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Reparameterization and invariant covariance matrices of factors in linear models

TÕNU MÖLS AND TATYANA NAHTMAN

ABSTRACT. Let the vector ζ consist of sampled random elements of factors in a linear mixed model. Let P be a permutation matrix. The covariance matrix $D(\zeta)$ is called P-invariant if $D(\zeta) = D(P\zeta)$. It will be demonstrated that there is a strong correspondence between the spectrum of $D(\zeta)$ and certain reparameterization conditions on the factors. In particular, the classical reparameterization condition $\sum \zeta_i = 0$ has a clear presentation through the eigenvalues of $D(\zeta)$. This correspondence is useful for modelling data.

1. Introduction

Consider the following linear statistical model

$$Y_{ijk} = \mu + \xi_i + \eta_j + \gamma_{ij} + \varepsilon_{ijk} \tag{1}$$

describing two factors ξ and η and their interaction γ (i and j refer here to factor levels). To make the meaning of parameters unique, the model terms ξ_i, η_j and γ_{ij} must be *reparameterized* by imposing certain constraints on

$$\beta = (\mu, \xi_1, \dots, \xi_l, \eta_1, \dots, \eta_m, \gamma_{11}, \gamma_{12}, \dots, \gamma_{lm}, \varepsilon_{111}, \varepsilon_{112}, \dots, \varepsilon_{lmn})'.$$

Classical reparameterization conditions are the null-sum condition $\sum_i \xi_i = 0$ and the condition $\xi_l = 0$, where ξ_l is the last component of ξ.

In the present paper the concept of invariance is used. According to this concept, an arbitrary permutation of levels of a factor must not affect the covariance matrix of that factor. The invariance with respect to the group of permutations implies a specific structure on the covariance matrix. The structure of patterned matrices which arise in statistics has been studied by a number of authors (Wilks, 1946; Votaw, 1948; Tong, 1997; etc.).

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It turns out, that the classical reparameterization conditions can be formulated as specific restrictions on the eigenvalues of an invariant covariance matrix. Earlier we have shown (Nahtman & Möls, 2003) that in the models with only one factor ξ, the classical reparameterization $\sum_i \xi_i = 0$ is equivalent to the equality $\lambda_2 = 0$, where λ_2 is the eigenvalue of the invariant covariance matrix of ξ, which has multiplicity 1. This result was partially generalized by Nahtman (2002) for interactions of two factors. In this case, the spectrum of an invariant covariance matrix of an interaction term γ_{ij} in (1) has four distinct eigenvalues, say λ_1, λ_2, λ_3, λ_4. The three classical reparameterization conditions

$$\textstyle\sum_i \gamma_{ij} = 0 \;\forall j, \quad \sum_j \gamma_{ij} = 0 \;\forall i, \quad \text{and} \quad \sum_{i,j} \gamma_{ij} = 0 \tag{2}$$

can respectively be expressed by

$$\lambda_2 = \lambda_4 = 0, \quad \lambda_3 = \lambda_4 = 0 \quad \text{and} \quad \lambda_2 = \lambda_3 = \lambda_4 = 0. \tag{3}$$

In the present paper we generalize these results to a higher number of factors.

2. Structure of invariant covariance matrices

The permutations we consider are only allowed to act within factors. Let $P^{(h)}$ denote the permutation that interchanges components of a factor $\xi^{(h)}$ $(h = 1, \ldots, g)$, and let $\gamma^{(s)}$ represent the vector of s-order interaction effects of factors $\xi^{(1)}, \ldots, \xi^{(g)}$ $(s = 1, \ldots, g)$. If n_h is the number of sampled levels of factor $\xi^{(h)}$, then $\gamma^{(s)}$ is of order $N = n_{i_1} \cdot n_{i_2} \cdot \ldots \cdot n_{i_s}$, where $\{i_1, \ldots, i_s\} \subseteq \{1, \ldots, g\}$. We number the components of $\gamma^{(s)}$ lexicographically. For example, for $s = 2, n_1 = m$ and $n_2 = n$ we have ordering $(1,1), (1,2), \ldots, (1,n), \ldots, (m,1), \ldots, (m,n)$.
The permutation matrix acting on $\gamma^{(s)}$ is given by

$$P_s = P^{(h_1)} \otimes \cdots \otimes P^{(h_s)}, \tag{4}$$

where $\otimes$ denotes the (right) Kronecker product and $\{h_1, \ldots, h_s\} \subseteq \{1, \ldots, g\}$. The permutation P_s will be called a *marginal permutation*.

Definition 2.1. The covariance matrix $D(\zeta)$ of a factor ζ is called *invariant with respect to a permutation* P (further simply P*-invariant*), if $D(\zeta) = D(P\zeta)$ or, equivalently, if $PD(\zeta)P' = D(\zeta)$.

In the next theorem we show that the invariance has strong implications on the structure of the covariance matrix. Denote, for convenience, $\Sigma_s = D(\gamma^{(s)})$.

Theorem 2.1. *If the covariance matrix Σ_s is invariant, with respect to all marginal permutations P_s, then it is defined by 2^s parameters and has the* *following structure:*

$$\Sigma_s = \sum_{\alpha_1=1}^{2} \cdots \sum_{\alpha_s=1}^{2} c_{\alpha_1,\ldots,\alpha_s} H_{1,\alpha_1} \otimes \cdots \otimes H_{s,\alpha_s}, \tag{5}$$

where, for all $k = 1,\ldots,s$, $H_{k,1}$ is the identity matrix I_{n_k} of order n_k, $H_{k,2}$ is an $n_k \times n_k$ matrix J_{n_k} of ones ($J_{n_k} = \mathbf{1}_{n_k}\mathbf{1}'_{n_k}$), and $c_{\alpha_1,\ldots,\alpha_s}$ are constants (parameters).

Proof. To see that Σ_s has structure (5), write it as

$$\begin{aligned}\Sigma_s &= \sum_{i_1,\ldots,i_s}\sum_{j_1,\ldots,j_s} \sigma_{(i_1 i_2\ldots i_s)(j_1 j_2\ldots j_s)}(e_{i_1}\otimes e_{i_2}\otimes\cdots\otimes e_{i_s})(e_{j_1}\otimes e_{j_2}\otimes\cdots\otimes e_{j_s})' \\ &= \sum_{i_1,\ldots,i_s}\sum_{j_1,\ldots,j_s} \sigma_{(i_1 i_2\ldots i_s)(j_1 j_2\ldots j_s)}(e_{i_1}e'_{j_1})\otimes(e_{i_2}e'_{j_2})\otimes\cdots\otimes(e_{i_s}e'_{j_s}),\end{aligned} \tag{6}$$

where e_{i_h} denotes the $n_{i_h} \times 1$ vector with 1 on the i_h-th place, and other components zeros, $\sigma_{(i_1 i_2\ldots i_s)(j_1 j_2\ldots j_s)}$ is the element of Σ_s in the k-th row and l-th column

$$\begin{aligned} k &= \sum_{h=1}^{s-1}(i_h - 1)n_{h+1}\cdot n_{h+2}\cdot\ldots\cdot n_s + i_s, \\ l &= \sum_{h=1}^{s-1}(j_h - 1)n_{h+1}\cdot n_{h+2}\cdot\ldots\cdot n_s + j_s. \end{aligned}$$

In the case of one factor $\xi^{(1)}$ (s=1)

$$\Sigma_1 = \sum_i\sum_j \sigma_{ij}(e_i e'_j) \tag{7}$$

and the condition $P_1\Sigma_1 P'_1 = \Sigma_1$, for all P_1 (P_1 is any permutation matrix affecting the ordering of components of factor $\xi^{(1)}$), implies

$$\sum_{ij}\sigma_{ij}e_i e'_j = \sum_{ij}\sigma_{ij}(P_1 e_i e'_j P'_1) = \sum_i \sigma_{ii}(P_1 e_i e'_i P'_1) + \sum_{i\neq j}\sigma_{ij}(P_1 e_i e'_j P'_1). \tag{8}$$

Equality (8) holds if and only if

$$\sigma_{ij} = \begin{cases}\tau_1, & \text{if } i = j,\\ \tau_2, & \text{if } i \neq j\end{cases}$$

and, therefore,

$$\Sigma_1 = (\tau_1 - \tau_2)I_{n_1} + \tau_2 J_{n_1} = c_1 I_{n_1} + c_2 J_{n_1}.$$

In the general case, if Σ_s is P_s-invariant, then applying (6) we can write

$$\Sigma_s = \sum_{\substack{i_1,\ldots,i_s\\ j_1,\ldots,j_s}} \sigma_{(i_1 i_2\ldots i_s)(j_1 j_2\ldots j_s)}(P^{(h_1)}e_{i_1}e'_{j_1}P^{(h_1)'})\otimes\cdots\otimes(P^{(h_s)}e_{i_s}e'_{j_s}P^{(h_s)'}). \tag{10}$$

Each component $P^{(h_l)}$ of the Kronecker product $P^{(h_1)} \otimes \cdots \otimes P^{(h_s)}$ acts on the component of $\gamma^{(s)}$ which is associated with the corresponding factor $\xi^{(h)}$. Thus, with respect to the first component $(P^{(h_1)}e_{i_1}e'_{i_1}P^{(h_1)'})$, the invariance of Σ_s implies

$$\begin{aligned}
\Sigma_s &= \sum_{i_1} \sum_{\substack{i_2,\dots,i_s \\ j_2,\dots,j_s}} \sigma_{(i_1 i_2 \dots i_s)(i_1 j_2 \dots j_s)} (P^{(h_1)}e_{i_1}e'_{i_1}P^{(h_1)'}) \otimes \cdots \otimes (P^{(h_s)}e_{i_s}e'_{j_s}P^{(h_s)'}) \\
&+ \sum_{i_1 \neq j_1} \sum_{\substack{i_2,\dots,i_s \\ j_2,\dots,j_s}} \sigma_{(i_1 i_2 \dots i_s)(j_1 j_2 \dots j_s)} (P^{(h_1)}e_{i_1}e'_{j_1}P^{(h_1)'}) \otimes \cdots \otimes (P^{(h_s)}e_{i_s}e'_{j_s}P^{(h_s)'}) \\
&= \sum_{\substack{i_2,\dots,i_s \\ j_2,\dots,j_s}} c^1_{1(i_2 \dots i_s, j_2 \dots j_s)} I_{n_1} \otimes (P^{(h_2)}e_{i_2}e'_{j_2}P^{(h_2)'}) \otimes \cdots \otimes (P^{(h_s)}e_{i_s}e'_{j_s}P^{(h_s)'}) \\
&+ \sum_{\substack{i_2,\dots,i_s \\ j_2,\dots,j_s}} c^1_{2(i_2 \dots i_s, j_2 \dots j_s)} J_{n_1} \otimes (P^{(h_2)}e_{i_2}e'_{j_2}P^{(h_2)'}) \otimes \cdots \otimes (P^{(h_s)}e_{i_s}e'_{j_s}P^{(h_s)'}),
\end{aligned} \tag{12}$$

where $c^1_{1(i_2 \dots i_s, j_2 \dots j_s)}$ and $c^1_{2(i_2 \dots i_s, j_2 \dots j_s)}$ are constants, defined as

$$\begin{aligned}
c^1_{0(i_2 \dots i_s, j_2 \dots j_s)} &= \sigma_{(i_1 i_2 \dots i_s)(j_1 j_2 \dots j_s)}, \text{ if } i_1 = j_1, \\
c^1_{2(i_2 \dots i_s, j_2 \dots j_s)} &= \sigma_{(i_1 i_2 \dots i_s)(j_1 j_2 \dots j_s)}, \text{ if } i_1 \neq j_1, \\
c^1_{1(i_2 \dots i_s, j_2 \dots j_s)} &= c^1_{0(i_2 \dots i_s, j_2 \dots j_s)} - c^1_{2(i_2 \dots i_s, j_2 \dots j_s)}.
\end{aligned} \tag{13}$$

If we continue and consider the next component $(P^{(h_2)}e_{i_2}e'_{j_2}P^{(h_2)'})$, then (12) becomes

$$\begin{aligned}
\Sigma_s &= \sum_{\substack{i_2,\dots,i_s \\ j_2,\dots,j_s}} c^1_{1(i_2 \dots i_s, j_2 \dots j_s)} I_{n_1} \otimes (P^{(h_2)}e_{i_2}e'_{j_2}P^{(h_2)'}) \otimes \cdots \otimes (P^{(h_s)}e_{i_s}e'_{j_s}P^{(h_s)'}) \\
&+ \sum_{\substack{i_2,\dots,i_s \\ j_2,\dots,j_s}} c^1_{2(i_2 \dots i_s, j_2 \dots j_s)} J_{n_1} \otimes (P^{(h_2)}e_{i_2}e'_{j_2}P^{(h_2)'}) \otimes \cdots \otimes (P^{(h_s)}e_{i_s}e'_{j_s}P^{(h_s)'}) \\
&= \sum_{\substack{i_3,\dots,i_s \\ j_3,\dots,j_s}} c^2_{11(i_3 \dots i_s, j_3 \dots j_s)} I_{n_1} \otimes I_{n_2} \otimes (P^{(h_3)}e_{i_s}e'_{j_s}P^{(h_3)'}) \otimes \cdots \otimes (P^{(h_s)}e_{i_s}e'_{j_s}P^{(h_s)'}) \\
&+ \sum_{\substack{i_3,\dots,i_s \\ j_3,\dots,j_s}} c^2_{12(i_3 \dots i_s, j_3 \dots j_s)} I_{n_1} \otimes J_{n_2} \otimes (P^{(h_3)}e_{i_s}e'_{j_s}P^{(h_3)'}) \otimes \cdots \otimes (P^{(h_s)}e_{i_s}e'_{j_s}P^{(h_s)'}) \\
&+ \sum_{\substack{i_3,\dots,i_s \\ j_3,\dots,j_s}} c^2_{21(i_3 \dots i_s, j_3 \dots j_s)} J_{n_1} \otimes I_{n_2} \otimes (P^{(h_3)}e_{i_s}e'_{j_s}P^{(h_3)'}) \otimes \cdots \otimes (P^{(h_s)}e_{i_s}e'_{j_s}P^{(h_s)'}), \\
&+ \sum_{\substack{i_3,\dots,i_s \\ j_3,\dots,j_s}} c^2_{22(i_3 \dots i_s, j_3 \dots j_s)} J_{n_1} \otimes J_{n_2} \otimes (P^{(h_3)}e_{i_s}e'_{j_s}P^{(h_3)'}) \otimes \cdots \otimes (P^{(h_s)}e_{i_s}e'_{j_s}P^{(h_s)'}),
\end{aligned}$$

where

$$
\begin{aligned}
c^1_{1(i_2\ldots i_s,j_2\ldots j_s)} &= c^2_{11(i_3\ldots i_s,j_3\ldots j_s)} = \sigma_{(i_1i_2\ldots i_s)(j_1j_2\ldots j_s)}, \text{ if } i_1 = j_1, i_2 = j_2,\\
c^1_{1(i_2\ldots i_s,j_2\ldots j_s)} &= c^2_{12(i_3\ldots i_s,j_3\ldots j_s)} = \sigma_{(i_1i_2\ldots i_s)(j_1j_2\ldots j_s)}, \text{ if } i_1 = j_1, i_2 \neq j_2,\\
c^1_{2(i_2\ldots i_s,j_2\ldots j_s)} &= c^2_{21(i_3\ldots i_s,j_3\ldots j_s)} = \sigma_{(i_1i_2\ldots i_s)(j_1j_2\ldots j_s)}, \text{ if } i_1 \neq j_1, i_2 = j_2,\\
c^1_{2(i_2\ldots i_s,j_2\ldots j_s)} &= c^2_{22(i_3\ldots i_s,j_3\ldots j_s)} = \sigma_{(i_1i_2\ldots i_s)(j_1j_2\ldots j_s)}, \text{ if } i_1 \neq j_1, i_2 \neq j_2.
\end{aligned}
$$

By continuing in the same manner we finally obtain that the covariance matrix Σ_s has the structure given in (5). □

Theorem 2.1 does not show the explicit form of the invariant covariance matrix Σ_s. In general, the structure of Σ_s is rather complicated. In practical data analysis, the second- and third-order interaction terms are often of main interest. The structure of the invariant covariance matrix of the second-order interaction effects can be found in Nahtman (2002). For the third-order interaction effects $\gamma^{(3)}$, the invariant covariance matrix Σ_3 can be constructed recursively in the following way.

Firstly, let

$$
\begin{aligned}
\tau_1 &= Cov(\gamma^{(3)}_{ijk}, \gamma^{(3)}_{ijk}),\\
\tau_2 &= Cov(\gamma^{(3)}_{ijk}, \gamma^{(3)}_{ijk'}), \quad k \neq k',\\
\tau_3 &= Cov(\gamma^{(3)}_{ijk}, \gamma^{(3)}_{ij'k}), \quad j \neq j',\\
\tau_4 &= Cov(\gamma^{(3)}_{ijk}, \gamma^{(3)}_{ij'k'}), \ j \neq j', k \neq k',\\
\tau_5 &= Cov(\gamma^{(3)}_{ijk}, \gamma^{(3)}_{i'jk}), \quad i \neq i',\\
\tau_6 &= Cov(\gamma^{(3)}_{ijk}, \gamma^{(3)}_{i'jk'}), \ i \neq i', k \neq k',\\
\tau_7 &= Cov(\gamma^{(3)}_{ijk}, \gamma^{(3)}_{i'j'k}), \ i \neq i', j \neq j',\\
\tau_8 &= Cov(\gamma^{(3)}_{ijk}, \gamma^{(3)}_{i'j'k'}), i \neq i', j \neq j', k \neq k',
\end{aligned}
$$

where $i, i' = 1, \ldots, n_3$, $j, j' = 1, \ldots, n_2$, $k, k' = 1, \ldots, n_1$, and construct

$$
\begin{aligned}
\Sigma^{(1)}_1 &= I_{n_1}(\tau_1 - \tau_2) + J_{n_1}\tau_2, & \Sigma^{(3)}_1 &= I_{n_1}(\tau_5 - \tau_6) + J_{n_1}\tau_6,\\
\Sigma^{(2)}_1 &= I_{n_1}(\tau_3 - \tau_4) + J_{n_1}\tau_4, & \Sigma^{(4)}_1 &= I_{n_1}(\tau_7 - \tau_8) + J_{n_1}\tau_8.
\end{aligned}
$$

Secondly, define

$$
\begin{aligned}
\Sigma^{(1)}_2 &= I_{n_2} \otimes (\Sigma^{(1)}_1 - \Sigma^{(2)}_1) + J_{n_2} \otimes \Sigma^{(2)}_1,\\
\Sigma^{(2)}_2 &= I_{n_2} \otimes (\Sigma^{(3)}_1 - \Sigma^{(4)}_1) + J_{n_2} \otimes \Sigma^{(4)}_1,
\end{aligned}
$$

and then

$$\Sigma_3 = I_{n_3} \otimes (\Sigma_2^{(1)} - \Sigma_2^{(2)}) + J_{n_3} \otimes \Sigma_2^{(2)} = \begin{pmatrix} \Sigma_2^{(1)} & \Sigma_2^{(2)} & \cdots & \Sigma_2^{(2)} \\ \Sigma_2^{(2)} & \Sigma_2^{(1)} & \cdots & \Sigma_2^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ \Sigma_2^{(2)} & \Sigma_2^{(2)} & \cdots & \Sigma_2^{(1)} \end{pmatrix}. \quad (14)$$

Alternatively, one may write Σ_3 in the explicit way

$$\begin{aligned} \Sigma_3 = I_{n_3} \otimes \Bigg[I_{n_2} \otimes \Big[(\tau_1 - \tau_2 - \tau_3 + \tau_4 - \tau_5 + \tau_6 + \tau_7 - \tau_8) I_{n_1} \\ + (\tau_2 - \tau_4 - \tau_6 + \tau_8) J_{n_1} \Big] + J_{n_2} \otimes \Big[(\tau_3 - \tau_4 - \tau_7 + \tau_8) I_{n_1} + (\tau_4 - \tau_8) J_{n_1} \Big] \Bigg] \\ + J_{n_3} \otimes \Bigg[I_{n_2} \otimes \Big[(\tau_5 - \tau_6 - \tau_7 + \tau_8) I_{n_1} + (\tau_6 - \tau_8) J_{n_1} \Big] \\ + J_{n_2} \otimes \Big[(\tau_7 - \tau_8) I_{n_1} + \tau_8 J_{n_1} \Big] \Bigg]. \end{aligned} \quad (15)$$

The algorithm used to construct the invariant covariance matrix Σ_3 presented above can be generalized to an arbitrary number of factors.

Theorem 2.2. *The matrix Σ_s in* (5) *can be written in a recursive form as*

$$\Sigma_s = I_{n_s} \otimes (\Sigma_{s-1}^{(1)} - \Sigma_{s-1}^{(2)}) + J_{n_s} \otimes \Sigma_{s-1}^{(2)}, \quad (16)$$

where

$$\Sigma_0^{(i_0)} = \tau_\nu, \quad \nu = 1, \ldots, 2^s, \quad (17)$$

$$\Sigma_k^{(i_k)} = I_{n_k} \otimes (\Sigma_{k-1}^{(2i_k-1)} - \Sigma_{k-1}^{(2i_k)}) + J_{n_k} \otimes \Sigma_{k-1}^{(2i_k)}, \quad (18)$$

$$i_k = 1, \ldots, 2^{s-k}, \ k = 1, \ldots, s-1,$$

where the constants τ_ν characterize the covariances between the components of $\gamma^{(s)}$.

3. Spectrum of the invariant covariance matrix

In the present section the spectrum of Σ_s is obtained using the spectra of matrices $\Sigma_{s-1}^{(1)}$ and $\Sigma_{s-1}^{(2)}$ in (16).

Theorem 3.1. *Let the covariance matrix Σ_s be defined as in* (16). *Let ω_h be an eigenvalue of $\Sigma_{s-1}^{(1)}$, ω'_h be an eigenvalue of $\Sigma_{s-1}^{(2)}$, $h = 1, \ldots, p$, $p = n_1 \cdot \ldots \cdot n_{s-1}$. Then the spectrum of Σ_s consists of eigenvalues $\omega_h + (n_s - 1)\omega'_{i_h}$ ($i_h = 1, \ldots, p$) and eigenvalues of the form $\omega_h - \omega'_{i_h}$.*

Proof. The matrices I_{n_s} and J_{n_s} commute. The construction of $\Sigma_{s-1}^{(1)}$ and $\Sigma_{s-1}^{(2)}$ in (16) implies that they commute. Hence, $I_{n_s} \otimes (\Sigma_{s-1}^{(1)} - \Sigma_{s-1}^{(2)})$ and $J_{n_s} \otimes \Sigma_{s-1}^{(2)}$ are normal matrices which commute. Therefore, they are simultaneously diagonalizable, i.e. there exists an orthogonal matrix Γ such that

$$\Gamma \Sigma_s \Gamma' = \Lambda_1 + \Lambda_2. \tag{19}$$

The diagonal matrix Λ_1 consists of eigenvalues $\omega_1 - \omega'_{i_1}, \ldots, \omega_p - \omega'_{i_p}$ of matrix $I_{n_s} \otimes (\Sigma_{s-1}^{(1)} - \Sigma_{s-1}^{(2)})$, each with multiplicity n_s. The diagonal matrix Λ_2 contains the spectrum of $J_{n_s} \otimes \Sigma_{s-1}^{(2)}$: $(n_s - 1)p$ zero eigenvalues and $n_s\omega'_{i_1}, \ldots, n_s\omega'_{i_p}$. Thus, the spectrum of Σ_s is the following: $\omega_1 - \omega'_{i_1}, \ldots, \omega_p - \omega'_{i_p}$ each with multiplicity $(n_s - 1)$ and $\omega_1 + (n_s - 1)\omega'_{i_1}, \ldots, \omega_p + (n_s - 1)\omega'_{i_p}$ each with multiplicity 1. □

As an example, the spectrum of the P_3-invariant covariance matrix Σ_3 is given in Table 1.

Table 1. Spectrum of Σ_3.

eigenvalue of Σ_3	*multiplicity*
$\lambda_1 = \tau_1 - \tau_2 - \tau_3 + \tau_4 - (\tau_5 - \tau_6 - \tau_7 + \tau_8)$	$(n_3 - 1)(n_2 - 1)(n_1 - 1)$
$\lambda_2 = \tau_1 - \tau_3 + (n_1 - 1)(\tau_2 - \tau_4)$ $-(\tau_5 - \tau_7 + (n_1 - 1)(\tau_6 - \tau_8))$	$(n_3 - 1)(n_2 - 1)$
$\lambda_3 = \tau_1 - \tau_2 + (n_2 - 1)(\tau_3 - \tau_4)$ $-(\tau_5 - \tau_6 + (n_2 - 1)(\tau_7 - \tau_8))$	$(n_3 - 1)(n_1 - 1)$
$\lambda_4 = -\lambda_1 + \lambda_2 + \lambda_3 + n_2 n_1(\tau_4 - \tau_8)$	$(n_3 - 1)$
$\lambda_5 = \tau_1 - \tau_2 - \tau_3 + \tau_4$ $+(n_3 - 1)(\tau_5 - \tau_6 - \tau_7 + \tau_8)$	$(n_2 - 1)(n_1 - 1)$
$\lambda_6 = \tau_1 - \tau_3 + (n_1 - 1)(\tau_2 - \tau_4)$ $+(n_3 - 1)(\tau_5 - \tau_7 + (n_1 - 1)(\tau_6 - \tau_8))$	$(n_2 - 1)$
$\lambda_7 = \tau_1 - \tau_2 + (n_2 - 1)(\tau_3 - \tau_4)$ $+(n_3 - 1)(\tau_5 - \tau_6 + (n_2 - 1)(\tau_7 - \tau_8))$	$(n_1 - 1)$
$\lambda_8 = -\lambda_5 + \lambda_6 + \lambda_7 + n_2 n_1(\tau_4 + (n_3 - 1)\tau_8)$	1

Eigenvectors corresponding to the eigenvalues of Σ_s have different structures $w_1, \ldots, w_8$:

$$\begin{aligned} w_1 &= v_{n_3} \otimes v_{n_2} \otimes v_{n_1}, & w_5 &= \mathbf{1}_{n_3} \otimes v_{n_2} \otimes v_{n_1}, \\ w_2 &= v_{n_3} \otimes v_{n_2} \otimes \mathbf{1}_{n_1}, & w_6 &= \mathbf{1}_{n_3} \otimes v_{n_2} \otimes \mathbf{1}_{n_1}, \\ w_3 &= v_{n_3} \otimes \mathbf{1}_{n_2} \otimes v_{n_1}, & w_7 &= \mathbf{1}_{n_3} \otimes \mathbf{1}_{n_2} \otimes v_{n_1}, \\ w_4 &= v_{n_3} \otimes \mathbf{1}_{n_2} \otimes \mathbf{1}_{n_1}, & w_8 &= \mathbf{1}_{n_3} \otimes \mathbf{1}_{n_2} \otimes \mathbf{1}_{n_1}, \end{aligned}$$

where $v'_{n_i}\mathbf{1}_{n_i} = 0$ $(i = 1, 2, 3)$.

Now, using the structure of Σ_3 in (15), and expressions of eigenvalues of Σ_3 (see Table 1), we can rewrite Σ_3 via its spectrum in the following way

$$\begin{aligned}\Sigma_3 = I_{n_3} \otimes \Big[I_{n_2} \otimes \Big[\lambda_1 I_{n_1} - \frac{1}{n_1}\{\lambda_1-\lambda_2\}J_{n_1}\Big] \\ - \frac{1}{n_2}J_{n_2} \otimes \Big[\{\lambda_1-\lambda_3\}I_{n_1} - \frac{1}{n_1}\{\lambda_1-\lambda_2-\lambda_3+\lambda_4\}J_{n_1}\Big]\Big] \\ - \frac{1}{n_3}J_{n_3} \otimes \Big[I_{n_2} \otimes \Big[\{\lambda_1-\lambda_5\}I_{n_1} - \frac{1}{n_1}\{\lambda_1-\lambda_2-\lambda_5+\lambda_6\}J_{n_1}\Big] \\ - \frac{1}{n_2}J_{n_2} \otimes \Big[\{\lambda_1-\lambda_3-\lambda_5+\lambda_7\}I_{n_1} \\ - \frac{1}{n_1}\{\lambda_1-\lambda_2-\lambda_3+\lambda_4-\lambda_5+\lambda_6+\lambda_7-\lambda_8\}J_{n_1}\Big]\Big]. \qquad (20)\end{aligned}$$

4. Reparameterization and spectrum of the covariance matrix of interaction effects

While arbitrary reparameterizations of a factor (in a linear model) may be mathematically acceptable, not all reparameterizations are equally reasonable for a given application. One of the most used reparameterization conditions for a factor ξ is the null-sum condition $\sum_i \xi_i = 0$. In this section we demonstrate how this reparameterization condition for a factor ξ can be expressed through the spectrum of the covariance matrix $D(\xi)$.

In the case when only one factor ξ is considered, the singularity of the P-invariant covariance matrix $D(\xi)$ of this factor is a necessary and sufficient condition for ξ to be reparameterized as $\sum_i \xi_i=0$ (see Nahtman, Möls, 2003). The situation with the s-order interaction effects is more complicated. The singularity of the P_s-invariant covariance matrix of $\gamma^{(s)}$ that represents s-order interaction effects does not, in general, imply a classical reparameterization of $\gamma^{(s)}$.

The next theorem, which is the main result of the paper, shows that imposing constraints on the spectrum of the singular P_3-invariant covariance matrix results in classical reparameterizations for $\gamma^{(3)}$. In the given context, under classical reparameterization conditions for $\gamma^{(3)}$ we mean the following conditions:

$$\sum_i \gamma^{(3)}_{ijk} = 0,\ \forall j,k, \quad \sum_j \gamma^{(3)}_{ijk} = 0,\ \forall\, i,k, \quad \sum_k \gamma^{(3)}_{ijk} = 0,\ \forall\, i,j.$$

Theorem 4.1. *Let $\gamma^{(3)}$: $(n_3n_2n_1)\times 1$ represent the third-order interaction effects of random factors. Assume $\gamma^{(3)}_{ijk} \neq \gamma^{(3)}_{i'jk}$ a.s. for all j and k, $\gamma^{(3)}_{ijk} \neq \gamma^{(3)}_{ij'k}$ a.s. for all i and k, and $\gamma^{(3)}_{ijk} \neq \gamma^{(3)}_{ijk'}$ a.s. for all i and j. Let $E(\gamma^{(3)}) = 0$ and let $\Sigma_3 = D(\gamma^{(3)})$ be P_3-invariant. Let $\lambda_1,\dots,\lambda_8$ be eigenvalues of Σ_3 as* *defined in Table* 1. *Then the following conditions hold:*

(i) $\sum_i \gamma_{ijk}^{(3)} = 0,\ \forall j,k,$ *iff* $\lambda_5 = \lambda_6 = \lambda_7 = \lambda_8 = 0,$

(ii) $\sum_j \gamma_{ijk}^{(3)} = 0,\ \forall i,k,$ *iff* $\lambda_3 = \lambda_4 = \lambda_7 = \lambda_8 = 0,$

(iii) $\sum_k \gamma_{ijk}^{(3)} = 0,\ \forall i,j,$ *iff* $\lambda_2 = \lambda_4 = \lambda_6 = \lambda_8 = 0.$

Proof. First, we show that condition (i) holds. Suppose $\sum_i \gamma_{ijk}^{(3)} = 0$ for all j and k, then

$$D(\sum_i \gamma_{ijk}^{(3)}) = n_3\tau_1 + n_3(n_3-1)\tau_5 = n_3(\tau_1 + (n_3-1)\tau_5) = 0,\ \forall j,k,$$

and

$$\tau_1 = -(n_3-1)\tau_5. \tag{21}$$

Condition $\sum_i \gamma_{ijk}^{(3)} = 0$, for all j and k, implies

$$\begin{aligned} \sum_i \sum_j \gamma_{ijk}^{(3)} &= 0,\ \forall k, \\ \sum_i \sum_k \gamma_{ijk}^{(3)} &= 0,\ \forall j, \\ \sum_i \sum_j \sum_k \gamma_{ijk}^{(3)} &= 0 \end{aligned}$$

and, consequently,

$$\begin{aligned} D(\sum_i \sum_j \gamma_{ijk}^{(3)}) &= n_3n_2\tau_1 + n_3(n_3-1)n_2\tau_5 + n_3n_2(n_2-1)\tau_3 \\ &+ n_3(n_3-1)n_2(n_2-1)\tau_7 = 0,\ \forall k, \qquad (22) \\ D(\sum_i \sum_k \gamma_{ijk}^{(3)}) &= n_3n_1\tau_1 + n_3(n_3-1)n_1\tau_5 + n_3n_1(n_1-1)\tau_2 \\ &+ n_3(n_3-1)n_2(n_2-1)\tau_6 = 0,\ \forall j, \qquad (23) \\ D(\sum_i \sum_j \sum_k \gamma_{ijk}^{(3)}) &= n_3n_2n_1\tau_1 + n_3(n_3-1)n_2n_1\tau_5 + n_3n_2(n_2-1)n_1\tau_3 \\ &+ n_3n_2n_1(n_1-1)\tau_2 + n_3(n_3-1)n_2(n_2-1)n_1\tau_7 \\ &+ n_3(n_3-1)n_2n_1(n_1-1)\tau_6 + n_3n_2(n_2-1)n_1(n_1-1)\tau_4 \\ &+ n_3(n_3-1)n_2(n_2-1)n_1(n_1-1)\tau_8 = 0. \qquad (24) \end{aligned}$$

Replacing τ_1 in (22) – (24) by (21) we get

$$\begin{aligned} \tau_2 &= -(n_3-1)\tau_6, \\ \tau_3 &= -(n_3-1)\tau_7, \\ \tau_4 &= -(n_3-1)\tau_8. \qquad (25) \end{aligned}$$

Substitution of obtained τ's into the expressions of eigenvalues, see Table 1, leads to $\lambda_5 = \lambda_6 = \lambda_7 = \lambda_8 = 0$, what proves the statement of (i) in one direction.

Now, suppose that $\lambda_5 = \lambda_6 = \lambda_7 = \lambda_8 = 0$. Then, it follows from (20)

$$\begin{aligned}\Sigma_3 &= \left[I_{n_3} - \frac{1}{n_3}J_{n_3}\right] \otimes \left[I_{n_2} \otimes \left[\lambda_1 I_{n_1} - \frac{1}{n_1}\{\lambda_1 - \lambda_2\}J_{n_1}\right]\right. \\ &\quad \left. - \frac{1}{n_2}J_{n_2} \otimes \left[\{\lambda_1 - \lambda_3\}I_{n_1} - \frac{1}{n_1}\{\lambda_1 - \lambda_2 - \lambda_3 + \lambda_4\}J_{n_1}\right]\right].\end{aligned}$$

Let $U = \mathbf{1}_{n_3} \otimes I_{n_2 n_1}$. Since $E(\gamma^{(3)}) = 0$, $E(U'\gamma^{(3)}) = 0$, and $D(U'\gamma^{(3)}) = U'\Sigma_3 U = 0$. Thus, $U'\gamma^{(3)} = 0$ a.s. what implies $\sum_i \gamma_{ijk}^{(3)} = 0$ for all j and k. This completes the proof of (i).

Condition (ii) is proved in a similar way. Using the condition $\sum_j \gamma_{ijk}^{(3)}=0$, for all i and k, it follows that $\sum_i \sum_j \gamma_{ijk}^{(3)} = 0$ for all k, and $\sum_j \sum_k \gamma_{ijk}^{(3)} = 0$ for all i. Furthermore,

$$\begin{aligned}D(\textstyle\sum_j \gamma_{ijk}^{(3)}) &= n_2\tau_1 + n_2(n_2-1)\tau_3 = 0, \ \forall i,k, \\ D(\textstyle\sum_i \sum_j \gamma_{ijk}^{(3)}) &= n_3(n_3-1)n_2\tau_5 + n_3(n_3-1)n_2(n_2-1)\tau_7 = 0, \ \forall k, \\ D(\textstyle\sum_j \sum_k \gamma_{ijk}^{(3)}) &= n_2 n_1(n_1-1)\tau_2 + n_2(n_2-1)n_1(n_1-1)\tau_4 = 0, \ \forall i, \\ D(\textstyle\sum_i \sum_j \sum_k \gamma_{ijk}^{(3)}) &= n_3(n_3-1)n_2 n_1(n_1-1)\tau_6 \\ &\quad + n_3(n_3-1)n_2(n_2-1)n_1(n_1-1)\tau_8 = 0\end{aligned}$$

and we obtain

$$\begin{aligned}\tau_1 &= -(n_2-1)\tau_3, \\ \tau_2 &= -(n_2-1)\tau_4, \\ \tau_5 &= -(n_2-1)\tau_7, \\ \tau_6 &= -(n_2-1)\tau_8.\end{aligned} \tag{26}$$

Taking these expressions for the τ's into account, Table 1 gives $\lambda_3 = \lambda_4 = \lambda_7 = \lambda_8 = 0$.

To show that $\lambda_3 = \lambda_4 = \lambda_7 = \lambda_8 = 0$ results in $\sum_j \gamma_{ijk}^{(3)} = 0$, for all i and k, notice

$$\begin{aligned}\Sigma_3 &= I_{n_3} \otimes \left[I_{n_2} - \frac{1}{n_2}J_{n_2}\right] \otimes \left[\lambda_1 I_{n_1} - \frac{1}{n_1}\{\lambda_1 - \lambda_2\}J_{n_1}\right] \\ &\quad - \frac{1}{n_3}J_{n_3} \otimes \left[I_{n_2} - \frac{1}{n_2}J_{n_2}\right] \otimes \left[\{\lambda_1 - \lambda_5\}I_{n_1} - \frac{1}{n_1}\{\lambda_1 - \lambda_2 - \lambda_5 + \lambda_6\}J_{n_1}\right].\end{aligned}$$

Define $U = I_{n_3} \otimes \mathbf{1}_{n_2} \otimes I_{n_1}$. Since $E(\gamma_3) = 0$,

$$E(U'\gamma^{(3)}) = 0, \; D(U'\gamma^{(3)}) = U'\Sigma_3 U = 0.$$

Thus, $U'\gamma^{(3)} = 0$ a.s. what implies $\sum_j \gamma_{ijk}^{(3)} = 0$ for all i and k.

To show that condition (iii) holds, notice that $\sum_k \gamma_{ijk}^{(3)} = 0$, for all i and j, implies $\sum_j \sum_k \gamma_{ijk}^{(3)} = 0$, for all i, $\sum_i \sum_k \gamma_{ijk}^{(3)} = 0$, for all j, and $\sum_i \sum_j \sum_k \gamma_{ijk}^{(3)} = 0$. Taking the variance of these sums we find after some simplifications that

$$\begin{aligned} \tau_1 &= -(n_1 - 1)\tau_2, \\ \tau_3 &= -(n_1 - 1)\tau_4, \\ \tau_5 &= -(n_1 - 1)\tau_6, \\ \tau_7 &= -(n_1 - 1)\tau_8. \end{aligned} \tag{27}$$

Using relationships (27) in the expressions of eigenvalues (see Table 1) leads to $\lambda_2 = \lambda_4 = \lambda_6 = \lambda_8 = 0$.

Finally, assume $\lambda_2 = \lambda_4 = \lambda_6 = \lambda_8 = 0$. In this case it follows from (20) that

$$\begin{aligned} \Sigma_3 = & \Bigg[I_{n_3} \otimes \Big[\lambda_1 I_{n_2} - \frac{1}{n_2}\{\lambda_1 - \lambda_3\} J_{n_2} \Big] - \frac{1}{n_3} J_{n_3} \otimes \Big[\{\lambda_1 - \lambda_5\} I_{n_2} \\ & - \frac{1}{n_2}\{(\lambda_1 - \lambda_3) - (\lambda_5 - \lambda_7)\} J_{n_2} \Big] \Bigg] \otimes \Big[I_{n_1} - \frac{1}{n_1} J_{n_1} \Big]. \end{aligned}$$

Define $U = I_{n_3} \otimes I_{n_2} \otimes \mathbf{1}_{n_1}$. Since $E(\gamma^{(3)}) = 0$,

$$E(U'\gamma^{(3)}) = 0, \; D(U'\gamma^{(3)}) = U'\Sigma_3 U = 0.$$

Thus, $U'\gamma^{(3)} = 0$ a.s. what implies $\sum_k \gamma_{ijk}^{(3)} = 0$ for all i and j. □

The next corollary follows from the proof of Theorem 4.1.

Corollary 4.1.

(i) $\sum_i \sum_j \gamma_{ijk}^{(3)} = 0, \; \forall k$, *iff* $\lambda_7 = \lambda_8 = 0$,

(ii) $\sum_j \sum_k \gamma_{ijk}^{(3)} = 0, \; \forall i$, *iff* $\lambda_4 = \lambda_8 = 0$,

(iii) $\sum_i \sum_k \gamma_{ijk}^{(3)} = 0, \; \forall j$, *iff* $\lambda_6 = \lambda_8 = 0$,

(iv) $\sum_i \sum_j \sum_k \gamma_{ijk}^{(3)} = 0$ *iff* $\lambda_8 = 0$.

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Institute of Mathematical Statistics, J. Liivi 2, 50409 Tartu, Estonia
E-mail address: tonu@zbi.ee
E-mail address: tnahtman@ut.ee