.036	0.020	0.014	0.028	0.022
	SCAD	0.064	0.076	0.246	0.199	0.149	0.064	0.123	0.180	0.174	0.123
	aLasso	0.361	**1.757**	**1.318**	**2.505**	**1.386**	0.866	0.908	**1.974**	**1.721**	**1.116**
RPE	CTFR	**12.338**	**1.191**	**2.573**	**16.630**	**10.936**	**8.255**	0.762	**6.301**	**23.682**	**34.628**
	MCP	0.161	0.265	0.228	**1.703**	**4.286**	0.360	0.291	0.150	**2.436**	**8.167**
	SCAD	0.112	0.219	**1.008**	**1.353**	**1.777**	0.132	0.368	**1.246**	**1.142**	**3.267**
	aLasso	0.509	**1.614**	**2.451**	**3.982**	0.807	0.461	**1.050**	**3.556**	**4.045**	0.512

Table 10 Simulation results for $p = 1000$ and $\rho = 0.8$

	α	0.1	0.3	0.5	0.7	0.9	0.1	0.3	0.5	0.7	0.9
		snr = 0.5					snr = 1				
RTP	CTFR	0.582	0.268	0.697	0.170	**1.033**	0.833	0.511	0.197	1.000	0.655
	MCP	**2.733**	0.143	0.427	0.091	0.107	0.483	**1.062**	0.223	0.202	0.164
	SCAD	0.759	0.633	0.505	0.293	0.576	0.745	0.879	0.875	0.691	0.197
	aLasso	**1.470**	0.286	**4.033**	**1.044**	**2.012**	0.202	**1.127**	**1.328**	**5.104**	**1.638**
RFP	CTFR	0.065	0.468	0.096	0.310	0.309	0.278	0.067	0.228	0.159	0.340
	MCP	0.036	0.037	0.040	0.056	0.048	0.046	0.027	0.060	0.018	0.118
	SCAD	0.064	0.403	0.073	0.402	0.206	0.377	0.054	0.264	0.097	0.299
	aLasso	0.991	**1.968**	**1.305**	**1.972**	**2.809**	**1.341**	**2.514**	**1.936**	**1.401**	**2.072**
RPE	CTFR	**1.502**	**1.170**	**1.705**	0.667	**2.097**	**1.834**	**2.234**	0.477	**6.729**	**1.310**
	MCP	**1.150**	0.610	**2.362**	0.911	0.628	0.840	0.647	**1.513**	**1.281**	**1.856**
	SCAD	0.398	0.988	**1.710**	**1.042**	0.734	**1.031**	0.347	**1.092**	**4.971**	0.274
	aLasso	**2.057**	**1.376**	**4.975**	**2.465**	**2.898**	0.814	**3.821**	**2.565**	**5.006**	**3.550**
		snr = 2					snr = 5				
RTP	CTFR	0.906	0.382	0.383	0.508	**1.103**	0.825	0.140	0.623	0.939	**2.294**
	MCP	0.552	0.938	0.491	0.336	0.230	0.735	0.825	0.229	0.353	0.521
	SCAD	0.272	0.828	**2.094**	0.382	0.510	0.307	0.794	**1.905**	0.355	0.66
	aLasso	0.409	0.487	**2.322**	**2.875**	**1.467**	0.288	0.485	**2.765**	**4.016**	**1.101**
RFP	CTFR	0.268	0.285	0.025	0.204	0.188	0.143	0.018	0.283	0.281	0.262
	MCP	0.025	0.029	0.033	0.043	0.037	0.009	0.015	0.036	0.035	0.036
	SCAD	0.097	0.147	0.083	0.227	0.126	0.051	0.046	0.248	0.159	0.146
	aLasso	**1.692**	**1.414**	**1.431**	**2.054**	**1.93**	**1.564**	**1.151**	**2.919**	**2.468**	**1.227**
RPE	CTFR	**2.688**	0.926	**3.577**	**1.259**	**4.694**	**3.573**	**1.127**	**2.03**	**2.677**	**6.923**
	MCP	0.560	**1.216**	0.900	**1.235**	**1.378**	0.307	0.618	0.599	**1.491**	**2.622**
	SCAD	0.254	**1.053**	**2.655**	0.725	**1.873**	0.197	0.534	**2.194**	0.813	**2.224**
	aLasso	**1.869**	**1.158**	**3.204**	**4.027**	**1.362**	**1.414**	**1.723**	**3.468**	**4.318**	**1.200**
		snr = 10					snr = 20				
RTP	CTFR	0.633	0.388	0.194	0.212	**1.217**	0.680	0.227	0.240	0.376	**1.617**
	MCP	0.416	**1.127**	0.829	0.419	0.207	0.599	**1.400**	0.813	0.525	0.163
	SCAD	0.207	0.807	**4.266**	0.898	0.231	0.243	0.898	**3.760**	0.712	0.395
	aLasso	0.127	0.418	**2.255**	**8.316**	**1.048**	0.170	0.417	**2.431**	**5.820**	**1.041**
RFP	CTFR	0.000	0.298	0.009	0.006	0.503	0.000	0.030	0.017	0.063	0.534
	MCP	0.020	0.122	0.017	0.025	0.046	0.011	0.020	0.015	0.029	0.071
	SCAD	0.046	0.226	0.084	0.074	0.167	0.012	0.044	0.039	0.054	0.283
	aLasso	0.300	**1.106**	**1.875**	**3.584**	**1.277**	0.488	0.755	**1.424**	**2.096**	**1.264**
RPE	CTFR	**6.281**	**1.475**	**6.634**	**15.067**	**6.288**	**16.466**	**3.31**	**12.632**	**13.979**	**5.139**
	MCP	0.688	**1.860**	0.435	**2.743**	**1.850**	0.132	0.796	0.443	**1.520**	**1.732**
	SCAD	0.265	**1.516**	**1.271**	**3.562**	**1.096**	0.065	0.450	**1.012**	**2.413**	**1.076**
	aLasso	0.544	**1.187**	**3.235**	**4.389**	**1.295**	0.580	**1.044**	**2.128**	**3.466**	**1.353**

3.3 Observations

In this section, we briefly summarize our simulation study in three aspects.

3.3.1 In terms of True Positives

- We see from simulation results that the performance of Lasso is superior to CTFR, MCP, and SCAD in terms of selecting true parameters when the true model is very sparse, the signal-to-noise ratio is low, and the predictors are uncorrelated.
- When the predictors are uncorrelated, as the model gets less sparse (for larger α) the TP performance of CTFR improves and in some cases outperforms Lasso.
- As the number of predictors increases, the true positive value of Lasso and MCP decreases. To put it differently, the variable selection performance of Lasso and MCP decreases under the higher dimensional settings.
- Overall, adaptive Lasso had better performance in variable selection compared to Lasso, but its performance was still inferior to that of CTFR and MCP.

3.3.2 In terms of False Positives

- CTFR and MCP outperformed Lasso in terms of FP under any sparsity, signal-to-noise ratio, and the correlation between predictors cases. This reflected the fact that a cross-validated Lasso tends to over select.
- SCAD also outperformed Lasso in terms of FP unless signal-to-noise ratio and the correlation between predictors are high. Therefore, for a two-stage variable selection procedure, applying CTFR or MCP in the second stage after applying Lasso in the first stage would help to eliminate the noise variables selected by Lasso.
- Under the presence of high correlation between predictors, FP of MCP was smaller than that of CTFR. In other words, MCP had better performance in screening out irrelevant variables than CTFR when predictors were highly correlated to each other.

3.3.3 In terms of Prediction Errors

- Lasso outperformed CTFR and aLasso under almost all simulation set-ups.
- Lasso's prediction performance is significantly better than CTFR as the model became less sparse, with higher signal-to-noise ratio, and greater correlation value in the design.

– In real data examples it is usually assumed that there are some signals in the data and predictors are not independent to each other. For this parameter range ($\rho = 0.2$ and snr = 2 or 5), MCP exhibits a better performance than Lasso in terms of false positive selection and prediction error performance.

3.4 Non-normal Error Distributions

In this section, we compare the variable selection and prediction performance of the Lasso and CTFR when the errors in the linear model, with $n = 100$ and $p = 500$, have a heavier tail. We only consider Cauchy and t-distribution with a degree of freedom 2.

In Table 11, we summarize the simulation results for some selected parameters when the errors come from Cauchy distribution. We observe that CTFR is no longer better than Lasso in terms of FP regardless of the sparsity level of model, signal-to-noise ratio and correlation level among predictors. On the other hand, it outperforms Lasso in terms of variable selection performance. CTFR has much lower prediction error than that of Lasso in all cases except the case that the model is very sparse and has high signal-to-noise ratio.

In Table 12, we summarize the simulation results for some selected parameters when the errors come from t-distribution with two degrees of freedom. When we compare the results in these two tables, we see that the prediction errors significantly decrease as the tail properties of the error distribution get closer to the normal distribution. In various combinations of sparsity level and the value of correlation among predictors, as long as signal-to-noise ratio increases, CTFR performs better than Lasso in terms of false positive selection; that is, it selects fewer noise variables.

Table 11 Errors in the linear models are Cauchy distributed

	Cauchy distribution					
	True Positive		False Positive		Prediction Error	
(α,ρ,snr)	Lasso	CTFR	Lasso	CTFR	Lasso	CTFR
(0.1,0.0,0.5)	0.08	0.34	3.10	56.22	2872	122
(0.1,0.0,20)	0.90	1.44	5.66	48.92	19, 632	70, 573
(0.1,0.8,0.5)	0.00	0.26	2.64	65.80	32, 902	488
(0.1,0.8,20)	0.46	0.90	4.76	55.54	1, 115, 701	21, 232
(0.5,0.0,0.5)	0.12	1.16	5.00	51.40	1662	108
(0.5,0.0,20)	1.26	2.52	7.12	40.08	1499	116
(0.5,0.8,0.5)	0.12	1.40	2.74	63.06	50, 765	986
(0.5,0.8,20)	0.42	1.66	6.42	54.50	6871	168

Table 12 Errors in the linear models are t-distributed with two degrees of freedom

	t distribution with two degrees of freedom					
	True Positive		False Positive		Prediction Error	
(α,ρ,snr)	Lasso	CTFR	Lasso	CTFR	Lasso	CTFR
(0.1,0.0,0.5)	0.56	0.84	10.34	18.26	6.95	3.89
(0.1,0.0,20)	1.98	2.00	14.00	4.68	6.51	8.54
(0.1,0.8,0.5)	0.18	0.34	5.38	31.44	10.87	3.81
(0.1,0.8,20)	1.16	1.02	13.28	11.24	10.8	6.32
(0.5,0.0,0.5)	0.72	1.26	7.66	21.40	6.78	4.08
(0.5,0.0,20)	6.02	4.28	25.24	5.26	16.31	14.38
(0.5,0.8,0.5)	0.40	0.64	10.40	27.38	8.79	3.62
(0.5,0.8,20)	2.60	2.22	16.60	12.30	6.75	6.03

4 Real Data Examples

In this section we apply the regression methods considered in this paper to two real data sets and summarize their results.

4.1 Prostate Data

In this section, we provide an application of each regression methods we studied in this paper on prostate cancer data. The data come from a study conducted by Stamey et al. [25]. The predictors in the data are log of cancer volume (lcavol), log of prostate weight (lweight), age, log of benign prostatic hyperplasia amount (lbph), seminal vesicle invasion (svi), log of capsular penetration (lcp), Gleason score (gleason), and percentage Gleason scores 4 or 5 (pgg45). The response of interest is log of prostate specific antigen (lpsa). The total number of observations in the dataset is 97. All the regression methods were applied after standardizing predictors.

In Table 13, we report estimated coefficients by different methods for the prostate data. Further, the average prediction errors (APEs) are shown therein. According to these results, the CTFR picks up four response variables; the Lasso, SCAD, and MCP do not eliminate any response variables but aLasso eliminates only one. We also observe that the aLasso has the minimum APE and then CTFR, MCP, Lasso, and SCAD follow, respectively. From Fig. 1, it looks like error distributions are symmetric, and inter-quartile ranges are almost the same for each method.

Table 13 Estimated coefficients and APEs for prostate data

	Lasso	CTFR	SCAD	MCP	aLasso
(Intercept)	2.478	2.478	2.478	2.478	2.478
lcavol	0.655	0.512	0.670	0.665	0.647
lweight	0.263	0.090	0.264	0.266	0.265
age	−0.148	0.000	−0.156	−0.158	−0.118
lbph	0.135	0.000	0.141	0.140	0.115
svi	0.305	0.115	0.312	0.315	0.276
lcp	−0.124	0.000	−0.147	−0.148	−0.044
gleason	0.032	0.000	0.005	0.036	0.067
pgg45	0.116	0.000	0.146	0.126	0.000
APE	0.589	0.527	0.593	0.574	0.511

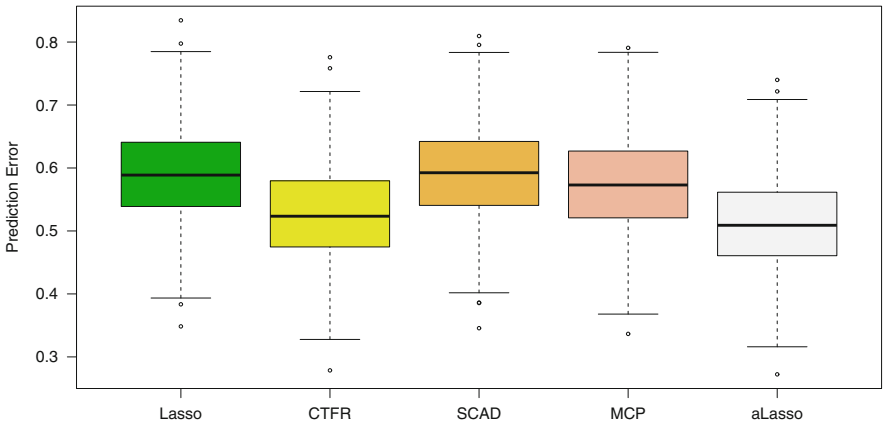

Fig. 1 Comparison of the estimators through prediction errors for prostate data

4.2 Production of Riboflavin in Bacillus subtilis Data

In [4], Bühlmann et al. made a data set on riboflavin production with *Bacillus subtilis* publicly available. In the data set, the logarithm of the riboflavin production rate is considered as the response variable corresponding to 4088 predictors which measure the logarithm of the expression level of 4088 genes. There are $n = 71$ samples. Therefore the design matrix for the dataset is $\mathbf{X} \in \mathbb{R}^{71\times 4088}$. We performed Lasso, SCAD, MCP, CTFR, aLasso to select a small subset of genes as the most important predictors for the model.

In Table 14, for each penalty estimator, we list the top 20 genes. Magnitude (absolute value) of the coefficient estimate was accompanied by each selected gene. For instance, in the case of CTFR, the absolute value of the coefficient estimate for the gene XHLA is 0.18. The table displays genes in a decreasing order with respect to their corresponding estimated values. As one can see, Lasso, SCAD, and aLasso selected more than 20 genes, while CTFR and MCP only selected 7 and 8 genes,

Table 14 Top 20 genes selected by each regression method from riboflavin data and their corresponding estimates

Lasso		CTFR		SCAD		MCP		aLasso	
gene	$\hat{\beta}$	gene	$\hat{\beta}$	gene	$\hat{\beta}$	gene	$\hat{\beta}$	alasso-gene	$\hat{\beta}$
YOAB	0.81	YOAB	0.23	YOAB	1.41	YOAB	1.45	YXLE	1.74
YEBC	0.53	XHLA	0.18	YHDZ	0.84	YHDZ	0.99	YXLF	1.25
LYSC	0.30	YXLD	0.13	SPOVAA	0.58	YXLD	0.46	YOAC	0.91
SPOVAA	0.26	YCKE	0.09	YEBC	0.51	SPOVAA	0.44	AADK	0.56
YQJU	0.23	LYSC	0.02	YXLD	0.44	CARA	0.39	PRKA	0.55
YXLD	0.22	YDAR	0.01	ARGF	0.36	XHLA	0.25	SPOVAB	0.54
YCLB	0.19	XTRA	0.01	XHLB	0.22	YSHB	0.06	YDDM	0.51
ARGF	0.19	YCGN	0.00	YTET	0.11	YEBC	0.04	YQJV	0.47
XHLB	0.16	AADK	0.00	YDDJ	0.08	AADK	0.00	YMFF	0.45
YFHE	0.15	AAPA	0.00	YQJU	0.08	AAPA	0.00	YYDB	0.44
YFIO	0.15	ABFA	0.00	YESJ	0.06	ABFA	0.00	PKSB	0.41
YHDS	0.14	ABH	0.00	YACN	0.06	ABH	0.00	YCLG	0.38
DNAJ	0.14	ABNA	0.00	YVDI	0.05	ABNA	0.00	ARGG	0.38
YBFI	0.14	ABRB	0.00	PTA	0.05	ABRB	0.00	YFIQ	0.36
YDDK	0.12	ACCA	0.00	YJCL	0.05	ACCA	0.00	YCLC	0.33
YKBA	0.11	ACCB	0.00	SPOIIAA	0.03	ACCB	0.00	YKVK	0.25
YYDA	0.11	ACCC	0.00	YHDS	0.02	ACCC	0.00	YCGP	0.25
PRIA	0.10	ACDA	0.00	YQIQ	0.02	ACDA	0.00	YLXX	0.24
YXLE	0.09	ACKA	0.00	YIST	0.02	ACKA	0.00	DNAK	0.22
YLXW	0.07	ACOA	0.00	KINA	0.02	ACOA	0.00	YQJU	0.19
APE	0.264		0.406		0.321		0.322		0.863

respectively. Lasso had the lowest average prediction errors among all five different penalty estimators.

From Fig. 2, we see that the error distributions are symmetric for Lasso, SCAD, and MCP, but it is left-skewed for CTFR and aLasso. CTFR and aLasso have a significantly larger inter-quartile range than those of Lasso, SCAD, and MCP.

Figure 3 depicts variable selection results for each penalty estimators. The blue line represents a general trend of the number of selected predictors by Lasso estimator for a given tuning parameter value. Each colored point represents the number of selected predictors with the corresponding tuning parameter value, which minimizes cross validation error. For instance, in the case of SCAD estimator, the estimator selected 26 predictors to minimize cross validation error. As CTFR's variable selection result is independent of the value of tuning parameter, the graph does not include it. However, from Table 14, one can observe that CTFR selected seven predictors, which is the least among all five penalty estimators of consideration.

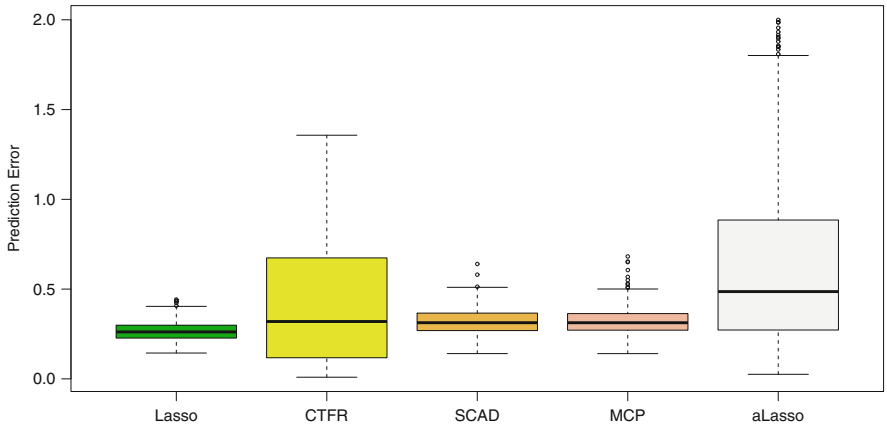

Fig. 2 Comparison of the estimators through prediction errors for Riboflavin data

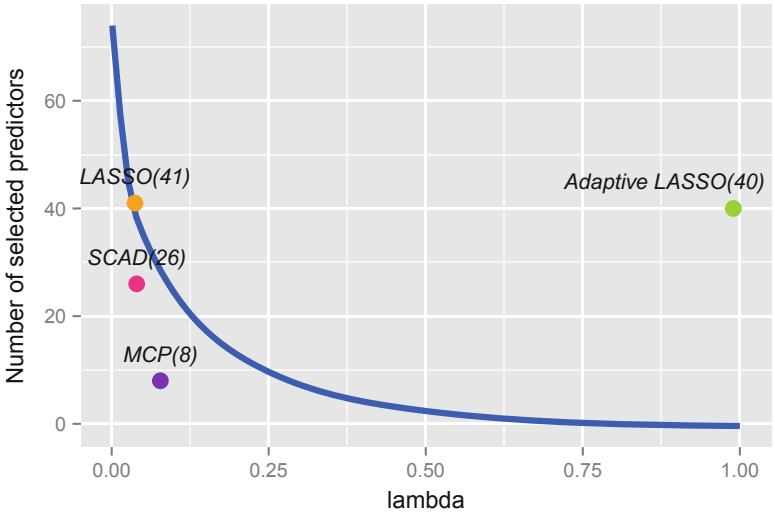

Fig. 3 The number of selected variables of each penalty estimators for the riboflavin data

5 Concluding Remarks and Future Research Directions

We have investigated the relative performance of high-dimensional regression strategies under the correlated design matrix and various signal-to-noise ratios. We have conducted an extensive simulation study to investigate the performance of the suggested strategies in terms of variable selection and prediction performance. The simulation results clearly demonstrate that none of the estimators considered here are better than their competitors under all possible correlation and signal-to-noise ratio scenarios.

As a future research project, one could investigate the distribution of the estimated parameters in CTFR and construction of confidence intervals for the estimated parameters. There are no theoretical results for CTFR in terms of variable selection performance so it is another research direction which needs to be explored.

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An Efficient Estimation Strategy in Autoregressive Conditional Poisson Model with Applications to Hospital Emergency Department Data

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Abstract Data in the form of time series of counts appear in a number of important applications such as health care services, financial markets, disease surveillance, and internet traffic modeling. One of the attractive models for this type of data is the so-called *autoregressive conditional Poisson model (ACP)*. In this work, we propose a Stein-type shrinkage estimation strategy for the regression coefficients of the ACP model. The proposed estimators are expected to improve over the existing maximum partial likelihood estimators (MPLE) in terms of efficiency. We illustrate the usefulness of the proposed methods by using a data set on the daily number of patients at the Emergency Department (ED) of a hospital at eight o'clock in the morning, recorded over a period of 7 years.

Keywords Integer-valued time series · Conditional autoregressive Poisson regression · Emergency department data · Shrinkage estimation

1 Introduction

An emerging area of research in statistics is the modeling and analysis of integer-valued time series. For instance, time series of counts, which is the topic of this work, appears in many fields of applications such as health care performance analysis (e.g., analysis of number of patients served at the ED of a hospital

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or admitted to the hospital); monitoring of environmental pollutants; analysis of data from financial markets (e.g., counts of daily transactions for a given stock); public health surveillance (e.g., surveillance of cause-specific mortality), among many other fields of applications. In the past two decades, the statistical analysis and modeling of such data has attracted a large host of researchers. For detailed discussions of this growing field of methodology and applications, we refer the reader to the recent handbook of [8].

Regression models for time series of counts can be classified into two main classes: parameter-driven (P-D) and observation-driven (O-D) models [5]. Generally speaking, a P-D model assumes that the temporal correlations in a time series of counts are driven by a latent random process (temporal random effect) while the O-D approach assumes that the dependence of the current observation on the past ones can be explained by including explicit functions of the past observed data in the model. For instance, [16] proposed a P-D model in which the conditional mean of the counts is specified as the product of a deterministic exponential function of known covariates and a latent stationary process with mean one. Zeger proposed an estimating equations approach for carrying out the inferences for his P-D model. However, the estimating equations approach of Zeger is numerically difficult to implement (see [4, 12]). In the observation-driven realm, a class of autoregressive conditional models studied by Kedem and Fokianos [13] among others handles the temporal dependence through a log-linear autoregressive specification of the conditional mean. In this model, in addition to the effects of known covariates, autoregressive and moving average components of some functions of the past responses as well as past conditional means are also included in the mean model. This class of O-D models is quite general and represents the temporal influence of the past observations by using an ARMA(p,q)-like specification. However, in many practical situations, the full ARMA(p,q) turns out to be over-parameterized and only the AR(p) portion is enough to explain the temporal dependence in the data. Furthermore, the effects of the various covariates in the full ARMA(p,q) model are not easily interpretable due to the moving average feedback process [10]. Another class of O-D models has been recently proposed by Davis et al. [7] where the conditional mean of the counts is modeled as an ARMA(p,q) series based on the model residuals, instead of the past observations of the process itself. Other approaches to the analysis of time series of counts are: the thinning operator approach, which transfers the usual Gaussian time series structures (e.g., ARMA, GARCH, etc.) to integer-valued observations (see [14]); and the recent approach of [6], which employs super-positioned renewal processes to produce a series of correlated counts with Poisson marginal distributions. Detailed review of these methodologies can be found in [9, 14].

In this paper we consider the autoregressive O-D Poisson regression model of [13] and propose a Stein-type shrinkage estimation strategy for the regression coefficients in the model. Besides many other examples that are available in the literature, our study was motivated by a data set on the number of patients at the ED of a hospital at eight o'clock in the morning, recorded for a period of 7 years. At some point in time, the hospital implemented an intervention aimed at improving

the flow of patients throughout the system and the hospital administration wanted to examine the effect of the intervention. In addition to conceivable factors (covariates) such as seasonal factors and factors related to the hospital services, the number of patients at an ED may also depend on the past history of the process itself for some latent reasons. For instance, the number of patients at the ED at 8 am in a given day may depend on the counts in days preceding. This gives rise to a possible autoregressive structure with a large number of autoregressive terms in addition to the known covariates. In many practical situations, the investigators may have some idea about the relevance of the various covariates based on subjective prior knowledge of the phenomena at hand. This may often encourage investigators to screen out some covariates and fit just a small model that seems appropriate based on their subjective judgement. Alternatively, one may develop a small and parsimonious regression model by using model selection techniques such as the lasso family or stepwise selection approaches based on AIC and BIC criteria. However, such model selection practices often lead to a full model (unrestricted) and a reduced submodel (restricted), leaving the investigators perplexed in choosing either of the two models. In fact, submodels, whether chosen by subjective screening or by model selection techniques, are prone to selection biases and inefficiencies thereof. Also, many recent selection methods tend to screen out covariates with weak effects on the response variable. However, when the discarded covariates are collectively significant, the selected submodel may be extremely inefficient. A way out of this dilemma is to use a shrinkage estimation strategy whereby the restricted and the unrestricted model estimators are combined in an attempt to obtain estimators that are more efficient than either of the merged estimators. Such strategies have been recently developed for many areas of applications. For instance, [2] studied shrinkage estimation strategies in the field of survival data analysis while [3] applied such strategies in linear regression models using M-estimators. A discussion of the shrinkage estimation methodologies and their relative merits can be found in [1]. In this latter reference, among other techniques, the author considered also a shrinkage and pre-test estimation approaches in Poisson regression with independent observations.

The rest of this paper is organized as follows: in Sect. 2, we will introduce our proposed shrinkage estimation strategies and discuss some of their analytical relative performances. In Sect. 3, we will carry out a simulation study to assess the performance the proposed estimators and illustrate their utility by analyzing the daily count of patients at the ED of a hospital. Finally, in Sect. 4, we will give some concluding remarks and future possible extensions.

2 The ACP Model and the Proposed Estimation Strategies

Following [13], let $\{y_t\}$, $t = 1, 2, \ldots, n$, denote a time series of counts, and let $\mu_t > 0$ denote the conditional mean process of y_t given the past information, $\mathscr{F}_{t-1}$. At every given time point, t, we assume that $\mathscr{F}_{t-1}$ is a σ–Algebra generated by the past

observations of the process y_t as well as the current values of covariate processes denoted by $x_t = (x_{1t}, x_{2t}, \ldots, x_{pt})$. That is, by setting $z_{t-1} = \{x_t, y_{t-1}, y_{t-2}, \ldots\}$, the past history that is available at time t is $\mathscr{F}_{t-1} = \sigma\{x_t, y_{t-1}, y_{t-2}, \ldots\} = \sigma\{z_{t-1}\}$, where $z_0 = 0$. The ACP model which we consider in this paper assumes that $y_t|\mathscr{F}_t \sim Poisson(\mu_t)$ where $\lambda_t = \ln(\mu_t) = \sum_{i=1}^{p} x_{it}\beta_i + \sum_{j=1}^{q} \alpha_j y_{t-j}$. The past observations may also be transformed (e.g., log transformed) before entering them to the model to avoid numerical instabilities. Now, we compact all the parameters in the model in a vector $\theta = [(\beta_1, \beta_2, \ldots, \beta_p), (\alpha_1, \ldots, \alpha_q)]$. Therefore, the Poisson log-partial likelihood for this model, given the past information, can be expressed as

$$\begin{aligned} l(\theta) &= \ln\Big(\prod_{t=1}^{n} f\,(y_t; \mu_t(\theta)|\mathscr{F}_{t-1})\Big) \\ &\propto \sum_{t=1}^{n} y_t \ln(\mu_t(\theta)) - \sum_{t=1}^{n} \mu_t(\theta) \\ &= \sum_{t=1}^{n} y_t \theta z_{t-1} - \sum_{t=1}^{n} \exp(\theta z_{t-1}). \end{aligned} \tag{1}$$

The MPLEs of the parameters in the model can be obtained numerically as a solution (if any exists) to the score estimating equations that result from the log-partial likelihood

$$S_n = \sum_{t=1}^{n} z_{t-1}(y_t - \exp(\theta z_{t-1}) = 0.$$

The solution of this equation (if the solution exists), in a model which contains all possible covariates, will be called the unrestricted maximum partial likelihood (UMPLE) estimator and it will be denoted by $\hat{\theta}^U$. Under some regularity conditions (assumption A in [13], pp. 16), these UMPLEs are consistent and asymptotically normal. That is, $\sqrt{n}(\hat{\theta}^U - \theta) \to \mathscr{N}_{p+q}(0, G^{-1}(\theta))$ and $\hat{\theta} \to \theta$ in probability, as $n \to \infty$, where $G(.)$ is the limiting information matrix of the normalized partial observed Fisher information. That is, $\frac{1}{n}G_n(\theta) = \sum_{t=1}^{n} z_{t-1}^{'} z_{t-1} \exp(\theta z_{t-1}) \to G(\theta)$.

Now suppose that, in general, one has $p + q$ covariates which constitute the largest affordable model and a smaller submodel is contemplated by using either a subjective judgement or a data-driven approach (such as AIC, BIC, and lasso criteria). Here, we will assume that the submodel is built on a smaller number of covariates and a smaller number of autoregression terms than the unrestricted model by setting some components of the vector θ to zero. In this ACP model, this would lead to partitioning the parameter space into zero and non-zero parts: $\theta = (\beta_1, \beta_2, \alpha_1, \alpha_2)$ and one would set $\beta_2 = 0, \alpha_2 = 0$. This can be expressed in

the form of a hypothesis such as $H_0 : \beta_2 = 0$ and $\alpha_2 = 0$ versus the alternative $H_a : \beta_2 \neq 0$ or $\alpha_2 \neq 0$. Here we assume that β_1, β_2 have, respectively, p_1, p_2 dimensions so that $p = p_1 + p_2$ and similarly, q_1 and q_2 are the dimensions of the partitioned α with $q = q_1 + q_2$. A more general contrast formulation of the submodel is usually preferable, which includes as special cases the hypotheses of the type described above, by setting $H_0 : H\theta = h$ vs $H_a : H\theta \neq h$, where H is a $(p_2 + q_2) \times (p + q)$ full-rank matrix of known contrasts, and h is a $((p_2 + q_2) \times 1)$ vector of known constants. Under such restriction, one can fit a reduced model whereby the above partial likelihood function is maximized only over the restricted space given by this null hypothesis. Let us denote the generic vector of model parameters under the restriction by θ_1 and denote the MPLE obtained under the restriction by $\hat{\theta}_1^R$. Let also $\hat{\theta}_1^U$ denote the UMPLE of the θ_1. This simply amounts to applying the contrast matrix H to the UMPLE $\hat{\theta}^U$. That is, $\hat{\theta}_1^U = H\hat{\theta}^U$. The hypothesis that the submodel is the true model can be tested by using a Wald-type test statistic given by $T_n = (H\hat{\theta}^U - h)'(HG^{-1}(\theta)H')^{-1}(H\hat{\theta}^U - h)$ where the parameter θ is eventually replaced by its restricted estimator. It turns out that this statistic follows a chi-squared distribution with $b = p_2 + q_2$ degrees of freedom [13].

In order to borrow strength from the unrestricted model and bring it to the smaller and more parsimonious model (which is represented by the null hypothesis above), we propose a Stein-type shrinkage estimator and its positive variant to estimate the parameter vector θ_1 as follows:

$$\hat{\theta}_1^S = \hat{\theta}_1^R + \left(\hat{\theta}_1^U - \hat{\theta}_1^R\right)\left\{1 - (p_2 + q_2 - 2)T_n^{-1}\right\}, \quad p_2 + q_2 \geq 3. \tag{2}$$

$$\theta_1^{PS} = \hat{\theta}_1^R + \left(\hat{\theta}_1^U - \hat{\theta}_1^R\right)\left\{1 - (p_2 + q_2 - 2)T_n^{-1}\right\}^+, \tag{3}$$

where $a^+ = \max\{0, a\}$.

These two estimators are known in the literature as the shrinkage and the positive shrinkage estimators, respectively. The rationale behind the second version is that, in some data sets, the shrinkage estimator suffers from a phenomenon known as over-shrinkage, whereby negative coordinates of $\hat{\theta}_1^U$ are obtained whenever $(T_n < p_2 + q_2 - 2)$. This problem is solved by truncating the weight function at zero, thus avoiding negative values of the combining weights.

The relative performance of shrinkage estimators with respect to the unrestricted and reduced model estimators is studied via their asymptotic quadratic risks (AQR). Such risks are calculated analytically as sample size increases under a sequence of local alternatives $H_{(an)}$ defined as:

$$H_{(an)} : H\theta = h + \frac{\delta}{\sqrt{n}}, \tag{4}$$

where δ is $(p_2 + q_2)$ vector of constants. For any estimator $\hat{\theta}_1^*$ of θ_1, let $Q(x)$ be the asymptotic distribution function of $\sqrt{n}(\hat{\theta}_1^* - \theta_1)$ under the local alternatives in (4). That is,

$$\boldsymbol{Q(x)} = \lim_{n\to\infty} P_{H_{(an)}}\left(\sqrt{n}(\hat{\theta}_1^* - \theta_1) \leq x\right). \tag{5}$$

Define also a weighted quadratic loss function

$$\begin{aligned} L(\theta_1^*, \theta_1) &= n(\theta_1^* - \theta_1)' M(\theta_1^* - \theta_1) \\ &= tr\left\{ M\left(n(\theta_1^* - \theta_1)(\theta_1^* - \theta_1)'\right)\right\}, \end{aligned} \tag{6}$$

where M is a $(p_1 + q_1) \times (p_1 + q_1)$ positive definite weight matrix. If $\sqrt{n}(\theta_1^* - \theta_1) \xrightarrow{D} T^*$, then the AQR is defined as

$$\begin{aligned} AQR(\theta_1^*, M) &= E\{T^{*\prime} M T^*\} \\ &= \int \left(x' M x\right) dQ(x). \end{aligned} \tag{7}$$

In general, the theory of the ACP, as described in [13], states that the conditional observed Fisher information matrix of the ACP model converges in probability to the unconditional Fisher information. This ensures that the asymptotic theory of the ACP model coincides with that of the usual Poisson regression. As a consequence of this fact, the AQR of the shrinkage estimators proposed above is identical to those described in [1]. Therefore, we will not re-iterate such risk expressions, while we expect that the above two estimators will have better performance in terms of asymptotic risks than the UMPLE ($\hat{\theta}_1^U$) in a neighborhood of the submodel and are as good as the UMPLE in the alternative parameter spaces, represented by H_{an}. On the other hand, the asymptotic risk behavior of the submodel estimator, $\hat{\theta}_1^R$, is well known in the literature. Intuitively, such an estimator is expected to outperform both of the shrinkage estimators above as well as the UMPLE near the submodel (i.e., in a neighborhood of the parameter space described by H_0). However, the performance of $\hat{\theta}_1^R$ deteriorates quickly as the true data generating model moves away from the submodel parameter space. This makes the restricted estimator unreliable, as one does not know a priori the true parameter space of the data generating process. The proposed shrinkage estimators can, however, provide safety in terms of overall AQR, regardless of the true parameter space on which the data generating process is based. It is worth noting here that the measure of closeness to the submodel space of the parameters is the Mahalanobis distance defined as $\Delta = \delta'(HG^{-1}(\theta)H')^{-1}\delta$.

In the next section we will illustrate the performance of the proposed shrinkage estimators by using a simulation study as well as the emergency department data set described earlier.

3 Numerical Studies

3.1 Simulation Study

In this section, we carry out a simulation study to examine the empirical performance of the shrinkage estimators when compared to the unrestricted and restricted model estimators. Our data generating model is the ACP with $n = 50, 150$ $p = 10, 15$ and $q = 10, 15, 20$. While the number of non-zero coefficients in the β vector was kept at $p_1 = 4$, the dimension of the non-zero coefficients in the autoregressive part, α, was varied over $q_1 = 4, 10, 15, 20$, in order to examine the effect of the autoregressive components on the performance of the estimators. The model intercept was set to $\beta_1 = 0.5$ while the rest of the non-zero coefficients in the β vector were all set to 1. The non-zero autoregressive coefficients were set to 0.001 so that their sum does not exceed unity. The latter is a condition for the validity of the asymptotic results for the ACP model. The zero coefficients are then increased by small increments so that the Mahalanobis distance, Δ, varies in $(0, 0.5)$ with steps of 0.01. In the autoregressive terms we used the log transformation $\ln(y_{t-i} + 1)$ to avoid numerical issues due to exponentially increasing counts. In all cases, the relative mean squared error (RMSE) of each estimator with respect to the UMPLE is computed based on 2000 Monte Carlo simulations. The results of these RMSEs are displayed in Figs. 1 and 2, where an RMSE greater than one indicates that the considered estimator is more efficient than the UMPLE. As theoretically expected, the restricted estimator (RE) for the submodel is the best in terms of MSE when the true model parameters are in a neighborhood of the null hypothesis. That is, when the submodel is nearly the true data generating model. However, as the true model moves away from the submodel space, the RE deteriorates rapidly and its RMSE approaches zero. This pattern is persistent throughout all the scenarios displayed in Figs. 1 and 2. On the other hand, the shrinkage and the positive shrinkage estimators (SE, PSE) are slightly less efficient than the RE but more efficient than the UMPLE near the submodel space. As we move away from the submodel, the shrinkage estimators become as efficient as the UMPLE. Figure 1 shows the effect of increasing the number of the zero elements in the vector α of the autoregressive coefficients from $q_2 = q - q_1 = 10 - 4 = 6$ to $q_2 = q - q_1 = 15 - 4 = 11$, for fixed sample sizes of $n = 50$ in the first row and $n = 150$ in the second row. Both panels show that the proposed estimators become more efficient for larger q_2, while increasing the sample size improves the UMPLE, which becomes comparable to the shrinkage estimators. That is, the shrinkage effect is more pronounced at small sample sizes. This is also intuitively expected, as for large sample sizes the UMPLE becomes more precise even for parameter components corresponding to the submodel, and hence the shrinkage effect will eventually fade out, and both SE and PSE become as efficient as the UMPLE. In other words, the interval of shrinkage estimators' dominance over the UMPLE becomes smaller and smaller. However, for obvious reasons, the same is not true for the submodel estimator when the true data generating process is not the submodel. Figure 2 reports simulation results

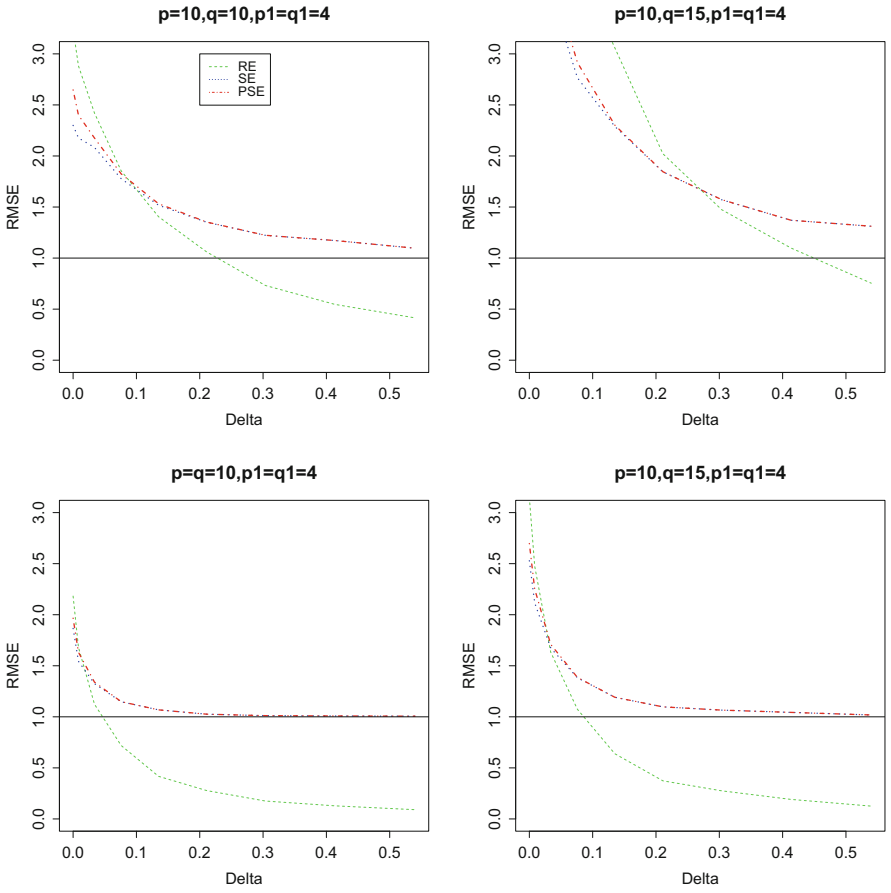

Fig. 1 Simulated RMSE of the restricted, and shrinkage estimators with respect to the UMPLE. Results for $n = 50, 150$ are, respectively, in the first and second rows of the figure

aimed at examining the performance of the SE and PSE with respect to the UMPLE when the number of non-zero components in the autoregressive vector, α, increases. For this part of the simulations, we fixed $n = 150$, $p = 10, p_1 = 4, q = 20$ and varied $q_1 = 4, 10, 15, 20$. The pattern here is quite simple: as the number of non-zero autoregressive components increases the efficiency of the estimators decreases, while maintaining the same relative dominance picture discussed earlier. For instance, when $q_1 = 20$, we can see that all the estimators start as efficient as the UMPLE and, while the SE and PSE remain as efficient as the UMPLE, the relative performance of the RE drops quickly. Therefore, we can conclude that high dimensional autoregression components can reduce the overall efficiency of all the estimators, regardless of the true data generating process, but the relative performance of the shrinkage estimators remains as theoretically predicted.

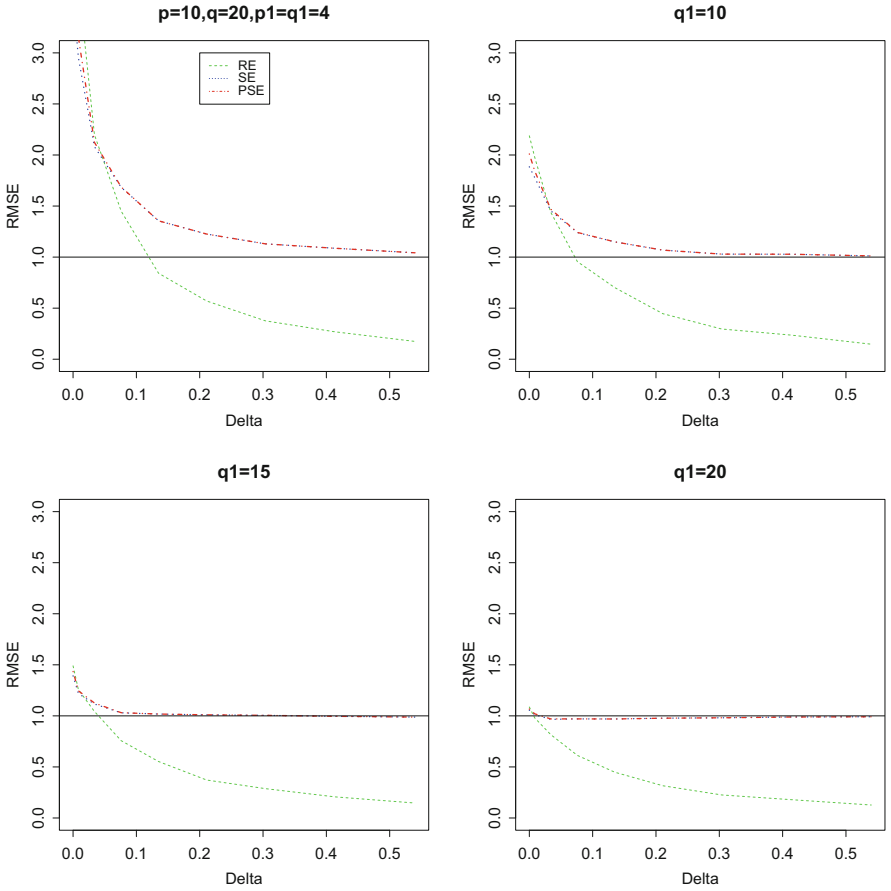

Fig. 2 Simulated RMSE of the restricted, and shrinkage estimators with respect to UMPLE. Here $n = 150$ and $p = 10, q = 20, p_1 = 4$ are fixed and q_1 is varied over the set 4, 10, 15, 20

3.2 Application to Emergency Department Data

To illustrate the practical use of the proposed estimation strategies, we consider a data set on patient flow at the ED of the Southlake Hospital in the province of Ontario, Canada. The hospital implemented a new technology that identified patient care status on monitors mounted throughout the hospital so that staff could readily see how many patients were waiting in the ED department for either treatments, admission, or other procedures like diagnostic imaging. The technology provided "visibility" of patient status to staff with the goal of informing staff who where patients were waiting for care in the hospital, so they could intervene more quickly to complete care procedures to support a more streamlined efficient flow of patients through the hospital system. The hospital's aim was to improve patient flow efficiency to increase capacity to treat patients with reduced wait times which

is an important *key performance indicator* (KPI) of hospital performance—ED wait times in particular is a KPI for hospitals in Ontario. The hospital administration wanted to examine the impact of the visibility technology solution on a number of important KPIs. Here we consider only one of the KPIs analyzed in the larger study. Namely, we will consider the number of patients at the ED at eight o'clock in the morning. Therefore, the main outcome in the data set to be analyzed here is y_t, the daily number of patients at the ED at eight o'clock in the morning, recorded over 7 years ($t = 1, 2, \ldots, 2436 = n$). The visibility technology (intervention) was implemented at some point in time when $t = 1756$. In addition to the intervention variable, the outcome y_t can be affected by many other factors such as seasonal variations (e.g., many admissions for falls during the winter months, admissions due to flu season), days of the week (e.g., weekends are busy due to primary care offices being closed), and seasonal variations such as holidays when other clinics or offices are unavailable and the only option for patients is to seek emergency department services. Beyond these conceivable covariates, the outcome may also depend on the past history of patient flow at the ED due to some latent reasons. Therefore, the data set in consideration had y_t as its main outcome, and the intervention indicator (interv), defined as zero for data before the intervention and one for data collected afterwards, as its main independent variable. In addition to these two key variables, we also defined the following groups of covariates: (1) Six dummy variables (Mon-Sat) with values 0 or 1 to indicate the day of the week (while assuming Sunday to be our baseline day); (2) Sine and cosine variables to tackle possible seasonal patterns in the counts. These variables were defined separately for yearly, quarterly, and monthly seasonality as $siny = sin(2\pi t/365)$, $sinq = sin(2\pi t/120)$ and $sinm = sin(2\pi t/30)$, respectively. The cosine functions were defined in a similar way; (3) Linear and quadratic time trends, $normt$, $normt2$ based on normalized time variable; (4) Autoregressive terms up to order seven, $Y7 = \ln(y_{t-7} + 1), \ldots, Y1 = \ln(y_{t-1} + 1)$.

As the autoregressive variables are usually not associable to apparent reasons, they can be legitimately considered as nuisance factors, which are needed to adjust the overall variability although the practitioners are not interested in their estimation. Therefore, it is always good practice to initially try out only a smaller number of autoregressive terms in the regression model, which justifies our choice of the autoregressive model with $q = 7$. Another appeal is our suspicion that dependence of the counts on its past history may go back only for a period of a week. An initial model (model #1) with all the above variables was fitted and reported below. This model seems to support the following significant effects: the indictors of the day of the week, the intervention variable (interv), the linear and quadratic time trends, the yearly cosine function, the yearly and quarterly sine functions, the autoregressive variables $Y1$, $Y2$, $Y3$, $Y6$, and $Y7$.

Since the effects of $Y6$ and $cosy$ are marginally significant, we fitted a second model (Model #2 below) in which these two variables along with $Y7$ and the rest of the nonsignificant effects were removed. Although $Y7$ was statistically significant in Model #1, it is not really intuitive or interpretable when past observations between the 3rd and the 7th are not significant. In other words, it is easier to convey that

Table 1 Estimated regression coefficients by using positive shrinkage strategy

Variable	Intercept	Mon	Tue	Wed	Thu	Fri	Sat	Interv
Coef	0.82	0.22	0.22	0.10	0.10	0.06	−0.31	−0.09
Variable	normt	normt2	siny	sinq	Y1	Y2	Y3	
Coef	−0.25	0.35	−0.02	−0.03	0.40	0.10	0.04	

the number of patients at the ED on any given day depends on the counts of the immediate past 3 days, than conveying that it also depends on the 7th day as well!

Now, in order to recover some efficiency from Model #1, we used our proposed shrinkage estimators and calculated their relative efficiency (with respect to the estimators of Model #1) by using a parametric bootstrapping based on the GLM residuals. The resulting bootstrapped relative efficiencies of the submodel (Model #2), the SEs and PSEs are, respectively, 0.9148982, 1.0059393, 1.0059393. Thus, the proposed shrinkage estimators are as efficient as those from the larger Model #1 and approximately 9% more efficient than the estimator obtained by just fitting the smaller Model #2. It is worth mentioning here that, while the bootstrapped relative efficiency may be reliable, the variances estimated via such bootstrapping in a GLM are not in general as reliable. A future research task to take up may be the development of methods for bootstrapping variances of the shrinkage estimators in the context of the ACP model. In any case, for this data set, we only report the coefficient estimators based on the positive shrinkage, which happen to coincide with those of the shrinkage strategy. These coefficient estimators are rounded to the second decimal place and reported in Table 1 below. We can see that the intervention was effective to some extent as the coefficient of its indicator variable is −0.09. This means that, if everything else is held fixed, the post-intervention period has approximately 10% smaller overall mean (exponential of the intercept) as compared to the pre-intervention period. Also, we can see that the average number of patients at the ED in weekdays is less than in weekends (Saturdays and Sundays). The peak days seem to be Mondays and Tuesdays and then it trends downward until it reaches its lowest on Saturdays.

```
Model #1:
Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept)  0.803186   0.049873  16.104  < 2e-16
mon          0.215468   0.025916   8.314  < 2e-16
tue          0.214688   0.026426   8.124 4.50e-16
wed          0.093726   0.026701   3.510 0.000448
thu          0.093426   0.026801   3.486 0.000490
fri          0.057099   0.026905   2.122 0.033817
sat         -0.304198   0.028392 -10.714  < 2e-16
interv      -0.085096   0.033869  -2.512 0.011989
normt       -0.237698   0.103780  -2.290 0.021998
normt2       0.340894   0.125257   2.722 0.006498
```

```
siny         -0.018497   0.009335  -1.982 0.047527
sinq         -0.024775   0.009212  -2.689 0.007160
Y1            0.401944   0.013919  28.878  < 2e-16
Y2            0.092629   0.013974   6.629 3.38e-11
Y3            0.036040   0.013789   2.614 0.008959
Y7            0.060107   0.012730   4.722 2.34e-06
Y6            0.022753   0.013590   1.674 0.094085
cosy         -0.016058   0.009242  -1.738 0.082296
cosm         -0.009082   0.009065  -1.002 0.316442
cosq         -0.005399   0.009165  -0.589 0.555794
sinm         -0.003106   0.009144  -0.340 0.734062
Y4            0.001535   0.013564   0.113 0.909888
Y5            0.019218   0.013485   1.425 0.154136
---
AIC: 15147

Model #2:
Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept)  0.955275   0.044034  21.694  < 2e-16
mon          0.237052   0.025594   9.262  < 2e-16
tue          0.246324   0.025856   9.527  < 2e-16
wed          0.114243   0.025977   4.398 1.09e-05
thu          0.099690   0.025386   3.927 8.60e-05
fri          0.051522   0.025589   2.013 0.044064
sat         -0.321918   0.028125 -11.446  < 2e-16
interv      -0.111673   0.033201  -3.364 0.000770
normt       -0.310959   0.102416  -3.036 0.002396
normt2       0.446304   0.122729   3.636 0.000276
siny        -0.023223   0.009297  -2.498 0.012496
sinq        -0.031211   0.009168  -3.404 0.000664
Y1           0.411477   0.013861  29.687  < 2e-16
Y2           0.100278   0.013888   7.220 5.18e-13
Y3           0.055145   0.012653   4.358 1.31e-05
---
AIC: 15189
```

4 Conclusion

In this work, we have explored the benefits of using a shrinkage strategy for estimating the regression coefficients in an ACP model for the analysis of time series of counts. We have indicated that the theoretical performance of the Stein-type shrinkage estimators, which has been proven elsewhere for the Poisson regression

with independent counts, holds also in the case of the ACP models. We have used a Monte Carlo simulation to confirm such performance and concluded that the autoregression in the GLM under the assumption of conditional Poisson model may reduce the overall efficiency at small sample sizes, but the relative performance of the shrinkage-type estimators, with respect to the unrestricted and restricted estimators, remains as theoretically expected. The proposed shrinkage estimators are useful in minimizing the loss of efficiency that may result from preferring a small and parsimonious model over a larger over-parameterized model. In such cases, the shrinkage estimators proposed in this work would borrow efficiency from the larger model while estimating only the smaller submodel, thus allowing better interpretation of the results. In this work we have used a parametric bootstrapping method, based on the GLM residuals. Although this approach may be useful in assessing the relative efficiencies of the various estimators considered in this work, it was not giving reasonable variances for the estimators. Finally, we illustrated the methodology by using data on the daily number of patients at the ED of a hospital over a period of 7 years. A future investigation shall undertake the task of developing a reasonable bootstrapping strategy for computing the variances of the shrinkage estimators. Unlike the case of independent counts' GLM, the task of bootstrapping an ACP model estimators is not straightforward, due to the temporal dependence of the counts. Instead of bootstrapping, one may also consider adopting a new post-selection estimation strategy which has been recently developed by Gao et al. [11]. A referee has also pointed out that there is a contemporary work that we were not aware of, which uses the general form of the autoregressive GLM and proposes a class of shrinkage estimators [15].

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