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Inference in Nonorthogonal Mixed Models

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Abstract.
The estimation of variance components and estimable vectors is carried out for nonorthogonal mixed models. To do that we use a decomposition of the design space in several orthogonal blocks. We assume the random vectors to have null mean vectors and null cross covariance matrices.

Keywords: Inference, mixed models
AMS: 62k15, 62E15,62H10, 62H15, 62J10

INTRODUCTION

There are many studies in estimation with mixed models; see, e.g., [2, 7, 8, 9]. However the estimation for fixed and random effects can be difficult to derive even in the case of orthogonal designs, see [1].

In this paper we will deal with mixed models

$$\boldsymbol{Y} = \sum_{i=0}^{w} \boldsymbol{X}_i \boldsymbol{\beta}_i, \tag{1}$$

where $\boldsymbol{\beta}_0$ is a fixed vector and $\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_w$ are random vectors. The $\boldsymbol{X}_i$ are known $n \times c_i$ design matrices. Usually it is assumed that:

a) the $\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_w$ have null mean vectors and variance-covariance matrices $\boldsymbol{\theta}_1 \boldsymbol{I}_{c_1} \dots \boldsymbol{\theta}_w \boldsymbol{I}_{c_w}$;
b) the models have orthogonal features, OF, expressed by matrices $\boldsymbol{M}_i = \boldsymbol{X}_i \boldsymbol{X}_i^\top, i = 1, \dots, w$, and $\boldsymbol{T} = \boldsymbol{X}_0(\boldsymbol{X}_0^\top \boldsymbol{X}_0)^+ \boldsymbol{X}_0^\top$, the orthogonal projection matrix on the range space $\Omega = R(\boldsymbol{X}_0)$ of $\boldsymbol{X}_0$, commuting.

These models have mean vector

$$\boldsymbol{\mu} = \boldsymbol{X}_0 \boldsymbol{\beta}_0, \tag{2}$$

and variance-covariance matrices

$$\boldsymbol{V}(\boldsymbol{\theta}) = \boldsymbol{\theta}^\top \boldsymbol{M} = \sum_{i=1}^{w} \theta_i \boldsymbol{M}_i. \tag{3}$$

We now intend to present a treatment to mixed models in which only a) holds. This is mixed models without OF.

In the next section we introduce some preliminary results on orthogonal matrices associated to families of symmetrical matrices before presenting, in section 3, the classes of models we consider. Finally, in sections 4, we consider the estimation of variance components and estimable vectors.

ORTHOGONAL MATRICES

Let $\boldsymbol{W}_1, \dots, \boldsymbol{W}_w$ be symmetric $n \times n$ matrices. These matrices will commute if, and only if, they are diagonalized by an orthogonal matrix $\boldsymbol{P}$, see Schott [10], pg 153.

Now, let $\boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_n$ be the row vectors of $\boldsymbol{P}$. These will also be eigenvectors of $\boldsymbol{W}_1, \dots, \boldsymbol{W}_w$. We put $\boldsymbol{\alpha}_i \tau \boldsymbol{\alpha}_l$ if $\boldsymbol{\alpha}_i$ and $\boldsymbol{\alpha}_l$ are associated to identical eigenvalues for all matrices of $\boldsymbol{W} = \{\boldsymbol{W}_1, \dots, \boldsymbol{W}_w\}$, thus defining an equivalence

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relation between eigenvectors. A τ equivalence class will be of first type if its eigenvectors are associated to a non null eigenvalue for at least one of the vectors, see [11].

Let $C_1,...,C_m$ be the sets of indexes of the eigenvalues belonging to the $m(\tau)$ first equivalence class. Then, the

$$Q_j = \sum_{l \in \mathscr{C}_j} \boldsymbol{\alpha}_l \boldsymbol{\alpha}_l, \quad j = 1,...,m \tag{4}$$

will be pairwise orthogonal orthogonal projection matrices, POOPM, that add up to $\boldsymbol{I}_n$. Moreover if $b_{i,j}$ is the eigenvalue of $\boldsymbol{W}_i$, $i = 1,...,w$, for the eigenvectors of the $j-$th class, $j = 1,...,m$, we have

$$\boldsymbol{W}_i = \sum_{j=1}^{m} b_{i,j} \boldsymbol{Q}_j, \quad i = 1,...,w, \tag{5}$$

as well as the transition matrix $\boldsymbol{B} = [b_{i,j}]$ which, see [6], play an important part in the structure of models with orthogonal features.

Moreover, with $\boldsymbol{A}_j = [\boldsymbol{\alpha}_l^\top; \ l \in C_j]$, $j = 1,...,m$, we have

$$\begin{cases} \boldsymbol{Q}_j = \boldsymbol{A}_j^\top \boldsymbol{A}_j, & j = 1,...,m \\ \boldsymbol{I}_{g_j} = \boldsymbol{A}_j \boldsymbol{A}_j^\top, & j = 1,...,m \end{cases}$$

with $g_j = rank(\boldsymbol{A}_j) = rank(\boldsymbol{Q}_j)$, $j = 1,...,m$. Thus

$$\boldsymbol{P} = [\boldsymbol{A}_1^\top .. \boldsymbol{A}_m^\top]^\top \tag{6}$$

will be an orthogonal matrix associated to the family $\boldsymbol{W}$ of commutative matrices. We point out that

$$\begin{cases} \boldsymbol{A}_j \left(\sum_{l=1}^m c_l \boldsymbol{Q}_l\right) \boldsymbol{A}_j^\top = c_l \boldsymbol{I}_{g_j}, & j = 1,...,m; \\ \boldsymbol{A}_j \left(\sum_{l=1}^m c_l \boldsymbol{Q}_l\right) \boldsymbol{A}_h^\top = \boldsymbol{0}_{g_j \times g_h}, & j \neq h. \end{cases}$$

In models with OF the orthogonal matrix $\boldsymbol{P}$ plays an important part, see Fonseca [5]. For instance if the matrices $\boldsymbol{M}_1,...,\boldsymbol{M}_w$ commute we will have

$$\boldsymbol{M}_i = \sum_{j=1}^{m} b_{i,j} \boldsymbol{A}_j^\top \boldsymbol{A}_j, \quad i = 1,...,w, \tag{7}$$

see again Fonseca [5].

MODELS AND SUB-MODELS

As mentioned above, models with OF have an associated orthogonal $n \times n$ matrix $\boldsymbol{P}$, as defined in (6), such that

$$\boldsymbol{A}_j \boldsymbol{M}_i \boldsymbol{A}_j^\top = b_{i,j} \boldsymbol{I}_{g_j}, \quad i = 1,...,w, \quad j = 1,...,m. \tag{8}$$

Besides this, for any classes of models with OF, we will have

$$\boldsymbol{A}_j \boldsymbol{M}_i \boldsymbol{A}_h^\top = \boldsymbol{0}_{g_j \times g_h}, \quad j \neq h, \tag{9}$$

since matrices $\boldsymbol{M}_1,...,\boldsymbol{M}_w$ commute in these models. However many times models do not have OF and so

$$\boldsymbol{A}_j \boldsymbol{M}_i \boldsymbol{A}_h^\top \neq \boldsymbol{0}_{g_j \times g_h}, \quad j \neq h. \tag{10}$$

But, on the other hand, see [3], whatever the family $\boldsymbol{W} = \{\boldsymbol{W}_1,...,\boldsymbol{W}_w\}$ of symmetric $n \times n$ matrices, there exists an orthogonal $n \times n$ matrix $\boldsymbol{P}$, as the one in (6), such that

$$\boldsymbol{A}_j \boldsymbol{W}_i \boldsymbol{A}_j^\top = b_{i,j} \boldsymbol{I}_{g_j}, \quad i = 1,...,w, \quad j = 1,...,m, \tag{11}$$

with

$$g_j = rank(\boldsymbol{A}_j) = rank(\boldsymbol{Q}_j), \tag{12}$$

where

$$\boldsymbol{Q}_j = \boldsymbol{A}_j^\top \boldsymbol{A}_j, \quad j = 1, ..., m. \tag{13}$$

Thus, if the model does not has OF one may use a decomposition of the design space in several orthogonal blocks, considering the sub-models

$$\boldsymbol{Y}_j = \boldsymbol{A}_j \boldsymbol{Y}, \quad j = 1, ..., m \tag{14}$$

with mean vectors

$$\boldsymbol{\mu}_j = \boldsymbol{X}_{0,j} \boldsymbol{\beta}_0, \quad j = 1, ..., m, \tag{15}$$

where $\boldsymbol{X}_{0,j} = \boldsymbol{A}_j \boldsymbol{X}_0$, $j = 1, ..., m$, and variance-covariance matrices

$$\boldsymbol{V}(\boldsymbol{Y}_j) = \boldsymbol{\gamma}_j \boldsymbol{I}_{g_j}, \quad j = 1, ..., m, \tag{16}$$

with

$$\boldsymbol{\gamma}_j = \sum_{i=1}^{w} b_{i,j} \boldsymbol{\theta}_i, \quad j = 1, ..., m, \tag{17}$$

$\dot{\boldsymbol{B}} = [\dot{b}_{i,j}]$, see [3]. In models with OF the $\dot{b}_{i,j}$ will be the elements of the transition matrices, see [4], while here they are the coefficients in the thesis of (11).

ESTIMATION OF VARIANCE COMPONENTS AND ESTIMABLE VECTORS

In this section we will show how to estimate the variance components $\boldsymbol{\theta}_1, ..., \boldsymbol{\theta}_w$ and the remaining estimable vectors. Starting by the variance components, let $\boldsymbol{P}_j$ and $\boldsymbol{P}_j^c$ be the orthogonal projection matrices on $\Omega_j = R(\boldsymbol{X}_{0,j})$, the range space of $\boldsymbol{X}_{0,j}$ and its orthogonal complement $\Omega_j^\perp$, $j = 1, ..., m$, respectively. With

$$\begin{cases} p_j = rank(\boldsymbol{P}_j) \\ p_j^c = rank(\boldsymbol{P}_j^c) \end{cases}, \tag{18}$$

$j = 1, ..., m$. Since the $\boldsymbol{Y}_j$, $j = 1, ..., m$, in (14) are homoscedastic, it is well known that the

$$\widetilde{\boldsymbol{\gamma}}_j = \frac{\boldsymbol{Y}_j^\top \boldsymbol{P}_j^c \boldsymbol{Y}_j}{p_j^c}, \tag{19}$$

are best quadratic unbiased estimators, BQUE, in the family of the quadratic estimators of $\boldsymbol{\gamma}_j$, derived from $\boldsymbol{Y}_j$, $j = 1, ..., m$.

Let $\boldsymbol{\gamma}$ have components $\boldsymbol{\gamma}_j$, then

$$\boldsymbol{\gamma} = \dot{\boldsymbol{B}}^\top \boldsymbol{\theta}. \tag{20}$$

So if the row vectors of $\dot{\boldsymbol{B}}$ are linearly independent we get

$$\boldsymbol{\theta} = (\dot{\boldsymbol{B}}^\top)^+ \boldsymbol{\gamma}, \tag{21}$$

where $\boldsymbol{A}^+$ indicates the MOORE-PENROSE inverse of matrix $\boldsymbol{A}$, and thus

$$\widetilde{\boldsymbol{\theta}} = (\dot{\boldsymbol{B}}^\top)^+ \widetilde{\boldsymbol{\gamma}}, \tag{22}$$

Now we will show how to estimate the remaining vectors. Let

$$\boldsymbol{\psi} = \boldsymbol{G} \boldsymbol{\beta}_0 \tag{23}$$

be an estimable vector. Since we were able to estimate $\boldsymbol{\theta}$ we can use the generalized least square estimator, GLSE,

$$\boldsymbol{\beta}_0(\widetilde{\boldsymbol{\theta}}) = \left(\boldsymbol{X}_0^\top \boldsymbol{V}(\widetilde{\boldsymbol{\theta}})^+ \boldsymbol{X}_0 \right)^+ \boldsymbol{X}_0^\top \boldsymbol{V}(\widetilde{\boldsymbol{\theta}})^+ \boldsymbol{Y}, \tag{24}$$

with

$$\boldsymbol{V}(\widetilde{\boldsymbol{\theta}}) = \sum_{i=1}^{w} \widetilde{\theta}_i \boldsymbol{M}_i, \tag{25}$$

to obtain the

$$\widetilde{\boldsymbol{\psi}}(\widetilde{\boldsymbol{\theta}}) = G \boldsymbol{\beta}_0(\widetilde{\boldsymbol{\theta}}), \tag{26}$$

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