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Abstract

The paper deals with the best unbiased estimators of the blocked compound symmetric covariance structure for $m-$variate observations over u sites under the assumption of multivariate normality. The free-coordinate approach is used to prove that the quadratic estimation of covariance parameters is equivalent to linear estimation with a properly defined inner product in the space of symmetric matrices. Complete statistics are then derived to prove that the estimators are best unbiased. Finally, strong consistency is proven. The proposed method is implemented with a real data set.

Keywords Best unbiased estimator, blocked compound symmetric covariance structure, doubly multivariate data, coordinate free approach.

JEL Classification: C13

1 Introduction

Blocked compound symmetric (BCS) covariance structure (defined in Section 2) for doubly multivariate observations (m dimensional observation vector repeatedly measured over u locations or time points), which is a multivariate generalization of compound symmetry covariance structure for multivariate observations, was introduced by Rao (1945, 1953) while classifying genetically different groups, and then Arnold (1979) studied this BCS covariance structure while developing general linear model with exchangeable and jointly normally distributed error vectors. Afterwards BCS covariance structure did not attract much attention in the literature for some time until Leiva (2007) developed classification rules for doubly multivariate observations and generalized Fishers linear discrimination method when the covariance matrix of the data is assumed to have a BCS structure. Leiva (2007) derived maximum likelihood estimates (MLEs) of the BCS covariance structure and developed classification rules using these MLEs. Lately, this covariance structure is starting to gain a lot of attention in the literature, especially in the area of high-dimensional estimation (see Roy and Leiva, 2011). Recently, Roy et al. (2015) obtained a natural extension of the Hotellings T^2 statistic, the Block T^2 statistic, a convolution of two T^2's, using unbiased estimates of the component matrices of the orthogonally transformed BCS covariance matrix while testing the equality of mean vectors for paired doubly multivariate observations. To the best knowledge of the authors, none of the previous studies have considered the estimation properties of the BCS covariance matrix. A natural question then is whether or not these estimators are "good" in some sense.

One measure of "good" is "unbiasedness." This article derives the unbiased estimators for parameters of mean vector and the BCS covariance structure following the same way as Roy et al. (2015), and addresses the issue of optimal properties of these unbiased estimators that is motivated by real-world applications. A characterization of BLUE given by Zmyślony (1978) and completeness in Zmýslony (1980) are used to derive the optimal properties of unbiased estimators. The derivation and computation of these estimators are developed using the coordinate free approach (see Kruskal (1968) and Drygas (1970)).

An important advantage of using BCS structure for doubly multivariate data is that the number of unknown parameters is only $m(m+1)$, which does not even depend on the number of repeated measures u, whereas the number of unknown parameters in the unstructured covariance matrix $\mathbf{\Omega}$ is $um(um+1)/2$, which can increase very rapidly with the increase of either m or u. Hence, BCS covariance structure allows the number of repeated measurements u to grow unrestrictedly, and thereby provides more information, while the number of unknown parameters remains the same.

Doubly multivariate data are very common in biological, biomedical, medical, environmental, engineering and many other fields. They require extraction of relevant information that is hidden in the data in order to model the data appropriately and accurately. In clinical trial study researchers often collect measurements on more than one response variable at different sites or over time. For example, suppose an investigator measures the mineral content of three bones, radius, humerus and ulna ($m = 3$) by photon absorptiometry to examine whether a particular dietary supplement would slow the bone loss in older women. All three measurements are also recorded on the dominant and non-dominant sides ($u = 2$) for each woman.

In this article we show that the unbiased estimates of the matrix parameters of the blocked compound symmetric (BCS) covariance structure are optimal. Unbiased estimates of the matrix parameters are needed for many statistical analysis, e.g., for testing the equality of mean vectors for doubly multivariate observation (Roy et al., 2015); thus it is important to get optimal unbiased estimates matrix parameters of blocked compound symmetric covariance structure. Another property of fixed effects estimators is that they do not depend directly on the normal distribution of the sample vector, like it is described in Zmyślony (1978), but solely on the covariance structure of the data. Strong consistency is also a property that arises from these estimators.

The rest of the article is organized as follows. Section 2 defines the BCS covariance structure. Unbiased estimate of this BCS structure is derived in Section 3. Optimal properties of estimates are derived in Section 4. Finally Sections 5 and 6 contain a real data example and a short conclusions.

2 Blocked compound symmetric covariance structure

The $(mu \times mu)-$dimensional BCS covariance structure is defined as

$$\begin{aligned} \mathbf{\Gamma} &= \begin{bmatrix} \mathbf{\Gamma}_0 & \mathbf{\Gamma}_1 & \dots & \mathbf{\Gamma}_1 \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \mathbf{\Gamma}_1 & \mathbf{\Gamma}_1 & \dots & \mathbf{\Gamma}_0 \end{bmatrix} \\ &= \mathbf{I}_u \otimes (\mathbf{\Gamma}_0 - \mathbf{\Gamma}_1) + \mathbf{J}_u \otimes \mathbf{\Gamma}_1, \end{aligned} \tag{2.1}$$

where $\mathbf{I}_u$ is the $u \times u$ identity matrix, $\mathbf{1}_u$ is a $u \times 1$ vector of ones, $\mathbf{J}_u = \mathbf{1}_u \mathbf{1}_u'$ and $\otimes$ represents the Kronecker product. We assume $\mathbf{\Gamma}_0$ is a positive definite symmetric $m \times m$ matrix, $\mathbf{\Gamma}_1$ is a symmetric $m \times m$ matrix, and the constraints $-\frac{1}{u-1}\mathbf{\Gamma}_0 \prec \mathbf{\Gamma}_1$ and $\mathbf{\Gamma}_1 \prec \mathbf{\Gamma}_0$, which mean that $\mathbf{\Gamma}_0 - \mathbf{\Gamma}_1$ and $\mathbf{\Gamma}_0 + (u-1)\mathbf{\Gamma}_1$ are positive definite matrices, so that the $um \times um$ matrix $\mathbf{\Gamma}$ is positive definite (for a proof, see Lemma 2.1 in Roy and Leiva (2011)). The $m \times m$ block diagonals $\mathbf{\Gamma}_0$ in $\mathbf{\Gamma}$ represent the variance-covariance matrix of the m response variables at any given site, whereas the $m \times m$ block off diagonals $\mathbf{\Gamma}_1$ in $\mathbf{\Gamma}$ represent the covariance matrix of the m response variables between any two sites. We also assume that $\mathbf{\Gamma}_0$ is constant for all sites and $\mathbf{\Gamma}_1$ is constant for all site pairs. The matrix $\mathbf{\Gamma}$ is also known as equicorrelated partitioned matrix with equicorrelation matrices $\mathbf{\Gamma}_0$ and $\mathbf{\Gamma}_1$ (Roy and Leiva, 2008). Roy and Leiva (2011) also tests the BCS covariance structure on doubly multivariate data.

Let $\boldsymbol{y}_{r,s}$ be a m-variate vector of measurements on the r^{th} individual at the s^{th} site; $r = 1, \ldots, n$, $s = 1, \ldots, u$. The n individuals are all independent. Let $\boldsymbol{y}_r = (\boldsymbol{y}_{r,1}', \ldots, \boldsymbol{y}_{r,u}')'$ be the mu-variate vector of all measurements corresponding to the r^{th} individual. Finally, let $\boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_n$ be a random sample of size n drawn from the population $N_{um}(\boldsymbol{\mu}, \mathbf{\Gamma})$, where $\boldsymbol{\mu} \in \mathbb{R}^{um}$ and $\mathbf{\Gamma}$ is assumed to be a $um \times um$ positive definite matrix. The following section derives the unbiased estimate of $\mathbf{\Gamma}$.

3 Unbiased Estimate of $\mathbf{\Gamma}$

In this section, unbiased estimates of $\mathbf{\Gamma}_0$ and $\mathbf{\Gamma}_1$ are obtained. Clearly, $\overline{\boldsymbol{y}} = (\overline{\boldsymbol{y}}_{\bullet 1}', \ldots, \overline{\boldsymbol{y}}_{\bullet u}')' \sim N_{um}\left(\boldsymbol{\mu}; \frac{1}{n}\mathbf{\Gamma}\right)$ with $\boldsymbol{\mu} = (\boldsymbol{\mu}_1', \ldots, \boldsymbol{\mu}_u')'$ and $\mathbf{\Gamma} = \operatorname{cov}(\boldsymbol{y}) = \mathbf{I}_u \otimes (\mathbf{\Gamma}_0 - \mathbf{\Gamma}_1) + \mathbf{J}_u \otimes \mathbf{\Gamma}_1$, where $\overline{\boldsymbol{y}}_{\bullet s} = \frac{1}{n}\sum_{r=1}^{n} \boldsymbol{y}_{r,s}$ for $s = 1, \ldots, u$. The equicorrelated hypothesis of $\mathbf{\Gamma}$ assures that

$$\mathrm{E}\left[\left(\boldsymbol{y}_{r,s} - \boldsymbol{\mu}_s\right)\left(\boldsymbol{y}_{r,s^*} - \boldsymbol{\mu}_{s^*}\right)'\right] = \begin{cases} \mathbf{\Gamma}_0 & \text{if} \quad s = s^* \\ \mathbf{\Gamma}_1 & \text{if} \quad s \neq s^*, \end{cases}$$

and

$$\mathrm{E}\left[\left(\overline{\boldsymbol{y}}_{\bullet s} - \boldsymbol{\mu}_s\right)\left(\overline{\boldsymbol{y}}_{\bullet s^*} - \boldsymbol{\mu}_{s^*}\right)'\right] = \operatorname{Cov}\left(\overline{\boldsymbol{y}}_{\bullet s}, \overline{\boldsymbol{y}}_{\bullet s^*}\right) = \begin{cases} \frac{1}{n}\mathbf{\Gamma}_0 & \text{if} \quad s = s^* \\ \frac{1}{n}\mathbf{\Gamma}_1 & \text{if} \quad s \neq s^*, \end{cases}$$

because $\boldsymbol{y}_{r,s}$ and $\boldsymbol{y}_{r^*,s^*}$ are independent if $r \neq r^*$. Now,

$$\begin{aligned}
\boldsymbol{C}_0 &= \sum_{s=1}^{u}\sum_{r=1}^{n}\left(\boldsymbol{y}_{r,s}-\overline{\boldsymbol{y}}_{\bullet s}\right)\left(\boldsymbol{y}_{r,s}-\overline{\boldsymbol{y}}_{\bullet s}\right)' \qquad (3.2)\\
&= \sum_{s=1}^{u}\sum_{r=1}^{n}\left[\left(\boldsymbol{y}_{r,s}-\boldsymbol{\mu}_s\right)-\left(\overline{\boldsymbol{y}}_{\bullet s}-\boldsymbol{\mu}_s\right)\right]\left[\left(\boldsymbol{y}_{r,s}-\boldsymbol{\mu}_s\right)-\left(\overline{\boldsymbol{y}}_{\bullet s}-\boldsymbol{\mu}_s\right)\right]'\\
&= \sum_{s=1}^{u}\sum_{r=1}^{n}\left(\boldsymbol{y}_{r,s}-\boldsymbol{\mu}_s\right)\left(\boldsymbol{y}_{r,s}-\boldsymbol{\mu}_s\right)'-\sum_{s=1}^{u}n\left(\overline{\boldsymbol{y}}_{\bullet s}-\boldsymbol{\mu}_s\right)\left(\overline{\boldsymbol{y}}_{\bullet s}-\boldsymbol{\mu}_s\right)',
\end{aligned}$$

then

$$\begin{aligned}
\mathrm{E}\left[\boldsymbol{C}_0\right] &= \sum_{s=1}^{u}\sum_{r=1}^{n}\mathrm{E}\left[\left(\boldsymbol{y}_{r,s}-\boldsymbol{\mu}_s\right)\left(\boldsymbol{y}_{r,s}-\boldsymbol{\mu}_s\right)'\right]-\sum_{s=1}^{u}n\mathrm{E}\left[\left(\overline{\boldsymbol{y}}_{\bullet s}-\boldsymbol{\mu}_s\right)\left(\overline{\boldsymbol{y}}_{\bullet s}-\boldsymbol{\mu}_s\right)'\right]\\
&= \sum_{s=1}^{u}\left(n\boldsymbol{\Gamma}_0-\boldsymbol{\Gamma}_0\right)=u\left(n-1\right)\boldsymbol{\Gamma}_0.
\end{aligned}$$

Therefore,

$$\mathrm{E}\left[\frac{1}{(n-1)u}\boldsymbol{C}_0\right]=\boldsymbol{\Gamma}_0.$$

Similarly,

$$\begin{aligned}
\boldsymbol{C}_1 &= \sum_{\substack{s=1\\ s\neq s^*}}^{u}\sum_{s^*=1}^{u}\sum_{r=1}^{n}\left(\boldsymbol{y}_{r,s}-\overline{\boldsymbol{y}}_{\bullet s}\right)\left(\boldsymbol{y}_{r,s^*}-\overline{\boldsymbol{y}}_{\bullet s^*}\right)' \qquad (3.3)\\
&= \sum_{\substack{s=1\\ s\neq s^*}}^{u}\sum_{s^*=1}^{u}\sum_{r=1}^{n}\left[\left(\boldsymbol{y}_{r,s}-\boldsymbol{\mu}_s\right)-\left(\overline{\boldsymbol{y}}_{\bullet s}-\boldsymbol{\mu}_s\right)\right]\left[\left(\boldsymbol{y}_{r,s^*}-\boldsymbol{\mu}_{s^*}\right)-\left(\overline{\boldsymbol{y}}_{\bullet s^*}-\boldsymbol{\mu}_{s^*}\right)\right]'\\
&= \sum_{\substack{s=1\\ s\neq s^*}}^{u}\sum_{s^*=1}^{u}\sum_{r=1}^{n}\left(\boldsymbol{y}_{r,s}-\boldsymbol{\mu}_s\right)\left(\boldsymbol{y}_{r,s^*}-\boldsymbol{\mu}_{s^*}\right)'-\sum_{\substack{s=1\\ s\neq s^*}}^{u}\sum_{s^*=1}^{u}n\left(\overline{\boldsymbol{y}}_{\bullet s}-\boldsymbol{\mu}_s\right)\left(\overline{\boldsymbol{y}}_{\bullet s^*}-\boldsymbol{\mu}_{s^*}\right)',
\end{aligned}$$

and then

$$\begin{aligned}
\mathrm{E}\left[\boldsymbol{C}_1\right] &= \sum_{\substack{s=1\\ s\neq s^*}}^{u}\sum_{s^*=1}^{u}\sum_{r=1}^{n}\mathrm{E}\left[\left(\boldsymbol{y}_{r,s}-\boldsymbol{\mu}_s\right)\left(\boldsymbol{y}_{r,s^*}-\boldsymbol{\mu}_{s^*}\right)'\right]-\sum_{\substack{s=1\\ s\neq s^*}}^{u}\sum_{s^*=1}^{u}n\mathrm{E}\left[\left(\overline{\boldsymbol{y}}_{\bullet s}-\boldsymbol{\mu}_s\right)\left(\overline{\boldsymbol{y}}_{\bullet s^*}-\boldsymbol{\mu}_{s^*}\right)'\right]\\
&= u(u-1)n\boldsymbol{\Gamma}_1-u(u-1)\boldsymbol{\Gamma}_1=u(u-1)\left(n-1\right)\boldsymbol{\Gamma}_1.
\end{aligned}$$

Hence,

$$\mathrm{E}\left[\frac{1}{(n-1)u(u-1)}\boldsymbol{C}_1\right]=\boldsymbol{\Gamma}_1.$$

Consequently, unbiased estimators of $\boldsymbol{\Gamma}_0$ and $\boldsymbol{\Gamma}_1$ are

$$\widetilde{\boldsymbol{\Gamma}}_0=\frac{1}{\left(n-1\right)u}\boldsymbol{C}_0, \qquad (3.4)$$

and

$$\widetilde{\boldsymbol{\Gamma}}_1 = \frac{1}{(n-1)\,u\,(u-1)}\boldsymbol{C}_1, \tag{3.5}$$

respectively. Therefore, an unbiased estimate of $\boldsymbol{\Gamma}$ is

$$\widetilde{\boldsymbol{\Gamma}} = \boldsymbol{I}_u \otimes \widetilde{\boldsymbol{\Gamma}}_0 + (\boldsymbol{J}_u - \boldsymbol{I}_u) \otimes \widetilde{\boldsymbol{\Gamma}}_1,$$

4 Optimal properties of estimates

In this section, optimal properties of unbiased estimators for parameters of mean vector and the covariance matrix of the following column vector

$$\underset{num\times 1}{\boldsymbol{y}} = \text{vec}(\underset{n\times um}{\boldsymbol{Y}}) \sim N\big((\mathbf{1}_n \otimes \boldsymbol{I}_{um})\boldsymbol{\mu}, \boldsymbol{I}_n \otimes \boldsymbol{\Gamma}_{um}\big).$$

are presented. This means that n independent random column vectors are identically distributed with $(um \times 1)-$dimensional unknown mean vector $\boldsymbol{\mu}$ and $(um \times um)-$dimensional variance covariance matrix $\boldsymbol{\Gamma}$ defined in (2.1). Define the projection matrix $\boldsymbol{P}$ as follows:

$$\boldsymbol{P} = \frac{1}{n}\mathbf{1}_n\mathbf{1}_n' \otimes \boldsymbol{I}_{um}, \tag{4.6}$$

where $\mathbf{1}_n$ is a vector with its n components equal to 1 and the data matrix $\underset{n\times um}{\boldsymbol{Y}} = (\boldsymbol{y}_1', \boldsymbol{y}_2', \ldots, \boldsymbol{y}_n')$. It is clear that $\boldsymbol{P}$ is an orthogonal projector on the subspace of the mean vector of $\boldsymbol{y}$. If $\boldsymbol{I}_n \otimes \boldsymbol{I}_{um} \in \boldsymbol{\vartheta}$, from (Gnot et al., 1977) it follows that $\boldsymbol{P}\boldsymbol{y}$ is the best linear unbiased estimator (BLUE) if and only if $\boldsymbol{P}$ commutes with all covariance matrices $\boldsymbol{V}$. Therefore, we have the following results.

Result 1. *The projection matrix $\boldsymbol{P}$ commutes with the covariance matrix $\boldsymbol{V}$, i.e., $\boldsymbol{P}\boldsymbol{V} = \boldsymbol{V}\boldsymbol{P}$, where $\boldsymbol{V} = \boldsymbol{I}_n \otimes \boldsymbol{\Gamma}$.*

Proof. $\boldsymbol{P}\boldsymbol{V} = (\frac{1}{n}\mathbf{1}_n\mathbf{1}_n' \otimes \boldsymbol{I})(\boldsymbol{I}_n \otimes \boldsymbol{\Gamma}) = \frac{1}{n}\mathbf{1}_n\mathbf{1}_n' \otimes \boldsymbol{\Gamma}$, and $\boldsymbol{V}\boldsymbol{P} = (\boldsymbol{I}_n \otimes \boldsymbol{\Gamma})(\frac{1}{n}\mathbf{1}_n\mathbf{1}_n' \otimes \boldsymbol{I}) = \frac{1}{n}\mathbf{1}_n\mathbf{1}_n' \otimes \boldsymbol{\Gamma}$. Thus, $\boldsymbol{P}$ and $\boldsymbol{V}$ commute. □

Lemma 1. *Let $\boldsymbol{\vartheta}$ denote the subspace spanned by $\boldsymbol{V}$, i.e., $\boldsymbol{\vartheta} = sp\{\boldsymbol{V}\}$. Then, $\boldsymbol{\vartheta}$ is a quadratic subspace; meaning that ϑ is a linear space and if $\boldsymbol{V} \in \vartheta$ then $\boldsymbol{V}^2 \in \vartheta$ (like it is defined in Seely (1971)).*

Proof. From the structure of the covariance matrix $\boldsymbol{V}$ it is clear the that $sp\{\boldsymbol{V}\}$ is a quadratic subspace if and only if $sp\{\boldsymbol{\Gamma}\}$ is a quadratic subspace. After simple calculations one can find that

$$\boldsymbol{\Gamma}^2 = \boldsymbol{I}_u \otimes (\boldsymbol{\Gamma}_0 - \boldsymbol{\Gamma}_1)^2 + \boldsymbol{J}_u \otimes [\boldsymbol{\Gamma}_1\boldsymbol{\Gamma}_0 + \boldsymbol{\Gamma}_0\boldsymbol{\Gamma}_1 + (u-2)\boldsymbol{\Gamma}_1^2]. \tag{4.7}$$

Defining $\boldsymbol{\Gamma}_0^* = \boldsymbol{\Gamma}_0^2 + (u-1)\boldsymbol{\Gamma}_1^2$ and $\boldsymbol{\Gamma}_1^* = \boldsymbol{\Gamma}_1\boldsymbol{\Gamma}_0 + \boldsymbol{\Gamma}_0\boldsymbol{\Gamma}_1 + (u-2)\boldsymbol{\Gamma}_1^2$, $\boldsymbol{\Gamma}^2$ in (4.7) can be rewritten as

$$\boldsymbol{\Gamma}^2 = \boldsymbol{I}_u \otimes (\boldsymbol{\Gamma}_0^* - \boldsymbol{\Gamma}_1^*) + \boldsymbol{J}_u \otimes \boldsymbol{\Gamma}_1^*. \tag{4.8}$$

It means that $sp\{\boldsymbol{\Gamma}\} = sp\{\boldsymbol{\Gamma}^2\}$, and this implies that $sp\{\boldsymbol{V}\}$ is a quadratic subspace. □

Let $\boldsymbol{M} = \boldsymbol{I} - \boldsymbol{P}$. So, $\boldsymbol{M}$ is idempotent. Now, since $\boldsymbol{PV} = \boldsymbol{VP}$, and $\boldsymbol{\vartheta}$ is a quadratic space, $\boldsymbol{M\vartheta M} = \boldsymbol{M\vartheta}$ is also a quadratic space. We now construct a base for the quadratic subspace $\boldsymbol{\vartheta}$. We define

$$\boldsymbol{A}_{ii} = \boldsymbol{E}_{ii} \quad \text{and} \quad \boldsymbol{A}_{ij} = \boldsymbol{E}_{ij} + \boldsymbol{E}_{ji}, \quad \text{for } i < j; \text{ and } \ j = 1, \ldots, m,$$

as a base for symmetric matrices $\boldsymbol{\Gamma}$. The $(m \times m)-$dimensional matrices $\boldsymbol{E}_{ij}$ has 1 only at the ijth element, and 0 at all other elements. Then, it is clear that the base for diagonal matrices of the form $\boldsymbol{I}_n \otimes \boldsymbol{I}_u \otimes \boldsymbol{\Gamma}_0$ is constituted by matrices

$$\boldsymbol{K}_{ij}^{(0)} = \boldsymbol{I}_n \otimes \boldsymbol{I}_u \otimes \boldsymbol{A}_{ij}, \quad \text{for } i \leq j, \quad j = 1, \ldots, m, \tag{4.9}$$

and the base for matrices of the form $\boldsymbol{I}_n \otimes (\boldsymbol{J}_u - \boldsymbol{I}_u) \otimes \boldsymbol{\Gamma}_1$ is constituted by matrices

$$\boldsymbol{K}_{ij}^{(1)} = \boldsymbol{I}_n \otimes (\boldsymbol{J}_u - \boldsymbol{I}_u) \otimes \boldsymbol{A}_{ij}, \quad \text{for } i \leq j, \quad j = 1, \ldots, m. \tag{4.10}$$

Result 2. *The complete and minimal sufficient statistics for the mean vector and the variance-covariance matrix are*

$$\boldsymbol{1}_n \otimes \boldsymbol{I}_{um}\boldsymbol{y} \tag{4.11}$$

$$\textit{and} \qquad \boldsymbol{y}'\boldsymbol{MK}_{ij}^{(l)}\boldsymbol{My}, \quad \textit{for } l = 0, 1 \tag{4.12}$$

where $\boldsymbol{M} = \boldsymbol{I} - \boldsymbol{P}$ and $\boldsymbol{P}$ is given in (4.6), see Fonseca et al. (2010), Seely (1977) and Zmyślony (1980).

Now, we give the following theorem to constitute the best unbiased estimators of $\boldsymbol{\mu}$ and $\boldsymbol{\Gamma}$ under the assumption of multivariate normality.

Theorem 1. *Assume that* $\boldsymbol{y}_{num\times 1} \sim N\big((\mathbf{1}_n \otimes \boldsymbol{I}_{um})\boldsymbol{\mu}, \boldsymbol{I}_n \otimes \boldsymbol{\Gamma}\big)$ *with BCS covariance structure on* $\boldsymbol{\Gamma}$*, i.e.,*

$$\begin{aligned}\boldsymbol{\Gamma} &= \boldsymbol{I}_u \otimes (\boldsymbol{\Gamma}_0 - \boldsymbol{\Gamma}_1) + \boldsymbol{J}_u \otimes \boldsymbol{\Gamma}_1 \\ &= \boldsymbol{I}_u \otimes \boldsymbol{\Gamma}_0 + (\boldsymbol{J}_u - \boldsymbol{I}_u) \otimes \boldsymbol{\Gamma}_1,\end{aligned}$$

where $\boldsymbol{\Gamma}_0$ *and* $\boldsymbol{\Gamma}_1$ *are* $m \times m$ *unknown symmetric matrices with* $\boldsymbol{\Gamma}_0$ *positive definite (defined in Section 2) such that* $\boldsymbol{\Gamma}$ *is positive definite. Then*

$$\widetilde{\boldsymbol{\mu}} = \frac{1}{n}\sum_{i=1}^{n} \boldsymbol{y}_i, \tag{4.13}$$

where $\underset{nmu\times 1}{\boldsymbol{y}} = (\boldsymbol{y}_1', \boldsymbol{y}_2', \ldots, \boldsymbol{y}_n')'$ *with* $\boldsymbol{y}_i = (\boldsymbol{y}_{i,1}', \ldots, \boldsymbol{y}_{i,u}')'$ *and* $\boldsymbol{y}_{i,j} = (\boldsymbol{y}_{i,j,1}, \ldots, \boldsymbol{y}_{i,j,m})'$ *and*

$$\widetilde{\boldsymbol{\Gamma}} = \boldsymbol{I}_u \otimes \widetilde{\boldsymbol{\Gamma}}_0 + (\boldsymbol{J}_u - \boldsymbol{I}_u) \otimes \widetilde{\boldsymbol{\Gamma}}_1, \tag{4.14}$$

where $\widetilde{\boldsymbol{\Gamma}}_0 = \frac{1}{(n-1)u}\boldsymbol{C}_0$ *and* $\widetilde{\boldsymbol{\Gamma}}_1 = \frac{1}{(n-1)u(u-1)}\boldsymbol{C}_1$*, are the best unbiased estimators (BUE) for* $\boldsymbol{\mu}$ *and* $\boldsymbol{\Gamma}$ *respectively. Here* $\boldsymbol{C}_0$ *and* $\boldsymbol{C}_1$ *are defined in (3.2) and (3.3) respectively.*

Proof. First we prove that $\widetilde{\boldsymbol{\mu}}$ is BLUE for $\boldsymbol{\mu}$. Note that putting $\boldsymbol{\Gamma}_0 = \boldsymbol{I}$ and $\boldsymbol{\Gamma}_1 = \mathbf{0}$ we see that the identity element belongs to the space generated by covariance matrices. This implies, according to well known theorem in linear mixed models (see Zmyślony, (1976, 1978, 1980)) that there exists BLUE for each estimable function of mean if and only if the orthogonal projector on the space generated by the mean vector commutes with all covariances matrices. Moreover, BLUE are least squares estimators (LSE), in our case $\boldsymbol{P} = \frac{1}{n}\mathbf{1}_n\mathbf{1}_n' \otimes \boldsymbol{I}_{um}$.

Now

$$\begin{aligned}\boldsymbol{P} &= (\mathbf{1}_n \otimes \boldsymbol{I}_{um})(\mathbf{1}_n \otimes \boldsymbol{I}_{um})^+ \\ &= (\mathbf{1}_n \otimes \boldsymbol{I}_{um})(\mathbf{1}_n^+ \otimes \boldsymbol{I}_{um}) \\ &= (\mathbf{1}_n \otimes \boldsymbol{I}_{um})(\frac{1}{n}\mathbf{1}_n' \otimes \boldsymbol{I}_{um}) \\ &= \frac{1}{n}\mathbf{1}_n\mathbf{1}_n' \otimes \boldsymbol{I}_{um}.\end{aligned}$$

Note that $(\frac{1}{n}\mathbf{1}_n\mathbf{1}_n' \otimes \boldsymbol{I}_{um})(\boldsymbol{I}_n \otimes \boldsymbol{\Gamma}) = \frac{1}{n}\mathbf{1}_n\mathbf{1}_n' \otimes \boldsymbol{\Gamma}$ is symmetric. It implies that the matrix $\boldsymbol{P}$ commutes with the covariance matrix of $\boldsymbol{y}$, and BLUE for $\boldsymbol{\mu}$ is LSE. Thus, $\widetilde{\boldsymbol{\mu}}$ is the unique solution of the following normal equation

$$(\mathbf{1}_n \otimes \boldsymbol{I}_{um})'(\mathbf{1}_n \otimes \boldsymbol{I}_{um})\boldsymbol{\mu} = (\mathbf{1}_n \otimes \boldsymbol{I}_{um})'\boldsymbol{y}, \quad \text{or}$$

$$n\boldsymbol{I}_{um}\boldsymbol{\mu} = [\boldsymbol{I}_{um}, \boldsymbol{I}_{um}, \ldots, \boldsymbol{I}_{um}]\boldsymbol{y},$$

which means that

$$\widetilde{\boldsymbol{\mu}} = \frac{1}{n}\sum_{i=1}^{n}\boldsymbol{y}_i.$$

Now we prove that $\widetilde{\boldsymbol{\Gamma}}_{um}$ is the best quadratic unbiased estimator (BQUE) for $\boldsymbol{\Gamma}$. Since $\boldsymbol{P}$ commutes with the covariance matrix of $\boldsymbol{y}$, for each parameter of quadratic covariance there exists BQUE if and only if

$$sp\{\boldsymbol{MVM}\}, \quad \text{where} \quad \boldsymbol{M} = \boldsymbol{I} - \boldsymbol{P},$$

is a quadratic subspace (see Zmyślony (1976, 1980) and Gnot et al. (1976, 1977a,c); or Jordan algebra, Jordan et al. (1934)), where $\boldsymbol{V}$ stands for the covariance matrix of $\boldsymbol{y}$. It is clear that if $sp\{\boldsymbol{V}\}$ is a quadratic subspace and if for each $\boldsymbol{\Sigma} \in sp\{\boldsymbol{V}\}$ commutativity $\boldsymbol{P\Sigma} = \boldsymbol{\Sigma P}$ holds, then $sp\{\boldsymbol{MVM}\} = sp\{\boldsymbol{MV}\}$ is also a quadratic subspace. According to the coordinate free approach, the expectation of $\text{vec}\{\boldsymbol{Myy'M}\} = \text{vec}(\boldsymbol{My})\text{vec}(\boldsymbol{My})'$ can be written as a linear combination of orthogonal vectors $\text{vec}(\boldsymbol{MK}_{ij}^{(0)})$ and $\text{vec}(\boldsymbol{MK}_{ij}^{(1)})$ with unknown coefficients $\sigma_{ij}^{(0)}$ and $\sigma_{ij}^{(1)}$ respectively. Note also that identity covariance operator of $\boldsymbol{yy'}$ belongs to $sp\{\text{cov}(\boldsymbol{yy'})\}$. It implies that the ordinary best quadratic estimators are least square estimators for corresponding parameters $\sigma_{ij}^{(0)}$ and $\sigma_{ij}^{(1)}$ and they are calculated independently from the following normal equations because of orthogonality

$$\begin{aligned}[\text{vec}(\boldsymbol{MK}_{ij}^{(l)})'\text{vec}(\boldsymbol{MK}_{ij}^{(l)})]\sigma_{ij}^{(l)} &= [\text{vec}(\boldsymbol{MK}_{ij}^{(l)})]'\text{vec}[(\boldsymbol{My})(\boldsymbol{My})'], \\ \text{for } \ l &= 0,1 \quad \text{and} \quad i \le j = 1, \ldots, m.\end{aligned}$$

Because $\boldsymbol{M}^2 = \boldsymbol{M}$, $\boldsymbol{M}$ commutes with $\boldsymbol{K}_{ij}^{(l)}$ and because $\text{vec}(\boldsymbol{A})'\text{vec}(\boldsymbol{B}) = \text{tr}(\boldsymbol{A}'\boldsymbol{B})$, one can easily find the above equations are equivalent to

$$\text{tr}\big(\boldsymbol{M}(\boldsymbol{K}_{ij}^{(l)})^2\big)\boldsymbol{\sigma}_{ij}^{l} = (\boldsymbol{My})'(\boldsymbol{K}_{ij}^{(l)})\boldsymbol{My} \quad \text{for } l = 0,1 \text{ and } i \le j = 1, \ldots, m,$$

and the explicit estimators are

$$\widetilde{\sigma}_{ij}^{(l)} = \frac{1}{\mathrm{tr}\big(\boldsymbol{M}(\boldsymbol{K}_{ij}^{(l)})^2\big)}(\boldsymbol{My})'(\boldsymbol{K}_{ij}^{(l)})(\boldsymbol{My}) \quad \text{for } l = 0, 1 \text{ and } i \le j = 1, \dots, m,$$

or, if $\boldsymbol{r}$ stands for the residual vector, i.e., $\boldsymbol{r} = \boldsymbol{My} = (\boldsymbol{I} - \boldsymbol{P})\boldsymbol{y}$. Then, the above estimators are of the form

$$\widetilde{\sigma}_{ij}^{(l)} = \frac{1}{\mathrm{tr}\big(\boldsymbol{M}(\boldsymbol{K}_{ij}^{(l)})^2\big)}\boldsymbol{r}'(\boldsymbol{K}_{ij}^{(l)})\boldsymbol{r} \quad \text{for } l = 0, 1 \text{ and } i \le j = 1, \dots, m. \tag{4.15}$$

Now, we consider the following four cases:

Case 1: for $l = 0, i = j$ we have

$$\begin{aligned}
\mathrm{tr}(\boldsymbol{M}(\boldsymbol{K}_{ii}^{(0)})^2) &= \mathrm{tr}[(\boldsymbol{I}_n - \frac{1}{n}\boldsymbol{J}_n) \otimes \boldsymbol{I}_u \otimes \boldsymbol{A}_{ii}^2] \\
&= \mathrm{tr}(\boldsymbol{I}_n - \frac{1}{n}\boldsymbol{J}_n)\mathrm{tr}(\boldsymbol{I}_u)\mathrm{tr}(\boldsymbol{A}_{ii}) = (n-1)u, \quad \text{and} \\
(\boldsymbol{My})'\boldsymbol{K}_{ii}^{(0)}\boldsymbol{My} &= \boldsymbol{r}'(\boldsymbol{I}_n \otimes \boldsymbol{I}_u \otimes \boldsymbol{A}_{ii})\boldsymbol{r} = \sum_{k=1}^{n}\sum_{p=1}^{u} r_{kpi}^2.
\end{aligned}$$

Case 2: for $l = 0, i < j$ we have

$$\begin{aligned}
\mathrm{tr}(\boldsymbol{M}(\boldsymbol{K}_{ij}^{(0)})^2) &= \mathrm{tr}[(\boldsymbol{I}_n - \frac{1}{n}\boldsymbol{J}_n) \otimes \boldsymbol{I}_u \otimes \boldsymbol{A}_{ij}^2] \\
&= \mathrm{tr}(\boldsymbol{A}_{ij}^2)\mathrm{tr}(\boldsymbol{I}_n - \frac{1}{n}\boldsymbol{J}_n)\mathrm{tr}(\boldsymbol{I}_u) = 2(n-1)u, \quad \text{for } i < j \ \text{ and} \\
(\boldsymbol{My})'\boldsymbol{K}_{ij}^{(0)}\boldsymbol{My} &= \boldsymbol{r}'(\boldsymbol{I}_n \otimes \boldsymbol{I}_u \otimes \boldsymbol{A}_{ij})\boldsymbol{r} \\
&= 2\sum_{k=1}^{n}\sum_{o=1}^{u} r_{koi}r_{koj} \quad \text{for } i < j.
\end{aligned}$$

Thus, in Cases 1 and 2, it follows that BQUE for $\sigma_{ij}^{(0)}$ in view of (4.15) are

$$\widetilde{\sigma}_{ij}^{(0)} = \frac{1}{(n-1)u}\sum_{k=1}^{n}\sum_{o=1}^{u} r_{koi}r_{koj} \quad \text{for } i \le j,$$

and BQUE for $\boldsymbol{\Gamma}_0$ we get $\widetilde{\boldsymbol{\Gamma}}_0 = \frac{1}{(n-1)u}\boldsymbol{C}_0$, where $\boldsymbol{C}_0$ is defined in (3.2). Cases 3 and 4 are similar to the previous ones for estimation of $\sigma_{ij}^{(1)}$ and $\boldsymbol{\Gamma}_1$.

Case 3: for $l = 1, i = j$, one gets the estimators by noting the following

$$\begin{aligned}
\mathrm{tr}(\boldsymbol{M}(\boldsymbol{K}_{ii}^{(1)})^2) &= \mathrm{tr}[(\boldsymbol{I}_n - \frac{1}{n}\boldsymbol{J}_n) \otimes (\boldsymbol{J}_u - \boldsymbol{I}_u)^2 \otimes \boldsymbol{A}_{ii}^2] \\
&= \mathrm{tr}(\boldsymbol{I}_n - \frac{1}{n}\boldsymbol{J}_n)\mathrm{tr}\{(\boldsymbol{J}_u - \boldsymbol{I}_u)^2\}\mathrm{tr}(\boldsymbol{A}_{ii}^2) = (n-1)u(u-1), \\
\text{and} \quad (\boldsymbol{M}\boldsymbol{y})'\boldsymbol{K}_{ii}^{(1)}\boldsymbol{M}\boldsymbol{y} &= \boldsymbol{r}'(\boldsymbol{I}_n \otimes (\boldsymbol{J}_u - \boldsymbol{I}_u) \otimes \boldsymbol{A}_{ii})\boldsymbol{r} \\
&= \sum_{k=1}^{n}\sum_{p=1}^{u}\sum_{q\neq p}^{u} r_{kpi}r_{kqi}.
\end{aligned}$$

Thus, in view of (4.15) we have

$$\widetilde{\sigma}_{ii}^{(1)} = \frac{1}{(n-1)u(u-1)}\sum_{k=1}^{n}\sum_{p=1}^{u}\sum_{q\neq p}^{u} r_{kpi}r_{kqi}.$$

Finally, in a similar way as in Case 2 we get Case 4 as follows:

Case 4: for $l = 1, i < j$

$$\begin{aligned}
\mathrm{tr}(\boldsymbol{M}(\boldsymbol{K}_{ij}^{(1)})^2) &= \mathrm{tr}[(\boldsymbol{I}_n - \frac{1}{n}\boldsymbol{J}_n) \otimes (\boldsymbol{J}_u - \boldsymbol{I}_u)^2 \otimes \boldsymbol{A}_{ij}^2] \\
&= \mathrm{tr}(\boldsymbol{I}_n - \frac{1}{n}\boldsymbol{J}_n)\mathrm{tr}\{(\boldsymbol{J}_u - \boldsymbol{I}_u)^2\}\mathrm{tr}(\boldsymbol{A}_{ij}^2) = 2(n-1)u(u-1), \quad \text{for} \quad i < j, \quad \text{and} \\
(\boldsymbol{M}\boldsymbol{y})'(\boldsymbol{K}_{ij}^{(1)})\boldsymbol{M}\boldsymbol{y} &= \boldsymbol{r}'(\boldsymbol{I}_n \otimes (\boldsymbol{J}_u - \boldsymbol{I}_u) \otimes \boldsymbol{A}_{ij})\boldsymbol{r} \\
&= 2\sum_{k=1}^{n}\sum_{p=1}^{u}\sum_{q\neq p}^{u} r_{kpi}r_{kqj}, \quad \text{for} \quad i < j.
\end{aligned}$$

Now, again in view of (4.15) we have

$$\widetilde{\sigma}_{ij}^{(1)} = \frac{1}{(n-1)u(u-1)}\sum_{k=1}^{n}\sum_{p=1}^{u}\sum_{q\neq p}^{u} r_{kpi}r_{kqj}, \quad \text{for} \quad i \leq j,$$

and as in the previous case we conclude that $\widetilde{\boldsymbol{\Gamma}}_1 = \frac{1}{(n-1)u(u-1)}\boldsymbol{C}_1$ where $\boldsymbol{C}_1$ is given in (3.3). Now, from Result 2 it follows that estimates for considered parameters are the best unbiased estimators BUEs as a function of complete sufficient statistics. □

Now we are able to make a statement that estimators presented in Theorem 1 are consistent and obviously the family of distribution of above estimators are complete.

Theorem 2. *Estimators given in (4.13) and (4.14) are consistent. Moreover, the family of distributions of these estimators is complete.*

Proof. Note that the variance of the quadratic forms $\boldsymbol{y}'\boldsymbol{A}\boldsymbol{y}$, where $\boldsymbol{y} \sim N(\boldsymbol{\mu}, \boldsymbol{V})$, is given by the following formula

$$\text{var}(\boldsymbol{y}'\boldsymbol{A}\boldsymbol{y}) = 2\text{tr}\big\{(\boldsymbol{AVAV}) + (\boldsymbol{AVA}\boldsymbol{\mu}\boldsymbol{\mu}' + \boldsymbol{\mu}\boldsymbol{\mu}'\boldsymbol{AVA})\big\}. \tag{4.16}$$

In a special case, if $\boldsymbol{A} = \boldsymbol{MAM}$, and if $\boldsymbol{MV} = \boldsymbol{VM}$ then $\boldsymbol{A}\boldsymbol{\mu}\boldsymbol{\mu}' = \boldsymbol{0}$, and (4.16) reduces to the following form

$$\text{var}(\boldsymbol{y}'\boldsymbol{A}\boldsymbol{y}) = 2\text{tr}(\boldsymbol{MAVAV}). \tag{4.17}$$

Now, making an use of (4.17), of the BCS structure of the covariance matrix of $\boldsymbol{y}$ and from (4.9), it follows that for any fixed $\boldsymbol{\Gamma}$

$$\text{var}(\widetilde{\sigma}_{ij}^{(0)}) = \frac{2}{(n-1)u^2}\text{tr}\big\{(\boldsymbol{I}_u \otimes \boldsymbol{A}_{ij})\boldsymbol{\Gamma}(\boldsymbol{I}_u \otimes \boldsymbol{A}_{ij})\boldsymbol{\Gamma}\big\} \to 0 \;\text{ if }\; n \to \infty$$

and from (4.10) it follows that for each fixed $\boldsymbol{\Gamma}$

$$\text{var}(\widetilde{\sigma}_{ij}^{(1)}) = \frac{2}{(n-1)u^2(u-1)^2}\text{tr}\big\{((\boldsymbol{J}_u - \boldsymbol{I}_u) \otimes \boldsymbol{A}_{ij})\boldsymbol{\Gamma}((\boldsymbol{J}_u - \boldsymbol{I}_u) \otimes \boldsymbol{A}_{ij})\boldsymbol{\Gamma}\big\} \to 0 \;\text{ if }\; n \to \infty$$

Estimators for $\boldsymbol{\mu}$ and estimators for elements of covariance matrix are one-to-one functions of minimal sufficient statistic given by (4.11) and (4.12). One can easily check that the $(rs)^{\text{th}}$ element of (3.2) is given by (4.11) for $l = 0$ and the rsth element of (3.3) is given by (4.12) for $l = 1$. Moreover, $\overline{\boldsymbol{y}}_{\bullet s}$ are part of $\widehat{\boldsymbol{\mu}}$ in both (3.2) and (3.3). □

Remark 1. *Note that the mean vector can be replaced by any vector* $\boldsymbol{a}$*. It means that* $E(\boldsymbol{y}) = \boldsymbol{a} \otimes \boldsymbol{\mu}$*.*

5 A real data Example

This data set is taken from Johnson and Wichern (2007, p. 43). An investigator measured the mineral content of bones (radius, humerus and ulna) by photon absorptiometry to examine whether dietary supplements would slow bone loss in 25 older women. Measurements were recorded for three bones on the dominant and non-dominant sides. Thus, the data is doubly multivariate, and clearly $m = 3$ and $u = 2$. We rearrange the variables in the data set by grouping together the mineral content of the dominant sides of radius, humerus and ulna as the first three variables, that is, the variables in the first location ($u = 1$) and then the mineral contents for the non-dominant side of the same bones ($u = 2$). Using the likelihood ratio test Roy and Leiva (2011) demonstrated that the data fail to reject the null hypothesis that the covariance structure is of the BCS form ($p-$value $= 0.5786$). Using the formula (4.13) presented in Section 4 the unbiased estimate of $\boldsymbol{\mu}$ is

$$\widetilde{\boldsymbol{\mu}} = \begin{bmatrix} 0.84380 & 1.79268 & 0.70440 & 0.81832 & 1.73484 & 0.69384 \end{bmatrix}.$$

Using Theorems 1 we say that the above estimate $\widetilde{\boldsymbol{\mu}}$ is BLUE for $\boldsymbol{\mu}$. Furthermore, using the formulas (3.4) and (3.5) presented in Section 3 the unbiased estimates of $\boldsymbol{\Gamma}_0$ and $\boldsymbol{\Gamma}_1$ are

$$\widetilde{\boldsymbol{\Gamma}}_0 = \begin{bmatrix} 0.01221 & 0.02172 & 0.00901 \\ 0.02172 & 0.07492 & 0.01682 \\ 0.00901 & 0.01682 & 0.01108 \end{bmatrix},$$

and

$$\widetilde{\boldsymbol{\Gamma}}_1 = \begin{bmatrix} 0.01038 & 0.01931 & 0.00824 \\ 0.01931 & 0.06678 & 0.01529 \\ 0.00824 & 0.01529 & 0.00807 \end{bmatrix},$$

respectively. Using the above estimates the unbiased estimate of $\boldsymbol{\Gamma}$ is

$$\begin{aligned} \widetilde{\boldsymbol{\Gamma}} &= \mathbf{I}_u \otimes \left(\widetilde{\boldsymbol{\Gamma}}_0 - \widetilde{\boldsymbol{\Gamma}}_1\right) + \mathbf{J}_u \otimes \widetilde{\boldsymbol{\Gamma}}_1 \\ &= \left[\begin{array}{cc} \begin{bmatrix} 0.01221 & 0.02172 & 0.00901 \\ 0.02172 & 0.07492 & 0.01682 \\ 0.00901 & 0.01682 & 0.01108 \end{bmatrix} & \begin{matrix} 0.01038 & 0.01931 & 0.00824 \\ 0.01931 & 0.06678 & 0.01529 \\ 0.00824 & 0.01529 & 0.00807 \end{matrix} \\ \begin{matrix} 0.01038 & 0.01931 & 0.00824 \\ 0.01931 & 0.06678 & 0.01529 \\ 0.00824 & 0.01529 & 0.00807 \end{matrix} & \begin{bmatrix} 0.01221 & 0.02172 & 0.00901 \\ 0.02172 & 0.07492 & 0.01682 \\ 0.00901 & 0.01682 & 0.01108 \end{bmatrix} \end{array}\right]. \end{aligned}$$

Using Theorems 1 and 2 we say that the above estimate $\widetilde{\boldsymbol{\Gamma}}$ is the best unbiased and complete estimate of $\boldsymbol{\Gamma}$.

6 Conclusions

Estimates of covariance matrices are needed for the principal component analysis and factor analysis, and are also involved in versions of regression analysis that treat the dependent variables in a data-set, jointly with the independent variable as the outcome of a random sample. Thus, optimal estimation of covariance matrices is very important aspect in any data analysis, and the obtained results demonstrate the optimality of estimates for both fixed effects and variance-covariance matrices using the coordinate free approach theory for estimation.

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