

Estimation in Multilevel Models with Block Circular Symmetric Covariance Structure

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Abstract

In this article we consider a multilevel model with block circular symmetric covariance structure. Maximum likelihood estimation of the parameters of this model is discussed. We show that explicit maximum likelihood estimators of variance components exist under certain restrictions on the parameter space.

Keywords: Circular block symmetry, Constrained model, Covariance matrix, Explicit solution, Maximum likelihood estimator, Multilevel model

1. Introduction

Very often data arise in natural hierarchies, for example, children are nested within families, students are grouped within classrooms and employees are clustered within workplaces. Many experimental designs also generate data having a hierarchical structure. The existence of such data hierarchies is not accidental and should be accounted for when conducting a statistical analysis. Multilevel models (Goldstein, 2003) refer to a class of multivariate statistical models developed for the analysis of hierarchically structured data. One can note the existence of many other names for these models, including, hierarchical linear model, random coefficients model, and hierarchical mixed linear model. To a certain extent, the emergence of names is due to the statistical properties of different modeling strategies used to analyze multilevel data.

The distinguishing feature of hierarchical data is that observations within a corresponding group (hierarchy) are usually more similar to one another than are observations from different groups (hierarchies). Moreover, hierarchical structures violate the independence assumption (because lack of independence between measurements), and techniques for dealing with this have to be developed.

In this article we consider the problem of estimation in multilevel models with a block circular symmetric covariance structure. In the framework of multilevel models, this structure has been utilized in many applications, to describe the situations with a spatial circular layout on one factor and an exchangeable feature on another factor. For example, in the signal processing problem in Olkin and Press (1969), one would

expect a circular symmetric structure for the covariances between the messages received by the receivers placed at these vertices. Furthermore, it is possible to collect an extended data structure which contains another symmetric factor (e.g., region) and the data has the circulant property in the receiver level and a symmetric pattern in the region level. Marin and Dhorne (2003) gave an example from experimental design: experiments where neighbourhood in space or in time is taken into account. The structure required on the experimental unit is cyclic, i.e. each experimental unit must have two neighbours, and the graph formed by joining neighbours is a single cycle. Additionally, a study can be designed to include one more symmetric factor with a block circular symmetric covariance structure.

Estimation in linear models with patterned covariance matrices has got a lot of attention. Olkin and Press (1969) and Olkin (1973) provided MLEs for the parameters in a circular symmetric model, but without patterned blocks. Szatrowski (1980) and Szatrowski and Miller (1980) discussed the multivariate normal model with a linear covariance structure and gave a necessary and sufficient condition of explicit MLEs for both the mean and covariance matrices. Marin and Dhorne (2002, 2003) gave a necessary and sufficient condition of an optimal unbiased estimator for statistical model with linear Toeplitz covariance structure. Ohlson and von Rosen (2010) studied linearly structured covariances in a classical growth curve model setting. In this article, we focus on the estimation of a covariance matrix which is block circular symmetric and has patterned blocks.

The organization of the article is as follows. Section 2 introduces the basic model, notation, necessary definitions and some results on ML estimation. In Section 3 the main results concerning the explicit estimation in multilevel models with a block circular symmetric covariance structure are presented, and explicit MLEs are derived. In section 4 the estimability of (co)variance components is discussed in terms of model reparameterization (restriction).

2. Preliminaries

In this section a balanced model with block circular covariance structure is introduced and spectral properties of the matrices corresponding to such a dependence structure are given. Let us consider a balanced (nested) mixed linear model with block circular symmetric covariance structure. In particular consider

$$\mathbf{y} = \mu \mathbf{1}_p + \mathbf{Z}_1 \boldsymbol{\gamma}_1 + \mathbf{Z}_2 \boldsymbol{\gamma}_2 + \mathbf{I}_p \boldsymbol{\epsilon}, \quad (1)$$

where μ is an unknown constant parameter, $\boldsymbol{\gamma}_1$, $\boldsymbol{\gamma}_2$ and $\boldsymbol{\epsilon}$ are independently normally distributed random variables with zero means and variances-covariance matrices $\boldsymbol{\Sigma}_1$, $\boldsymbol{\Sigma}_2$, and $\sigma^2 \mathbf{I}_p$, respectively. Here $\mathbf{Z}_1 = \mathbf{I}_{n_2} \otimes \mathbf{1}_{n_1}$, $\mathbf{Z}_2 = \mathbf{I}_{n_2} \otimes \mathbf{I}_{n_1}$, $\mathbf{1}_s$ is a column vector of size s with all elements equal to one and \mathbf{I}_s is the identity matrix of order s ,

$p = n_1 n_2$. The symbol \otimes denotes the Kronecker product. Thus,

$$\mathbf{y} \sim N_p(\mu \mathbf{1}_p, \boldsymbol{\Sigma}), \quad (2)$$

$$\boldsymbol{\Sigma} = \mathbf{Z}_1 \boldsymbol{\Sigma}_1 \mathbf{Z}_1' + \boldsymbol{\Sigma}_2 + \sigma^2 \mathbf{I}_p. \quad (3)$$

In our model we suppose that the covariance matrix $\boldsymbol{\Sigma}_1 : n_2 \times n_2$ has the following structure (compound symmetry):

$$\boldsymbol{\Sigma}_1 = a \mathbf{I}_{n_2} + b(\mathbf{J}_{n_2} - \mathbf{I}_{n_2}), \quad (4)$$

where a and b are unknown parameters. The covariance matrix $\boldsymbol{\Sigma}_2 : p \times p$ has a block compound symmetric pattern with a symmetric circular Toeplitz (SC-Toeplitz) matrix in each block, i.e.

$$\boldsymbol{\Sigma}_2 = \mathbf{I}_{n_2} \otimes \boldsymbol{\Sigma}^{(1)} + (\mathbf{J}_{n_2} - \mathbf{I}_{n_2}) \otimes \boldsymbol{\Sigma}^{(2)}, \quad (5)$$

where the SC-Toeplitz matrix $\boldsymbol{\Sigma}^{(h)} = (\sigma_{ij}^{(h)})$ depends on $[n_1/2] + 1$ parameters, the symbol $[\bullet]$ stands for the integer part, and for $i, j = 1, \dots, n_1$, $h = 1, 2$,

$$\sigma_{ij}^{(h)} = \begin{cases} \tau_{|j-i|+(h-1)([n_1/2]+1)}, & \text{if } |j-i| \leq [n_1/2], \\ \tau_{n_1-|j-i|+(h-1)([n_1/2]+1)}, & \text{otherwise,} \end{cases} \quad (6)$$

and τ_q 's are unknown parameters, $q = 0, \dots, 2[n_1/2] + 1$.

The covariance matrix $\boldsymbol{\Sigma}$ given in (3) is a sum of three symmetric matrices $\mathbf{Z}_1 \boldsymbol{\Sigma}_1 \mathbf{Z}_1'$, $\boldsymbol{\Sigma}_2$ and $\sigma^2 \mathbf{I}_p$, which as will be shown commute in the next lemma, and hence can be simultaneously diagonalized. This property will be utilized to obtain the eigenvalues of $\boldsymbol{\Sigma}$, which in turn can be used to derive explicit maximum likelihood estimators of the unknown parameters. The next auxiliary lemma provides an important property of $\mathbf{Z}_1 \boldsymbol{\Sigma}_1 \mathbf{Z}_1'$ and $\boldsymbol{\Sigma}_2$.

Lemma 2.1. *The matrices $\mathbf{Z}_1 \boldsymbol{\Sigma}_1 \mathbf{Z}_1'$ and $\boldsymbol{\Sigma}_2$ are commuting normal matrices.*

Proof. Since $\mathbf{Z}_1 \boldsymbol{\Sigma}_1 \mathbf{Z}_1'$ and $\boldsymbol{\Sigma}_2$ both are symmetric they are also normal matrices. Now, using the structure of $\boldsymbol{\Sigma}_1$ given in (4), we first observe that

$$\begin{aligned} \mathbf{Z}_1 \boldsymbol{\Sigma}_1 \mathbf{Z}_1' &= (\mathbf{I}_{n_2} \otimes \mathbf{1}_{n_1})(a \mathbf{I}_{n_2} + b(\mathbf{J}_{n_2} - \mathbf{I}_{n_2}))(\mathbf{I}_{n_2} \otimes \mathbf{1}'_{n_1}) \\ &= a \mathbf{I}_{n_2} \otimes \mathbf{J}_{n_1} + b(\mathbf{J}_{n_2} - \mathbf{I}_{n_2}) \otimes \mathbf{J}_{n_1}. \end{aligned} \quad (7)$$

Next we calculate

$$\begin{aligned} &\mathbf{Z}_1 \boldsymbol{\Sigma}_1 \mathbf{Z}_1' \boldsymbol{\Sigma}_2 \\ &= (a \mathbf{I}_{n_2} \otimes \mathbf{J}_{n_1} + b(\mathbf{J}_{n_2} - \mathbf{I}_{n_2}) \otimes \mathbf{J}_{n_1}) \left(\mathbf{I}_{n_2} \otimes \boldsymbol{\Sigma}^{(1)} + (\mathbf{J}_{n_2} - \mathbf{I}_{n_2}) \otimes \boldsymbol{\Sigma}^{(2)} \right) \\ &= a \mathbf{I}_{n_2} \otimes \left(\mathbf{J}_{n_1} \boldsymbol{\Sigma}^{(1)} \right) + a(\mathbf{J}_{n_2} - \mathbf{I}_{n_2}) \otimes \left(\mathbf{J}_{n_1} \boldsymbol{\Sigma}^{(2)} \right) \\ &\quad + b(\mathbf{J}_{n_2} - \mathbf{I}_{n_2}) \otimes \left(\mathbf{J}_{n_1} \boldsymbol{\Sigma}^{(1)} \right) + b[(n_2 - 2)\mathbf{J}_{n_2} + \mathbf{I}_{n_2}] \otimes \left(\mathbf{J}_{n_1} \boldsymbol{\Sigma}^{(2)} \right). \end{aligned}$$

Since both $\boldsymbol{\Sigma}^{(1)}$ and $\boldsymbol{\Sigma}^{(2)}$ commute with \mathbf{J}_{n_1} , it is straightforward to obtain that $\mathbf{Z}_1 \boldsymbol{\Sigma}_1 \mathbf{Z}_1' \boldsymbol{\Sigma}_2 = \boldsymbol{\Sigma}_2 \mathbf{Z}_1 \boldsymbol{\Sigma}_1 \mathbf{Z}_1'$. ■

Since symmetric circular Toeplitz matrices are important for the subsequent inference, several of their properties will be reviewed. In the next theorem we give the eigenvalues and eigenvectors of a SC-Toeplitz matrix.

Theorem 2.2. Let $\mathbf{T} = \{t_{ij}\} : n \times n$ be a SC-Toeplitz matrix, i.e.

$$t_{ij} = \begin{cases} t_{|j-i|}, & \text{if } |j-i| \leq \lfloor \frac{n}{2} \rfloor, \\ t_{n-|j-i|}, & \text{otherwise.} \end{cases} \quad (8)$$

The eigenvalues of \mathbf{T} are given by

$$\lambda_k = \sum_{j=0}^{n-1} t_j \cos\left(\frac{2\pi}{n}(k-1)(n-j)\right), k = 1, \dots, n. \quad (9)$$

The corresponding eigenvectors $\mathbf{w}^1, \dots, \mathbf{w}^n$ are defined through

$$\mathbf{w}_j^k = \frac{1}{\sqrt{n}} \left[\cos\left(\frac{2\pi}{n}(j-1)(k-1)\right) + \sin\left(\frac{2\pi}{n}(j-1)(k-1)\right) \right], \quad (10)$$

$j, k = 1, \dots, n.$

Corollary 2.3. The matrix \mathbf{T} defined in (8) have the following properties.

- (i) $t_{ij} = t_{in-j+2}$, $j = 2, \dots, n$.
- (ii) $\lambda_i = \lambda_{n-i+2}$, $i = 2, \dots, n$.
- (iii) The eigenvectors of \mathbf{T} defined in (10) are independent of the elements of \mathbf{T} .
- (iv) Let $\mathbf{W} = (\mathbf{w}^1, \dots, \mathbf{w}^n)$, with $\mathbf{w}^k = (w_1^k, \dots, w_n^k)'$, $k = 1, \dots, n$. Then $\mathbf{W}\mathbf{W}' = \mathbf{I}_n$ and $\mathbf{1}'_n \mathbf{W} = (\sqrt{n}, 0, \dots, 0)$.

Eigenvalues of the matrices $\mathbf{Z}_1 \boldsymbol{\Sigma}_1 \mathbf{Z}'_1$ and $\boldsymbol{\Sigma}_2$ together with the corresponding eigenvectors will be presented in the following theorems.

Theorem 2.4. A symmetric matrix $\mathbf{Z}_1 \boldsymbol{\Sigma}_1 \mathbf{Z}'_1 : n_1 n_2 \times n_1 n_2$ of the form given in (7) has three distinct eigenvalues:

$$\begin{aligned} \lambda_1 &= n_1(a-b) + n_2 n_1 b && \text{with multiplicity } 1, \\ \lambda_2 &= n_1(a-b) && \text{with multiplicity } (n_2 - 1), \\ \lambda_3 &= 0 && \text{with multiplicity } n_2(n_1 - 1). \end{aligned}$$

The following set $(\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_{n_2}, \mathbf{v}_{n_2+1}, \dots, \mathbf{v}_{n_1 n_2})$ comprises the eigenvectors of $\mathbf{Z}_1 \boldsymbol{\Sigma}_1 \mathbf{Z}'_1$ which are of the form

$$\mathbf{v}_h = \mathbf{w}_2^{i_2} \otimes \mathbf{w}_1^{i_1}, \quad (11)$$

where elements of the vectors $\mathbf{w}_k^{i_k}$ are defined by (10), $i_k = 1, \dots, n_k$, $h = 1, \dots, n_1 n_2$, and $k = 1, 2$. Moreover, the eigenvector corresponding to λ_1 is $\mathbf{v}_1 = \mathbf{w}_2^1 \otimes \mathbf{w}_1^1 = (n_1 n_2)^{-1/2} \mathbf{1}_{n_2} \otimes \mathbf{1}_{n_1}$; the eigenvectors corresponding to λ_2 are $\mathbf{v}_h = \mathbf{w}_2^{h_2} \otimes \mathbf{w}_1^1 = \mathbf{w}_2^{h_2} \otimes n_1^{-1/2} \mathbf{1}_{n_1}$, $h_2 = 2, \dots, n_2$; and the eigenvectors corresponding to λ_3 are $\mathbf{v}_i = \mathbf{w}_2^{h_2} \otimes \mathbf{w}_1^{h_1}$, where $h_2 = 1, \dots, n_2$, $h_1 = 2, \dots, n_1$.

Proof. Let us define the following orthogonal matrix

$$\mathbf{\Gamma} = \mathbf{\Gamma}_2 \otimes \mathbf{\Gamma}_1,$$

where the matrix $\mathbf{\Gamma}_k$ comprises of eigenvectors of a SC-Toeplitz matrix of order n_k which are specified by (10), i.e. $\mathbf{\Gamma}_k = (\mathbf{w}_k^1, \dots, \mathbf{w}_k^{n_k})$, $k = 1, 2$. Observing that the first column in $\mathbf{\Gamma}_k$ is $\mathbf{w}_k^1 = n_k^{-1/2} \mathbf{1}_{n_k}$, it follows that

$$\mathbf{\Gamma}'_k \mathbf{J}_{n_k} \mathbf{\Gamma}_k = \begin{pmatrix} n_k & 0 \\ 0 & \mathbf{0}_{n_k-1} \end{pmatrix},$$

where $\mathbf{0}_{n_k-1} : (n_k - 1) \times (n_k - 1)$ is a matrix with all elements equal to zero. Then

$$\begin{aligned} & \mathbf{\Gamma}' \mathbf{Z}_1 \mathbf{\Sigma}_1 \mathbf{Z}'_1 \mathbf{\Gamma} \\ &= (\mathbf{\Gamma}'_2 \otimes \mathbf{\Gamma}'_1) (a \mathbf{I}_{n_2} \otimes \mathbf{J}_{n_1} + b (\mathbf{J}_{n_2} - \mathbf{I}_{n_2}) \otimes \mathbf{J}_{n_1}) (\mathbf{\Gamma}_2 \otimes \mathbf{\Gamma}_1) \\ &= (a - b) \mathbf{I}_{n_2} \otimes \mathbf{\Gamma}'_1 \mathbf{J}_{n_1} \mathbf{\Gamma}_1 + b \mathbf{\Gamma}'_2 \mathbf{J}_{n_2} \mathbf{\Gamma}_2 \otimes \mathbf{\Gamma}'_1 \mathbf{J}_{n_1} \mathbf{\Gamma}_1 \\ &= (a - b) \mathbf{I}_{n_2} \otimes \begin{pmatrix} n_1 & 0 \\ 0 & \mathbf{0}_{n_1-1} \end{pmatrix} + b \begin{pmatrix} n_2 & 0 \\ 0 & \mathbf{0}_{n_2-1} \end{pmatrix} \otimes \begin{pmatrix} n_1 & 0 \\ 0 & \mathbf{0}_{n_1-1} \end{pmatrix}. \end{aligned}$$

This is a diagonal matrix and therefore the eigenvalues follow immediately.

Due to the structure of the matrix $\mathbf{Z}_1 \mathbf{\Sigma}_1 \mathbf{Z}'_1$ it is straightforward to verify that the vectors defined in (11) are indeed eigenvectors of $\mathbf{Z}_1 \mathbf{\Sigma}_1 \mathbf{Z}'_1$. \blacksquare

In the next theorem the eigenvalues and the eigenvectors of the matrix $\mathbf{\Sigma}_2$ are presented using the block structure of $\mathbf{\Sigma}_2$.

Theorem 2.5. *Let $\mathbf{\Sigma}_2$ have the structure specified in (5), and $\lambda_1^{(i)}, \dots, \lambda_{n_1}^{(i)}$ be the eigenvalues given in Theorem 2.2 of a SC-Toeplitz matrix $\mathbf{\Sigma}^{(i)}$ in (6), $i = 1, 2$. Then, $\mathbf{\Sigma}_2$ has eigenvalues*

$$\lambda_{1h} = \lambda_h^{(1)} + (n_2 - 1) \lambda_h^{(2)}, \quad (12)$$

$$\lambda_{2h} = \lambda_h^{(1)} - \lambda_h^{(2)}, \quad (13)$$

where $h = 1, \dots, n_1$.

Furthermore, if n_1 is odd, the multiplicity of λ_{i1} is $(n_2 - 1)^{i-1}$, the eigenvalues $\lambda_{i2}, \dots, \lambda_{in_1}$ are of the multiplicity $2(n_2 - 1)^{i-1}$, $i = 1, 2$. If n_1 is even, the multiplicities of both λ_{i1} and $\lambda_{i \frac{n_1}{2}}$ are $(n_2 - 1)^{i-1}$ and other eigenvalues $\lambda_{i2}, \dots, \lambda_{in_1}$ are of the multiplicity $2(n_2 - 1)^{i-1}$, $i = 1, 2$. Thus, the number of distinct eigenvalues for $\mathbf{\Sigma}_2$ is $2(\lfloor n_1/2 \rfloor + 1)$. The set $(\mathbf{v}_1^1, \dots, \mathbf{v}_1^{n_1}, \mathbf{v}_2^1, \dots, \mathbf{v}_2^{n_1(n_2-1)})$ comprises the eigenvectors of $\mathbf{\Sigma}_2$ which are of the following form:

$$\mathbf{v}_1^i = \mathbf{w}_2^1 \otimes \mathbf{w}_1^{h_1} = n_2^{-1/2} \mathbf{1}_{n_2} \otimes \mathbf{w}_1^{h_1}, \quad i, h_1 = 1, \dots, n_1, \quad (14)$$

$$\mathbf{v}_2^j = \mathbf{w}_2^{h_2} \otimes \mathbf{w}_1^{h_1}, \quad j = 1, \dots, n_1(n_2 - 1), h_2 = 2, \dots, n_2, \quad (15)$$

where elements of the vectors $\mathbf{w}_k^{i_k}$ are defined in (10), $i_k = 1, \dots, n_k$ and $k = 1, 2$.

Proof. Let us define the following orthogonal matrix

$$\mathbf{\Gamma} = \mathbf{\Gamma}_2 \otimes \mathbf{\Gamma}_1 = (\mathbf{v}_1^1 \dots, \mathbf{v}_1^{n_1}, \mathbf{v}_2^1, \dots, \mathbf{v}_2^{n_1(n_2-1)}),$$

where the matrix $\mathbf{\Gamma}_k$ consists of eigenvectors of a SC-Toeplitz matrix of order n_k which are specified in (10), i.e. $\mathbf{\Gamma}_k = (\mathbf{w}_k^1, \dots, \mathbf{w}_k^{n_k})$, $k = 1, 2$, and

$$\mathbf{\Gamma}_1' \mathbf{\Sigma}^{(i)} \mathbf{\Gamma}_1 = \mathbf{\Lambda}^{(i)} = \text{diag}(\lambda_1^{(i)}, \lambda_2^{(i)}, \dots, \lambda_{n_1}^{(i)}), \quad i = 1, 2. \quad (16)$$

Observing that the first column in $\mathbf{\Gamma}_k$ is $\mathbf{w}_k^1 = n_k^{-1/2} \mathbf{1}_{n_k}$, $k = 1, 2$, it follows that

$$\mathbf{\Gamma}_k' \mathbf{J}_{n_k} \mathbf{\Gamma}_k = \begin{pmatrix} n_k & 0 \\ 0 & \mathbf{0}_{n_k-1} \end{pmatrix}.$$

Then

$$\begin{aligned} \mathbf{\Gamma}' \mathbf{\Sigma}_2 \mathbf{\Gamma} &= (\mathbf{\Gamma}_2' \otimes \mathbf{\Gamma}_1') \left[\mathbf{I}_{n_2} \otimes \left(\mathbf{\Sigma}^{(1)} - \mathbf{\Sigma}^{(2)} \right) + \mathbf{J}_{n_2} \otimes \mathbf{\Sigma}^{(2)} \right] (\mathbf{\Gamma}_2 \otimes \mathbf{\Gamma}_1) \\ &= \mathbf{I}_{n_2} \otimes \left(\mathbf{\Gamma}_1' \mathbf{\Sigma}^{(1)} \mathbf{\Gamma}_1 - \mathbf{\Gamma}_1' \mathbf{\Sigma}^{(2)} \mathbf{\Gamma}_1 \right) + (\mathbf{\Gamma}_2' \mathbf{J}_{n_2} \mathbf{\Gamma}_2) \otimes \left(\mathbf{\Gamma}_1' \mathbf{\Sigma}^{(2)} \mathbf{\Gamma}_1 \right) \\ &= \mathbf{I}_{n_2} \otimes (\mathbf{\Lambda}^{(1)} - \mathbf{\Lambda}^{(2)}) + \begin{pmatrix} n_2 & 0 \\ 0 & \mathbf{0}_{n_2-1} \end{pmatrix} \otimes \mathbf{\Lambda}^{(2)}. \end{aligned} \quad (17)$$

From the last expression in (17) the eigenvalues with corresponding multiplicities can be obtained.

To verify that \mathbf{v}_i^h is a eigenvector of $\mathbf{\Sigma}_2$ corresponding to the eigenvalue λ_{ih} , $i = 1, 2$ one should check that $\mathbf{\Sigma}_2 \mathbf{v}_i^h = \lambda_{ih} \mathbf{v}_i^h$, $h = 1, \dots, n_1$. Indeed, for $\mathbf{v}_1^h = \mathbf{w}_2^1 \otimes \mathbf{w}_1^{h_1} = n_2^{-1/2} \mathbf{1}_{n_2} \otimes \mathbf{w}_1^{h_1}$,

$$\begin{aligned} \mathbf{\Sigma}_2 \mathbf{v}_1^h &= \left(\mathbf{I}_{n_2} \otimes \mathbf{\Sigma}^{(1)} + (\mathbf{J}_{n_2} - \mathbf{I}_{n_2}) \otimes \mathbf{\Sigma}^{(2)} \right) (n_2^{-1/2} \mathbf{1}_{n_2} \otimes \mathbf{w}_1^{h_1}) \\ &= n_2^{-1/2} \mathbf{1}_{n_2} \otimes \mathbf{\Sigma}^{(1)} \mathbf{w}_1^{h_1} + n_2^{-1/2} (n_2 - 1) \mathbf{1}_{n_2} \otimes \mathbf{\Sigma}^{(2)} \mathbf{w}_1^{h_1} \\ &= n_2^{-1/2} \mathbf{1}_{n_2} \otimes (\lambda_h^{(1)} \mathbf{w}_1^{h_1}) + n_2^{-1/2} (n_2 - 1) \mathbf{1}_{n_2} \otimes (\lambda_h^{(2)} \mathbf{w}_1^{h_1}) \\ &= (\lambda_h^{(1)} + (n_2 - 1) \lambda_h^{(2)}) (n_2^{-1/2} \mathbf{1}_{n_2} \otimes \mathbf{w}_1^{h_1}) \\ &= \lambda_{1h} \mathbf{v}_1^{h_1}, \end{aligned}$$

where $h_1 = 1, \dots, n_1$. Similarly, one can verify that $\mathbf{\Sigma}_2 \mathbf{v}_2^h = \lambda_{2h} \mathbf{v}_2^h$, $h = 1, \dots, n_1(n_2 - 1)$. ■

An alternative formulation of the spectrum of $\mathbf{\Sigma}_2$ in Theorem 2.5 is given in the following corollary.

Corollary 2.6. *Let $\boldsymbol{\tau}$ and $\boldsymbol{\lambda}$ be the vectors representing distinct elements and distinct eigenvalues of $\mathbf{\Sigma}_2$, given in (6) and Theorem 2.5, respectively. Then*

$$\boldsymbol{\lambda} = \mathbf{B}_2 \boldsymbol{\tau}, \quad (18)$$

where the nonsingular coefficient matrix \mathbf{B}_2 has the following form:

$$\mathbf{B}_2 = \begin{pmatrix} \mathbf{A} & (n_2 - 1)\mathbf{A} \\ \mathbf{A} & -\mathbf{A} \end{pmatrix}, \quad (19)$$

where $\mathbf{A} = \{a_{ij}\}$ is a $(\lfloor \frac{n_1}{2} \rfloor + 1) \times (\lfloor \frac{n_1}{2} \rfloor + 1)$ matrix and

$$a_{ij} = 2^{\mathbf{1}_{\{1 < j < \lfloor n_1/2 \rfloor + 1\}}} \cos(2\pi(i-1)(n_1-j+1)/n_1),$$

$i, j = 1, \dots, n_1$. Moreover, by inverting \mathbf{B}_2 , $\boldsymbol{\tau}$ can be expressed as follows:

$$\boldsymbol{\tau} = \mathbf{B}_2^{-1}\boldsymbol{\lambda},$$

where, since $\mathbf{A}^2 = n_1\mathbf{I}_{n_1}$,

$$\mathbf{B}_2^{-1} = \frac{1}{n_1 n_2} \begin{pmatrix} \mathbf{A} & (n_2 - 1)\mathbf{A} \\ \mathbf{A} & -\mathbf{A} \end{pmatrix}.$$

3. Estimation

This section deals with ML estimation of parameters of the model given in (1). Suppose that we have a sample of n independent, identically distributed observations $\mathbf{y}_1, \dots, \mathbf{y}_n$ from a multivariate normal distribution with mean $\mu\mathbf{1}_p$ and covariance matrix $\boldsymbol{\Sigma}$, i.e. $\mathbf{y}_i \sim N_p(\mu\mathbf{1}_p, \boldsymbol{\Sigma})$, $i = 1, \dots, n$. We are interested in obtaining maximum likelihood estimators of μ and $\boldsymbol{\Sigma}$ when the covariance matrix $\boldsymbol{\Sigma}$ has a particular linear pattern.

Definition 3.1. *A positive-definite covariance matrix $\boldsymbol{\Sigma}$ has a linear pattern (Anderson, 1973) when $\boldsymbol{\Sigma} = \sum_{i=0}^r \theta_i \mathbf{G}_i$, where the \mathbf{G}_i 's are linearly independent symmetric matrices and $\theta_0, \dots, \theta_r$ are scalars.*

Later it will be shown that with the spectral decomposition, $\boldsymbol{\Sigma}$ given by (3) is of this form where the \mathbf{G}_i 's are known and the $\theta_0, \dots, \theta_r$ are unknown. It is fairly easy to imagine that $\boldsymbol{\Sigma}$ follows a linear structure but it is more difficult to imagine that the \mathbf{G}_i 's are linearly independent.

Concerning estimation of variance components, Harville (1977) discussed the maximum likelihood and restricted maximum likelihood approaches for normal mixed effects models, and gave formulae for special cases. For a two-level model, Mason, Wong & Entwistle (1984) obtained restricted maximum likelihood estimates using the EM algorithm. Fuller & Battese (1973) showed how noniterative but consistent moment estimators of the error variances for a simple three-level model can be obtained and used it in generalized least squares estimation. Szatrowski (1980) gave necessary and sufficient conditions on linear patterns so that explicit maximum likelihood estimators for μ and the covariance matrix $\boldsymbol{\Sigma}$ exist.

Theorem 3.1. *Szatrowski (1980) Let \mathbf{X} be $p \times r$, $r \leq p$ of full rank. A necessary and sufficient condition for*

$$(\mathbf{X}'\boldsymbol{\Sigma}^{-1}\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\Sigma}^{-1}\mathbf{y} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} \quad (20)$$

is that the columns of \mathbf{X} are linear combinations of r eigenvectors of $\boldsymbol{\Sigma}$.

The condition implies that there must be r eigenvectors of $\boldsymbol{\Sigma}$ which form a basis of $\mathcal{C}(\mathbf{X})$, where $\mathcal{C}(\bullet)$ stands for the column vector space. Hence, we have a condition for the equality between an ordinary least square (OLS) estimator and a generalized least square (GLS) estimator.

Theorem 3.2. *Szatrowski (1980) Assume that the MLE of μ has an explicit representation and that \mathbf{G} 's in $\boldsymbol{\Sigma} = \sum_{i=0}^r \theta_i \mathbf{G}_i$ are all diagonal in the canonical form. Then the MLE of $\boldsymbol{\theta}$ has an explicit representation if and only if the eigenvalues of $\boldsymbol{\Sigma}$ consist of exactly $r + 1$ linearly independent combinations of the $\boldsymbol{\theta}$.*

3.1. Spectral properties of $\boldsymbol{\Sigma}$

In this section we will present the spectral properties of $\boldsymbol{\Sigma}$ given in (3) which will be used when deriving MLEs for the variance-covariance parameters.

Theorem 3.3. *Let the matrix $\boldsymbol{\Sigma}$ be defined as in (3). Then there exists an orthogonal matrix \mathbf{Q} such that $\mathbf{Q}'\boldsymbol{\Sigma}\mathbf{Q} = \mathbf{D}$, where \mathbf{D} is an diagonal matrix containing the eigenvalues of $\boldsymbol{\Sigma}$. Moreover,*

$$\mathbf{D} = \text{Diag}\{\mathbf{D}_1, \mathbf{I}_{n_2-1} \otimes \mathbf{D}_2\}, \quad (21)$$

where

$$\mathbf{D}_1 = \text{diag}(\sigma^2 + n_1 a + n_1(n_2 - 1)b + \lambda_{11}, \sigma^2 + \lambda_{12}, \dots, \sigma^2 + \lambda_{1n_1}), \quad (22)$$

$$\mathbf{D}_2 = \text{diag}(\sigma^2 + n_1(a - b) + \lambda_{21}, \sigma^2 + \lambda_{22}, \dots, \sigma^2 + \lambda_{2n_1}), \quad (23)$$

and λ_{ih} are given by (12)-(13) in Theorem 2.5, $i = 1, 2$, $h = 1, \dots, n_1$.

The matrix \mathbf{Q} which columns are the eigenvectors of $\boldsymbol{\Sigma}$ equals

$$\mathbf{Q} = \mathbf{V}_{\mathbf{D}_1} \otimes \mathbf{V}_{\mathbf{D}_2}, \quad (24)$$

where

$$\mathbf{V}_{\mathbf{D}_1} = (\mathbf{w}_2^1, \dots, \mathbf{w}_2^{n_2}), \quad \mathbf{V}_{\mathbf{D}_2} = (\mathbf{w}_1^1, \dots, \mathbf{w}_1^{n_1}), \quad (25)$$

and the vectors \mathbf{w}_k^i are given by (10), $k = 1, 2$, $i = 1, \dots, n_k$.

Proof. Recall that Σ is a sum of three symmetric commuting matrices $\sigma^2 \mathbf{I}_p$, $\mathbf{Z}_1 \Sigma_1 \mathbf{Z}'_1$ and \mathbf{Z}_2 , and hence they can be simultaneously diagonalized. Define \mathbf{Q} as in (24) and then we obtain

$$\begin{aligned}
\mathbf{Q}' \Sigma \mathbf{Q} &= \mathbf{Q}' (\sigma^2 \mathbf{I}_p + \mathbf{Z}_1 \Sigma_1 \mathbf{Z}'_1 + \Sigma_2) \mathbf{Q} \\
&= \sigma^2 \mathbf{I}_p + (\mathbf{V}'_{D_1} \otimes \mathbf{V}'_{D_2}) [(a-b) \mathbf{I}_{n_2} \otimes \mathbf{J}_{n_1} + b \mathbf{J}_{n_2} \otimes \mathbf{J}_{n_1}] (\mathbf{V}_{D_1} \otimes \mathbf{V}_{D_2}) \\
&\quad + (\mathbf{V}'_{D_1} \otimes \mathbf{V}'_{D_2}) (\mathbf{I}_{n_2} \otimes \Sigma^{(1)} + (\mathbf{J}_{n_2} - \mathbf{I}_{n_2}) \otimes \Sigma^{(2)}) (\mathbf{V}_{D_1} \otimes \mathbf{V}_{D_2}) \\
&= \sigma^2 \mathbf{I}_p + [(a-b) (\mathbf{I}_{n_2} \otimes \mathbf{V}'_{D_2} \mathbf{J}_{n_1} \mathbf{V}_{D_2}) \\
&\quad \quad \quad + b (\mathbf{V}'_{D_1} \mathbf{J}_{n_2} \mathbf{V}_{D_1}) \otimes (\mathbf{V}'_{D_2} \mathbf{J}_{n_1} \mathbf{V}_{D_2})] \\
&\quad + \mathbf{I}_{n_2} \otimes (\mathbf{V}'_{D_2} (\Sigma^{(1)} - \Sigma^{(2)}) \mathbf{V}_{D_2}) + (\mathbf{V}'_{D_1} \mathbf{J}_{n_2} \mathbf{V}_{D_1}) \otimes (\mathbf{V}'_{D_2} \Sigma^{(2)} \mathbf{V}_{D_2}) \\
&= \sigma^2 \mathbf{I}_p + \left[\mathbf{I}_{n_2} \otimes \begin{pmatrix} (a-b)n_1 & 0 \\ 0 & \mathbf{0}_{n_1-1} \end{pmatrix} + \begin{pmatrix} n_2 & 0 \\ 0 & \mathbf{0}_{n_2-1} \end{pmatrix} \otimes \begin{pmatrix} bn_1 & 0 \\ 0 & \mathbf{0}_{n_1-1} \end{pmatrix} \right] \\
&\quad + \left[\mathbf{I}_{n_2} \otimes (\Lambda^{(1)} - \Lambda^{(2)}) + \begin{pmatrix} n_2 & 0 \\ 0 & \mathbf{0}_{n_2-1} \end{pmatrix} \otimes \Lambda^{(2)} \right],
\end{aligned}$$

where $\Lambda^{(i)}$, $i = 1, 2$ are defined in (16). From the last expression, the distinct eigenvalues η_i of Σ with the corresponding multiplicities m_i , $i = 1, \dots, 2([\frac{n_1}{2}] + 1)$, can be obtained directly.

Both of the two following tables present the spectrum of Σ . It is seen from Table 1, there are four types of eigenvalues of Σ . There is a clear picture of how the results of Theorem 2.4 and Theorem 2.5 are connected and build up the eigenstructure of Σ .

Table 1. Eigenvalues d_i for Σ given in (3) with corresponding eigenvectors \mathbf{u}_i and multiplicities m_i , $i = 1, \dots, n_1 n_2$. Here $\mathbf{w}_k^1 = \mathbf{1}_{n_k}$, and vectors $\mathbf{w}_k^{h_k}$ are defined in (10), $h_k = 2, \dots, n_k$, $k = 1, 2$. The eigenvalues λ_{kh_1} are defined in Theorem 2.5.

d_i	m_i	\mathbf{u}_i
$\sigma^2 + n_1(a-b) + n_2 n_1 b + \lambda_{11}$	1	$\mathbf{w}_2^1 \otimes \mathbf{w}_1^1$
$\sigma^2 + \lambda_{1h_1}$	1	$\mathbf{w}_2^1 \otimes \mathbf{w}_1^{h_1}$
$\sigma^2 + n_1(a-b) + \lambda_{21}$	$n_2 - 1$	$\mathbf{w}_2^{h_2} \otimes \mathbf{w}_1^1$
$\sigma^2 + \lambda_{2h_1}$	$n_2 - 1$	$\mathbf{w}_2^{h_2} \otimes \mathbf{w}_1^{h_1}$

However, taking into account that $\lambda_{ks} = \lambda_{kr}$, where $r = n_1 - s + 2$, $k = 1, 2$, $s = 2, \dots, n_1$, in Table 2 the distinct eigenvalues of Σ are presented.

Table 2. Distinct eigenvalues η_i of Σ given in (3) with corresponding multiplicities m_i .

η_i	m_i	
	odd n_1	even n_1
η_1	1	1
$\eta_2, \dots, \eta_{\lfloor \frac{n_1}{2} \rfloor + 1}$	2	2, $\eta_{\frac{n_1}{2}}$ has multiplicity 1.
$\eta_{\lfloor \frac{n_1}{2} \rfloor + 2}$	$n_2 - 1$	$n_2 - 1$
$\eta_{\lfloor \frac{n_1}{2} \rfloor + 3}, \dots, \eta_{2(\lfloor \frac{n_1}{2} \rfloor + 1)}$	$2(n_2 - 1)$	$2(n_2 - 1)$, η_{n_1+1} has multiplicity $n_2 - 1$.

The eigenvectors for Σ corresponding to the distinct eigenvalues provided in Table 2 can be easily verified. We have to check that $\Sigma \mathbf{u}_i = \eta_i \mathbf{u}_i$, $i = 1, \dots, n_1 n_2$.

For $\mathbf{u}_1 = \mathbf{w}_2^1 \otimes \mathbf{w}_1^1 = (n_1 n_2)^{-1/2} \mathbf{1}_{n_2} \otimes \mathbf{1}_{n_1}$ we have

$$\begin{aligned}
\Sigma \mathbf{u}_1 &= \sigma^2 \mathbf{I}_p (n_1 n_2)^{-1/2} \mathbf{1}_{n_2 n_1} + (a \mathbf{I}_{n_2} \otimes \mathbf{J}_{n_1} + b(\mathbf{J}_{n_2} - \mathbf{I}_{n_2}) \otimes \mathbf{J}_{n_1}) (n_1 n_2)^{-1/2} \mathbf{1}_{n_2 n_1} \\
&\quad + (\mathbf{I}_{n_2} \otimes \Sigma^{(1)} + (\mathbf{J}_{n_2} - \mathbf{I}_{n_2}) \otimes \Sigma^{(2)}) (n_1 n_2)^{-1/2} \mathbf{1}_{n_2 n_1} \\
&= \sigma^2 (n_1 n_2)^{-1/2} \mathbf{1}_{n_2 n_1} + a n_1 (n_1 n_2)^{-1/2} \mathbf{1}_{n_2 n_1} + b n_1 (n_2 - 1) (n_1 n_2)^{-1/2} \mathbf{1}_{n_2 n_1} \\
&\quad + (n_1 n_2)^{-1/2} \mathbf{1}_{n_2} \otimes (\Sigma^{(1)} \mathbf{1}_{n_1}) + (n_2 - 1) (n_1 n_2)^{-1/2} \mathbf{1}_{n_2} \otimes (\Sigma^{(2)} \mathbf{1}_{n_1}) \\
&= \sigma^2 (n_1 n_2)^{-1/2} \mathbf{1}_{n_2 n_1} + a n_1 (n_1 n_2)^{-1/2} \mathbf{1}_{n_2 n_1} + b n_1 (n_2 - 1) (n_1 n_2)^{-1/2} \mathbf{1}_{n_2 n_1} \\
&\quad + (n_1 n_2)^{-1/2} \mathbf{1}_{n_2} \otimes (\lambda_1^{(1)} \mathbf{1}_{n_1}) + (n_2 - 1) (n_1 n_2)^{-1/2} \mathbf{1}_{n_2} \otimes (\lambda_2^{(1)} \mathbf{1}_{n_1}) \\
&= (\sigma^2 + a n_1 + b n_1 (n_2 - 1) + \lambda_1^{(1)} + (n_2 - 1) \lambda_2^{(1)}) (n_1 n_2)^{-1/2} (\mathbf{1}_{n_2} \otimes \mathbf{1}_{n_1}) \\
&= \eta_1 \mathbf{u}_1.
\end{aligned}$$

Thus, $\Sigma \mathbf{u}_1 = \eta_1 \mathbf{u}_1$. To check $\Sigma \mathbf{u}_i = \eta_i \mathbf{u}_i$, where $\mathbf{u}_i = \mathbf{w}_2^1 \otimes \mathbf{w}_1^{h_1} = n_2^{-1/2} \mathbf{1}_{n_2} \otimes \mathbf{w}_1^{h_1}$, $h_1 = 2, \dots, n_1$, we calculate

$$\begin{aligned}
\Sigma \mathbf{u}_i &= \sigma^2 \mathbf{I}_p (n_2^{-1/2} \mathbf{1}_{n_2} \otimes \mathbf{w}_1^{h_1}) + (a \mathbf{I}_{n_2} \otimes \mathbf{J}_{n_1} + b(\mathbf{J}_{n_2} - \mathbf{I}_{n_2}) \otimes \mathbf{J}_{n_1}) (n_2^{-1/2} \mathbf{1}_{n_2} \otimes \mathbf{w}_1^{h_1}) \\
&\quad + (\mathbf{I}_{n_2} \otimes \Sigma^{(1)} + (\mathbf{J}_{n_2} - \mathbf{I}_{n_2}) \otimes \Sigma^{(2)}) (n_2^{-1/2} \mathbf{1}_{n_2} \otimes \mathbf{w}_1^{h_1}) \\
&= \sigma^2 (n_2^{-1/2} \mathbf{1}_{n_2} \otimes \mathbf{w}_1^{h_1}) + n_2^{-1/2} \mathbf{1}_{n_2} \otimes (\Sigma^{(1)} \mathbf{w}_1^{h_1}) + (n_2 - 1) n_2^{-1/2} \mathbf{1}_{n_2} \otimes (\Sigma^{(2)} \mathbf{w}_1^{h_1}) \\
&= \sigma^2 (n_2^{-1/2} \mathbf{1}_{n_2} \otimes \mathbf{w}_1^{h_1}) + n_2^{-1/2} \mathbf{1}_{n_2} \otimes (\lambda_{h_1}^{(1)} \mathbf{w}_1^{h_1}) + (n_2 - 1) n_2^{-1/2} \mathbf{1}_{n_2} \otimes (\lambda_{h_1}^{(2)} \mathbf{w}_1^{h_1}) \\
&= (\sigma^2 + \lambda_{h_1}^{(1)} + (n_2 - 1) \lambda_{h_1}^{(2)}) (n_2^{-1/2} \mathbf{1}_{n_2} \otimes \mathbf{w}_1^{h_1}).
\end{aligned}$$

Similarly, for $\mathbf{u}_i = \mathbf{w}_2^{h_2} \otimes n_1^{-1/2} \mathbf{1}_{n_1}$ and $\mathbf{u}_i = \mathbf{w}_2^{h_2} \otimes \mathbf{w}_1^{h_1}$, $h_k = 2, \dots, n_k$, $k = 1, 2$, we can verify that $\Sigma \mathbf{u}_i = \eta_i \mathbf{u}_i$ where $\eta_i = \sigma^2 + n_1(a - b) + \lambda_{21}$ and $\eta_i = \sigma^2 + \lambda_{2h_1}$, respectively. Thus, the proof of Theorem 3.3 is completed. \blacksquare

Let $\boldsymbol{\theta}$ be a vector of unknown (co)variance parameters, i.e.

$$\boldsymbol{\theta} = (\sigma^2, a, b, \tau_0, \dots, \tau_{2[n_1/2]+1})'.$$

Now the main theorem for obtaining MLEs is presented.

Theorem 3.4. *Let $\boldsymbol{\eta}$ be the vector representing the distinct eigenvalues of Σ given in (3). $\boldsymbol{\eta}$ as in Table 2 can be expressed as follows:*

$$\boldsymbol{\eta} = \mathbf{L}\boldsymbol{\theta}, \tag{26}$$

where $\mathbf{L} = (\mathbf{B}_1 : \mathbf{B}_2)$, the matrix \mathbf{B}_2 is given in Corollary 2.6,

$$\mathbf{B}_1 = \begin{pmatrix} 1 & n_1 & n_1(n_2 - 1) \\ \mathbf{1}_{[n_1/2]} & \mathbf{0}_{[n_1/2]} & \mathbf{0}_{[n_1/2]} \\ 1 & n_1 & -n_1 \\ \mathbf{1}_{[n_1/2]} & \mathbf{0}_{[n_1/2]} & \mathbf{0}_{[n_1/2]} \end{pmatrix},$$

and $\mathbf{1}_{[n_1/2]}$ and $\mathbf{0}_{[n_1/2]}$ are vectors of length $\lfloor \frac{n_1}{2} \rfloor$.

3.2. Maximum Likelihood Estimation

In this section MLEs for parameters of the model given in (1) will be derived. Let $\mathbf{y}_1, \dots, \mathbf{y}_n$ be a random sample from $N_p(\mu \mathbf{1}_p, \Sigma)$, and

$$\mathbf{Y} = (\mathbf{y}_1, \dots, \mathbf{y}_n) \sim N_{p,n}(\mu \mathbf{1}_p \mathbf{1}'_n, \Sigma, \mathbf{I}_n),$$

i.e., \mathbf{Y} is matrix normal distributed and the columns of \mathbf{Y} are independent normally distributed p -vectors with an unknown covariance matrix Σ and expectation of \mathbf{Y} equals $\mu \mathbf{1}_p \mathbf{1}'_n$. It is equivalent to

$$\text{vec} \mathbf{Y} \sim N_{pn}(\mu \mathbf{1}_{pn}, \mathbf{I}_n \otimes \Sigma), \tag{27}$$

where $\text{vec}(\mathbf{Y})$ denotes the vectorization of the matrix \mathbf{Y} .

The log-likelihood function is given by

$$\ln L(\mu, \Sigma) = c - \frac{1}{2} |\mathbf{I}_n \otimes \Sigma| - \frac{1}{2} [(\text{vec} \mathbf{Y} - \mu \mathbf{1}_{pn})' (\mathbf{I}_n \otimes \Sigma)^{-1} (\text{vec} \mathbf{Y} - \mu \mathbf{1}_{pn})],$$

where $c = -\frac{1}{2} pn \ln(2\pi)$.

First we consider the MLE of μ . The partial derivative,

$$\frac{\partial \ln L}{\partial \mu} = \mathbf{1}'_{pn}(\mathbf{I}_n \otimes \boldsymbol{\Sigma})^{-1} \text{vec} \mathbf{Y} - \mathbf{1}'_{pn}(\mathbf{I}_n \otimes \boldsymbol{\Sigma})^{-1} \mathbf{1}_{pn} \mu, \quad (28)$$

yields the normal equation

$$\mathbf{1}'_{pn}(\mathbf{I}_n \otimes \boldsymbol{\Sigma})^{-1} \text{vec} \mathbf{Y} = \mathbf{1}'_{pn}(\mathbf{I}_n \otimes \boldsymbol{\Sigma})^{-1} \mathbf{1}_{pn} \mu,$$

and then the MLE of μ is given by

$$\hat{\mu} = [\mathbf{1}'_{pn}(\mathbf{I}_n \otimes \boldsymbol{\Sigma}^{-1}) \mathbf{1}_{pn}]^{-1} \mathbf{1}'_{pn}(\mathbf{I}_n \otimes \boldsymbol{\Sigma}^{-1}) \text{vec} \mathbf{Y}, \quad (29)$$

if $\boldsymbol{\Sigma}$ is known. From Theorem 3.1, (29) becomes the least square estimator if $\mathbf{1}_p$ is an eigenvector of $\boldsymbol{\Sigma}$. From Theorem 3.3, we know that this is the case. Thus, the MLE equals

$$\hat{\mu} = (\mathbf{1}'_{pn} \mathbf{1}_{pn})^{-1} \mathbf{1}'_{pn} \text{vec} \mathbf{Y}. \quad (30)$$

Next we will estimate $\boldsymbol{\Sigma}$. Since $\boldsymbol{\Sigma}$ is a symmetric matrix, by utilizing the spectral decomposition of $\boldsymbol{\Sigma}$, it can be decomposed as $\boldsymbol{\Sigma} = \mathbf{Q} \mathbf{D} \mathbf{Q}'$, where \mathbf{Q} is an orthogonal matrix whose p columns are orthonormal eigenvectors of $\boldsymbol{\Sigma}$, $\mathbf{D}(\boldsymbol{\eta})$ is a $p \times p$ diagonal matrix with all eigenvalues of $\boldsymbol{\Sigma}$ and $\boldsymbol{\eta} = (\eta_1, \dots, \eta_{2(\lfloor \frac{n_1}{2} \rfloor + 1)})$ are the $2(\lfloor \frac{n_1}{2} \rfloor + 1)$ distinct nonzero eigenvalues with multiplicity m_i given in Table 2. Moreover, \mathbf{Q} given in (24) is independent of \mathbf{D} . The likelihood function can be written in the following way:

$$L(\mu, \boldsymbol{\eta}) \leq L(\hat{\mu}, \boldsymbol{\eta}) = (2\pi)^{-\frac{1}{2}pn} |\mathbf{D}(\boldsymbol{\eta})|^{-\frac{n}{2}} e^{-\frac{1}{2} \text{tr} \{ [\mathbf{D}(\boldsymbol{\eta})]^{-1} [\mathbf{Q}'(\mathbf{Y} - \hat{\mu} \mathbf{1}_p \mathbf{1}'_n)(\mathbf{Y} - \hat{\mu} \mathbf{1}_p \mathbf{1}'_n)' \mathbf{Q}] \}},$$

when μ is replaced by its MLE and tr denotes the trace. Now,

$$\begin{aligned} L(\hat{\mu}, \boldsymbol{\eta}) &= (2\pi)^{-\frac{1}{2}pn} |\mathbf{D}(\boldsymbol{\eta})|^{-\frac{n}{2}} e^{-\frac{1}{2} \text{tr} \{ [\mathbf{D}(\boldsymbol{\eta})]^{-1} \mathbf{H} \}} \\ &= (2\pi)^{-\frac{1}{2}pn} |\mathbf{D}(\boldsymbol{\eta})|^{-\frac{n}{2}} e^{-\frac{1}{2} \text{tr} \{ [\mathbf{D}(\boldsymbol{\eta})]^{-1} \mathbf{H}_d \}}, \end{aligned} \quad (31)$$

where

$$\mathbf{H} = \mathbf{Q}'(\mathbf{Y} - \hat{\mu} \mathbf{1}_p \mathbf{1}'_n)(\mathbf{Y} - \hat{\mu} \mathbf{1}_p \mathbf{1}'_n)' \mathbf{Q} \text{ and } \mathbf{H}_d = \text{diag}(\mathbf{H}) = \{h_j\}.$$

Thus,

$$L(\hat{\mu}, \boldsymbol{\eta}) = (2\pi)^{-\frac{1}{2}pn} \prod_{i=1}^{2(\lfloor \frac{n_1}{2} \rfloor + 1)} \eta_i^{-\frac{nm_i}{2}} \exp \left\{ -\frac{1}{2} \sum_{i=1}^{2(\lfloor \frac{n_1}{2} \rfloor + 1)} \eta_i^{-1} \sum_{j=1}^{m_i} h_j \right\}.$$

By taking the derivative with respect to η_i , $i = 1, \dots, 2(\lfloor \frac{n_1}{2} \rfloor + 1)$, the MLE of η_i is obtained by solving the normal equation

$$-\frac{nm_i}{2\eta_i} + \frac{\sum_{j=1}^{m_i} h_j}{2\eta_i^2} = 0. \quad (32)$$

Theorem 3.5. *The MLEs of the distinct eigenvalues η_i of Σ are*

$$\hat{\eta}_i = \frac{\sum_{j=1}^{m_i} h_j}{nm_i}, \quad i = 1, \dots, 2(\lfloor n_1/2 \rfloor + 1), \quad (33)$$

where h_j is j -th diagonal element of the matrix \mathbf{H}_d in (31) and m_i is the multiplicity of η_i given in Table 2.

Corollary 3.6. *The MLE of Σ given in (3) is*

$$\hat{\Sigma} = \mathbf{Q}\mathbf{D}(\hat{\boldsymbol{\eta}})\mathbf{Q}', \quad (34)$$

where $\hat{\boldsymbol{\eta}} = (\hat{\eta}_1, \dots, \hat{\eta}_{2(\lfloor n_1/2 \rfloor + 1)})$ and $\mathbf{D}(\hat{\boldsymbol{\eta}})$ is a $p \times p$ diagonal matrix.

Example 3.1:

Let us consider model (1) in the case when $n_2 = 2$ and $n_1 = 4$, $\mathbf{y}_j \sim N_8(\mathbf{1}_8\boldsymbol{\mu}, \Sigma)$, $j = 1, \dots, n$. Model (1) can be written as

$$\mathbf{y}_j = \mathbf{1}_8\boldsymbol{\mu} + (\mathbf{I}_2 \otimes \mathbf{1}_4)\boldsymbol{\gamma}_1 + \mathbf{I}_8\boldsymbol{\gamma}_2 + \boldsymbol{\epsilon},$$

and the covariance matrix of the observation vector is

$$\Sigma = \sigma^2\mathbf{I}_8 + \Sigma_1 \otimes \mathbf{J}_4 + \Sigma_2,$$

where $\Sigma_1 = a\mathbf{I}_2 + b(\mathbf{J}_2 - \mathbf{I}_2)$ and

$$\Sigma_2 = \mathbf{I}_{n_2} \otimes \Sigma^{(1)} + (\mathbf{J}_{n_2} - \mathbf{I}_{n_2}) \otimes \Sigma^{(2)},$$

with

$$\Sigma^{(1)} = \begin{pmatrix} \tau_0 & \tau_1 & \tau_2 & \tau_1 \\ \tau_1 & \tau_0 & \tau_1 & \tau_2 \\ \tau_2 & \tau_1 & \tau_0 & \tau_1 \\ \tau_1 & \tau_2 & \tau_1 & \tau_0 \end{pmatrix}, \quad \Sigma^{(2)} = \begin{pmatrix} \tau_3 & \tau_4 & \tau_5 & \tau_4 \\ \tau_4 & \tau_3 & \tau_4 & \tau_5 \\ \tau_5 & \tau_4 & \tau_3 & \tau_4 \\ \tau_4 & \tau_5 & \tau_4 & \tau_3 \end{pmatrix}.$$

The vector of (co)variance components is $\boldsymbol{\theta} = (\sigma^2, a, b, \tau_0, \tau_1, \tau_2, \tau_3, \tau_4, \tau_5)'$ and the spectral decomposition of Σ gives the following eigenvalues

$$\begin{aligned} \eta_1 &= \sigma^2 + 4(a + b) + \tau_0 + 2\tau_1 + \tau_2 + \tau_3 + 2\tau_4 + \tau_5, \\ \eta_2 &= \sigma^2 + \tau_0 - 2\tau_1 + \tau_2 + \tau_3 - 2\tau_4 + \tau_5, \\ \eta_3 &= \sigma^2 + \tau_0 - \tau_2 + \tau_3 - \tau_5, \\ \eta_4 &= \sigma^2 + 4(a - b) + \tau_0 + 2\tau_1 + \tau_2 - \tau_3 - 2\tau_4 - \tau_5, \\ \eta_5 &= \sigma^2 + \tau_0 - 2\tau_1 + \tau_2 - \tau_3 + 2\tau_4 - \tau_5, \\ \eta_6 &= \sigma^2 + \tau_0 - \tau_2 - \tau_3 + \tau_5. \end{aligned}$$

The multiplicities of eigenvalues are 1, 1, 2, 1, 1 and 2, and the corresponding orthonormal eigenvectors define the matrix \mathbf{Q} in the following way,

$$\mathbf{Q} = \begin{pmatrix} \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} \\ \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} \\ \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \\ \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \\ \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \\ \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \\ \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} \\ \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} \end{pmatrix}. \quad (35)$$

Using (30), the MLE of μ is

$$\hat{\mu} = \frac{\sum_{j=1}^n \sum_{i=1}^8 y_{ij}}{8n}, \quad (36)$$

and the MLEs of η_k , $k = 1, \dots, 6$ are

$$\begin{aligned} \hat{\eta}_1 &= \frac{1}{n} \left[\sum_{j=1}^n (\mathbf{v}'_1 \mathbf{y}_j)^2 - 8n\hat{\mu}^2 \right], \\ \hat{\eta}_2 &= \frac{1}{n} \sum_{j=1}^n (\mathbf{v}'_2 \mathbf{y}_j)^2, \\ \hat{\eta}_3 &= \frac{1}{2n} \left[\sum_{j=1}^n (\mathbf{v}'_3 \mathbf{y}_j)^2 + \sum_{j=1}^n (\mathbf{v}'_4 \mathbf{y}_j)^2 \right], \\ \hat{\eta}_4 &= \frac{1}{n} \sum_{j=1}^n (\mathbf{v}'_5 \mathbf{y}_j)^2, \\ \hat{\eta}_5 &= \frac{1}{n} \sum_{j=1}^n (\mathbf{v}'_6 \mathbf{y}_j)^2, \\ \hat{\eta}_6 &= \frac{1}{2n} \left[\sum_{j=1}^n (\mathbf{v}'_7 \mathbf{y}_j)^2 + \sum_{j=1}^n (\mathbf{v}'_8 \mathbf{y}_j)^2 \right], \end{aligned}$$

where \mathbf{v}_p are $p = 1, \dots, 8$ are columns of the matrix \mathbf{Q} given in (35).

The MLE of Σ has been calculated as $\hat{\Sigma} = \sum_{k=1}^6 \hat{\eta}_k \mathbf{E}_k$, where

$$\begin{aligned} \mathbf{E}_1 &= \frac{1}{8} \mathbf{1}_8 \mathbf{1}'_8, & \mathbf{E}_2 &= \mathbf{J}_2 \otimes \begin{pmatrix} \frac{1}{8} & -\frac{1}{8} & \frac{1}{8} & -\frac{1}{8} \\ -\frac{1}{8} & \frac{1}{8} & -\frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & -\frac{1}{8} & \frac{1}{8} & -\frac{1}{8} \\ -\frac{1}{8} & \frac{1}{8} & -\frac{1}{8} & \frac{1}{8} \end{pmatrix}, \\ \mathbf{E}_3 &= \mathbf{J}_2 \otimes \begin{pmatrix} \frac{1}{4} & 0 & -\frac{1}{4} & 0 \\ 0 & \frac{1}{4} & 0 & -\frac{1}{4} \\ -\frac{1}{4} & 0 & \frac{1}{4} & 0 \\ 0 & -\frac{1}{4} & 0 & \frac{1}{4} \end{pmatrix}, & \mathbf{E}_4 &= \mathbf{I}_2 \otimes \frac{1}{4} \mathbf{J}_4 - \mathbf{J}_2 \otimes \frac{1}{8} \mathbf{J}_4, \\ \mathbf{E}_5 &= \mathbf{I}_2 \otimes \begin{pmatrix} \frac{1}{8} & -\frac{1}{8} & \frac{1}{8} & -\frac{1}{8} \\ -\frac{1}{8} & \frac{1}{8} & -\frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & -\frac{1}{8} & \frac{1}{8} & -\frac{1}{8} \\ -\frac{1}{8} & \frac{1}{8} & -\frac{1}{8} & \frac{1}{8} \end{pmatrix} + (\mathbf{J}_2 - \mathbf{I}_2) \otimes \begin{pmatrix} -\frac{1}{8} & \frac{1}{8} & -\frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & -\frac{1}{8} & \frac{1}{8} & -\frac{1}{8} \\ -\frac{1}{8} & \frac{1}{8} & -\frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & -\frac{1}{8} & \frac{1}{8} & -\frac{1}{8} \end{pmatrix}, \\ \mathbf{E}_6 &= \mathbf{I}_2 \otimes \begin{pmatrix} \frac{1}{4} & 0 & -\frac{1}{4} & 0 \\ 0 & \frac{1}{4} & 0 & -\frac{1}{4} \\ -\frac{1}{4} & 0 & \frac{1}{4} & 0 \\ 0 & -\frac{1}{4} & 0 & \frac{1}{4} \end{pmatrix} + (\mathbf{J}_2 - \mathbf{I}_2) \otimes \begin{pmatrix} -\frac{1}{4} & 0 & \frac{1}{4} & 0 \\ 0 & -\frac{1}{4} & 0 & \frac{1}{4} \\ \frac{1}{4} & 0 & -\frac{1}{4} & 0 \\ 0 & \frac{1}{4} & 0 & -\frac{1}{4} \end{pmatrix}. \end{aligned}$$

The covariance matrix Σ is a function of

$$\boldsymbol{\theta} = (\sigma^2, a, b, \tau_0, \dots, \tau_{2[\frac{n_1}{2}]+1})',$$

i.e. $\Sigma = \Sigma(\boldsymbol{\theta})$. It can be shown that the system of linear equations given in (26) is consistent. If the condition in Theorem 3.2 holds, i.e. the number of elements in $\boldsymbol{\eta}$ equals the number of elements in $\boldsymbol{\theta}$, the MLE of $\boldsymbol{\theta}$ has an explicit expression, which is obtained by solving the linear system in (26). If the number of elements in $\boldsymbol{\eta}$ is less than the number elements in $\boldsymbol{\theta}$, $\boldsymbol{\theta}$ is estimable only under some constraints on $\boldsymbol{\theta}$.

For the balanced circular symmetric model with patterned blocks, the following theorem can be stated. In the next theorem we prove that in the balanced circular symmetric model with patterned blocks given in (1), $\boldsymbol{\theta}$ is non-estimable unless some constraints will be imposed on it.

Theorem 3.7. *Let s_1 be the number of the distinct eigenvalues of Σ defined in (3), and s_2 be the number of unknown parameters in Σ , then $\Delta \equiv s_2 - s_1 = 3$.*

Proof. According to the definition of Σ in (3), the number of unknown parameters is $3 + 2([\frac{n_1}{2}] + 1)$, i.e. it is $n_1 + 4$ for the odd n_1 and $n_1 + 5$ for the even n_1 . Moreover,

recall that Σ given in (3) is the sum of three matrices:

$$\Sigma = \underbrace{\sigma^2 \mathbf{I}}_{1 \text{ parameter}} + \underbrace{\mathbf{Z}_1 \Sigma_1 \mathbf{Z}_1'}_{2 \text{ parameters}} + \underbrace{\Sigma_2}_{2(\lfloor \frac{n_1}{2} \rfloor + 1) \text{ parameters}} \quad (37)$$

From Table 2, it follows that there are $2(\lfloor \frac{n_1}{2} \rfloor + 1)$ distinct eigenvalues. So, $\Delta = 3$. ■

4. Concluding remarks and future studies

From Theorem 3.7, it follows that θ is non-estimable for the unconstrained model given in (1). The question is what kind of constraints can be imposed on Σ or whether there is any natural way of reparametrizing Σ ? It deserves our further studies. Firstly, we note that imposing constraints on Σ means introducing some constraints on \mathbf{y} elements in model (1), since elements of Σ describe dependence between the elements of \mathbf{y} . Secondly, altering the dependence structure of \mathbf{y} can result in change in the structure of Σ which can violate the assumption of invariance. Thirdly, it is important to recall that Σ is the sum of three matrices characterizing dependence structures of three factors. Thus, imposing constraints on Σ can be done via imposing constraints on some or all of these components, equivalently, imposing constraints on some or all factors in model (1). This option seems to be feasible since one often has information about factors in the model. The question which remains is what kind of constraints can be imposed. From the interpretation point of view, it is of special interest to see whether the usual “sum-to-zero” restriction, which preserves the group invariance, can lead explicit MLEs of θ in model (1). Notice that the “set-to-zero” restriction does not preserve the group invariance. In future studies, we are going to find necessary conditions in terms of constrained models for existence of explicit MLEs.

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