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Reparameterization of second-order interaction effects through the covariance matrix

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ABSTRACT. It is demonstrated that the reparameterization of second-order interaction terms in ANOVA can be achieved by means of constraints on the covariance matrix. In particular, classical reparameterization conditions for fixed factors can be formulated in this way. The approach stresses the common nature of fixed and random factors in mixed linear analysis.

1. Introduction

Mixed linear statistical models contain both fixed and random factors. During the history of the Analysis of Variance, various mixed model formulations have been proposed and the discussion around this topic is still continuing (Scheffè 1959 [7], Searle 1971 [5], Harville 1978 [1], Seely and El-Houssainy 1988 [6], Khuri et al. 1998 [3]). In models of this type fixed and random factors are clearly distinguishable and the interactions between fixed and random factors are considered as independent random effects. Fixed factors are treated as constants while levels of random factors are represented as random variables, possibly with a restricted covariance structure.

In the present paper we consider an approach to imposing constraints on the second-order interaction effects through the covariance matrix of sampled levels. In this context, the goal is to find out conditions under which the covariance matrix would provide a reparameterization of the corresponding factor. This approach is advantageous, for instance, from the point of view of simulation studies where levels of fixed factors must be generated randomly so that classical reparameterization conditions hold.

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2. Results

Let ξ be an $m \times 1$ vector of sampled levels of a factor α, η be an $n \times 1$ vector of sampled levels of a factor β. Let γ be an $mn \times 1$ vector of sampled levels of the factor that represents second-order interaction effects of ξ and η and let Σ_γ be the covariance matrix of γ. Introduce a permutation matrix P_ξ that interchanges levels of factor ξ. A matrix P_η is defined analogously. The permutation matrix $P_\gamma = P_\xi \otimes P_\eta$ interchanges levels of γ with respect to the changes in ξ and η.

Definition 1. The covariance matrix Σ_γ is called invariant with respect to the permutation P_γ of the factor γ (further simply P_γ-invariant) if

$$\Sigma_\gamma = D(\gamma) = D(P_\gamma \gamma).$$

Obviously, the P_γ-invariance can be considered as a property of the covariance matrix Σ_γ, i.e., Σ_γ is P_γ-invariant if and only if $P_\gamma \Sigma_\gamma P'_\gamma = \Sigma_\gamma$.

The invariance has strong implications for the covariance matrix.

Lemma 1. *If the matrix Σ_γ is invariant with respect to all permutations P_γ, then it has the following structure:*

$$\mathbf{\Sigma}_\gamma = \begin{pmatrix} \Sigma & \Sigma_2 & \dots & \Sigma_2 \\ \Sigma_2 & \Sigma & \dots & \Sigma_2 \\ \vdots & \vdots & \ddots & \vdots \\ \Sigma_2 & \Sigma_2 & \dots & \Sigma \end{pmatrix} = I_m \otimes \Sigma_1 + J_m \otimes \Sigma_2, \tag{1}$$

where I_m is the identity matrix of order m and $J_m = \mathbf{1} \cdot \mathbf{1}'$, where $\mathbf{1}$ is an $m \times 1$ vector of ones. The matrices Σ, Σ_1 and Σ_2 are here defined as

$$\Sigma = \begin{pmatrix} \tau & \tau_1 & \dots & \tau_1 \\ \tau_1 & \tau & \dots & \tau_1 \\ \vdots & \vdots & \ddots & \vdots \\ \tau_1 & \tau_1 & \dots & \tau \end{pmatrix} = (\tau - \tau_1) I_n + \tau_1 J_n, \tag{2}$$

$$\Sigma_2 = \begin{pmatrix} \tau_2 & \tau_3 & \dots & \tau_3 \\ \tau_3 & \tau_2 & \dots & \tau_3 \\ \vdots & \vdots & \ddots & \vdots \\ \tau_3 & \tau_3 & \dots & \tau_2 \end{pmatrix} = (\tau_2 - \tau_3) I_n + \tau_3 J_n, \tag{3}$$

$$\Sigma_1 = \Sigma - \Sigma_2 = (\tau - \tau_1 - \tau_2 + \tau_3) I_n + (\tau_1 - \tau_3) J_n \tag{4}$$

and

$$\begin{aligned} \tau &= Cov(\gamma_{ij}, \gamma_{ij}), \\ \tau_1 &= Cov(\gamma_{ij}, \gamma_{ij'}), \quad j \neq j', \\ \tau_2 &= Cov(\gamma_{ij}, \gamma_{i'j}), \quad i \neq i', \\ \tau_3 &= Cov(\gamma_{ij}, \gamma_{i'j'}), \quad i \neq i', j \neq j', \end{aligned} \tag{5}$$

where $i = 1, \dots, m$ *and* $j = 1, \dots n$.

Proof. The proof follows by applying P_γ to γ. This corresponds to interchanging some elements of γ, what implies permutations of certain elements in Σ_γ. As a result of the rearrangement, the structure of Σ_γ must not be changed. □

The proof of the following lemma is straightforward.

Lemma 2. *If the matrix* Σ_γ *has the structure* (1), *then its spectrum of eigenvalues and corresponding eigenvectors is the following:*

eigenvalue	*multiplicity*	*structure of eigenvectors*
$\lambda_1 = \tau - \tau_1 - \tau_2 + \tau_3$	$(m-1)(n-1)$	$w_1 = u \otimes v$
$\lambda_2 = \tau - \tau_2 + (n-1)(\tau_1 - \tau_3)$	$(m-1)$	$w_2 = u \otimes 1_n$
$\lambda_3 = \tau - \tau_1 + (m-1)(\tau_2 - \tau_3)$	$(n-1)$	$w_3 = 1_m \otimes v$
$\lambda_4 = \tau + (n-1)(\tau_1 - \tau_3) + (m-1)(\tau_2 - \tau_3) + (mn-1)\tau_3$	1	$w_4 = 1_m \otimes 1_n$

where u *and* v *are vectors satisfying* $\sum_{i=1}^m u_i = 0$ *and* $\sum_{j=1}^n v_j = 0$.

Next we show that the classical reparameterization conditions imply a specific form for the P_γ-invariant covariance matrix Σ_γ.

Lemma 3. *If the covariance matrix* Σ_γ *of* γ *is* P_γ*-invariant, then the reparameterization of* γ *leads to the following structure of* Σ_γ*:*

(a) $\sum_{i=1}^m \gamma_{ij} = 0,\ \forall j \ \Rightarrow\ \Sigma_\gamma = \frac{m}{m-1}(I_m - \frac{1}{m}J_m) \otimes ((\tau - \tau_1)I_n + \tau_1 J_n)$,

(b) $\sum_{j=1}^n \gamma_{ij} = 0,\ \forall i \ \Rightarrow\ \Sigma_\gamma = \frac{n}{n-1}((\tau - \tau_2)I_m + \tau_2 J_m) \otimes (I_n - \frac{1}{n}J_n)$,

(c) $\sum \gamma_{ij} = 0,\ \forall i$ *and* $\forall j \ \Rightarrow\ \Sigma_\gamma = \frac{mn}{(m-1)(n-1)}\tau(I_m - \frac{1}{m}J_m) \otimes (I_n - \frac{1}{n}J_n)$.

Proof. First, using the condition $\sum_{i=1}^m \gamma_{ij} = 0$ for all j, we have

$$D(\sum_{i=1}^m \gamma_{ij}) = m\tau + m(m-1)\tau_2 = 0$$

and

$$D(\sum_{i=1}^m \sum_{j=1}^n \gamma_{ij}) = mn\tau + mn(n-1)\tau_1 + m(m-1)n\tau_2 + m(m-1)n(n-1)\tau_3 = 0. \quad (6)$$

Hence,

$$\tau_2 = -\frac{\tau}{m-1} \quad \text{and} \quad \tau_3 = -\frac{\tau_1}{m-1}. \tag{7}$$

Substituting these expressions for τ_2 and τ_3 into (1)–(4), we get

$$\begin{aligned}
\Sigma_\gamma &= I_m \otimes ((\tau - \tau_1 + \tfrac{\tau}{m-1} - \tfrac{\tau_1}{m-1})I_n + (\tau_1 + \tfrac{\tau_1}{m-1})J_n) \\
&\quad + J_m \otimes (-\tfrac{\tau}{m-1} + \tfrac{\tau_1}{m-1})I_n - \tfrac{\tau_1}{m-1})J_n) \\
&= \tfrac{m}{m-1}(\tau - \tau_1)(I_m - \tfrac{1}{m}J_m) \otimes I_n + \tfrac{m}{m-1}\tau_1(I_m - \tfrac{1}{m}J_m) \otimes J_n \\
&= \tfrac{m}{m-1}(I_m - \tfrac{1}{m}J_m) \otimes ((\tau - \tau_1)I_n + \tau_1 J_n).
\end{aligned}$$

Next, because of $\sum_{j=1}^{n} \gamma_{ij} = 0$ for all i,

$$D(\sum_{j=1}^{n} \gamma_{ij}) = n\tau + n(n-1)\tau_1 = 0.$$

Therefore, using this result and (6), we get,

$$\tau_1 = -\frac{\tau}{n-1} \quad \text{and} \quad \tau_3 = -\frac{\tau_2}{n-1}. \tag{8}$$

In this case the matrix Σ_γ is rewritten as

$$\begin{aligned}
\Sigma_\gamma &= I_m \otimes ((\tau + \tfrac{\tau}{n-1} - \tau_2 - \tfrac{\tau_2}{n-1})I_n + (-\tfrac{\tau}{n-1} + \tfrac{\tau_2}{n-1})J_n) \\
&\quad + J_m \otimes ((\tau_2 + \tfrac{\tau_2}{n-1})I_n - \tfrac{\tau_2}{n-1})J_n) \\
&= \tfrac{n}{n-1}(\tau - \tau_2)I_m \otimes (I_n - \tfrac{1}{n}J_n) + \tfrac{n}{n-1}\tau_2 J_m \otimes (I_n - \tfrac{1}{n}J_n) \\
&= \tfrac{n}{n-1}((\tau - \tau_2)I_m + \tau_2 J_m) \otimes (I_n - \tfrac{1}{n}J_n).
\end{aligned}$$

Finally, applying the conditions $\sum \gamma_{ij} = 0$, for all i and j, and (6), the parameters τ_1, τ_2 and τ_3 are expressed as

$$\tau_1 = -\frac{\tau}{n-1}, \quad \tau_2 = -\frac{\tau}{m-1}, \quad \tau_3 = \frac{\tau}{(m-1)(n-1)}. \tag{9}$$

Substituting expressions (9) for the parameters τ_1, τ_2, τ_3 into (1)–(4), the covariance matrix Σ_γ becomes

$$\Sigma_\gamma = \tfrac{mn}{(m-1)(n-1)}\tau(I_m - \tfrac{1}{m}J_m) \otimes (I_n - \tfrac{1}{n}J_n).$$

□

As a consequence of Lemma 3, if the factor γ of second-order interaction effects is reparameterized according to the conditions in (a), (b) or (c), then its covariance matrix is singular.

In case when only one factor ξ is considered, the singularity of the P_ξ-invariant covariance matrix of this factor would be a necessary and sufficient condition for ξ to be reparameterized (see [4]). The situation with the second-order interaction effects is more complicated. The singularity of the

P_γ-invariant covariance matrix of γ that represents the second-order interaction effects does not, in general, imply the classical reparameterization of γ. The next result provides conditions under which eigenvalues of the P_γ-invariant covariance matrix lead to the classical reparameterization for the vector of second-order interaction effects.

Theorem. *Let $\gamma = (\gamma_{11}, \dots, \gamma_{mn})'$ represent the interaction effects of factors ξ and η. Assume $\gamma_{ij} \neq \gamma_{kj}$ for all j and $\gamma_{ij} \neq \gamma_{is}$ for all i a.s. Let $E(\gamma) = 0$ and let Σ_γ be P_γ-invariant. Let λ_k $(k = 1, \dots, 4)$ be an eigenvalue of Σ_γ as defined by Lemma 2. Then the following conditions hold:*

(i) $\sum_i \gamma_{ij} = 0,\ \forall j \quad \Leftrightarrow \lambda_3 = \lambda_4 = 0,$

(ii) $\sum_j \gamma_{ij} = 0,\ \forall i \quad \Leftrightarrow \lambda_2 = \lambda_4 = 0,$

(iii) $\sum_i \gamma_{ij} = 0,\ \forall j,$ *and* $\sum_j \gamma_{ij} = 0,\ \forall i \quad \Leftrightarrow \lambda_2 = \lambda_3 = \lambda_4 = 0.$

Proof. We first show that condition (i) holds. Since $\sum_i \gamma_{ij} = 0$ for all j,

$$\tau_2 = -\frac{\tau}{m-1} \quad \text{and} \quad \tau_3 = -\frac{\tau_1}{m-1}$$

(see the proof of Lemma 3, (7)). Then

$$\begin{aligned} \lambda_3 &= \tau - \tau_1 + (m-1)(\tau_2 - \tau_3) \\ &= \tau - \tau_1 + (m-1)\left(-\frac{\tau}{m-1} + \frac{\tau_1}{m-1}\right) = 0, \\ \lambda_4 &= \tau + (n-1)(\tau_1 - \tau_3) + (m-1)(\tau_2 - \tau_3) + (mn-1)\tau_3 \\ &= \tau + (n-1)\left(\tau_1 + \frac{\tau_1}{m-1}\right) - (\tau - \tau_1) - (mn-1)\frac{\tau_1}{m-1} = 0. \end{aligned}$$

In case $\lambda_3 = \lambda_4 = 0$, the set of n linearly independent eigenvectors that correspond to zero eigenvalues can be given by columns of the matrix $U = \mathbf{1}_m \otimes I_n$. Since $E(\gamma) = 0$,

$$E(U'\gamma) = 0, \;\; D(U'\gamma) = U'D(\gamma)U = 0.$$

Thus, $U'\gamma = 0$ a.s. what implies the classical reparameterization of the factor γ:

$$\sum_{i=1}^{m} \gamma_{ij} = 0, \quad \forall j.$$

Next we prove condition (ii). Suppose $\sum_j \gamma_{ij} = 0$ for all i. Then, from the proof of Lemma 3, we find

$$\tau_1 = -\frac{\tau}{n-1} \quad \text{and} \quad \tau_3 = -\frac{\tau_2}{n-1}.$$

According to Lemma 2,

$$\begin{aligned}\lambda_2 &= \tau - \tau_2 + (n-1)(\tau_1 - \tau_3) = \tau - \tau_2 + (n-1)(-\frac{\tau}{n-1} + \frac{\tau_2}{n-1}) = 0.\\ \lambda_4 &= \tau + (n-1)(\tau_1 - \tau_3) + (m-1)(\tau_2 - \tau_3) + (mn-1)\tau_3\\ &= \tau - (\tau - \tau_2) + (m-1)(\tau_2 + \frac{\tau_2}{n-1}) - (mn-1)\frac{\tau_2}{n-1} = 0.\end{aligned}$$

If $\lambda_2 = \lambda_4 = 0$, then according to the specific form of Σ_γ (see Lemma 3), the set of m linearly independent eigenvectors that correspond to zero eigenvalues can be given by columns of the matrix $V = I_m \otimes \mathbf{1}_n$. Since $E(\gamma) = 0$,

$$E(V'\gamma) = 0, \; D(V'\gamma) = V'D(\gamma)V = 0.$$

Thus, $V'\gamma = 0$ a.s. what implies the reparameterization of γ with

$$\sum_{j=1}^{n} \gamma_{ij} = 0, \; \forall i.$$

The proof of (iii) goes similarly. Conditions $\sum_j \gamma_{ij} = 0$, for all i, and $\sum_i \gamma_{ij} = 0$, for all j, lead to

$$\tau_1 = -\frac{\tau}{n-1}, \quad \tau_2 = -\frac{\tau}{m-1}, \quad \tau_3 = \frac{\tau}{(m-1)(n-1)}$$

(see the proof of Lemma 3). Therefore,

$$\begin{aligned}\lambda_2 &= \tau - \tau_2 + (n-1)(\tau_1 - \tau_3)\\ &= \tau + \frac{\tau}{m-1} + (n-1)(-\frac{\tau}{n-1} - \frac{\tau}{(m-1)(n-1)}) = 0,\\ \lambda_3 &= \tau - \tau_1 + (m-1)(\tau_2 - \tau_3)\\ &= \tau + \frac{\tau}{n-1} + (m-1)(-\frac{\tau}{m-1} - \frac{\tau}{(m-1)(n-1)}) = 0,\\ \lambda_4 &= \tau + (n-1)(\tau_1 - \tau_3) + (m-1)(\tau_2 - \tau_3) + (mn-1)\tau_3\\ &= \tau - (\tau - \tau_2) - (\tau - \tau_1) + (mn-1)\tau_3 = -\tau + \tau_1 + \tau_2 + (mn-1)\tau_3\\ &= -\tau - \frac{\tau}{n-1} - \frac{\tau}{m-1} + (mn-1)\frac{\tau}{(m-1)(n-1)} = 0.\end{aligned}$$

Results from the proofs of conditions (i) and (ii) in case $\lambda_2 = \lambda_3 = \lambda_4 = 0$ lead to the reparameterization $\sum_j \gamma_{ij} = 0$, for all i, and $\sum_i \gamma_{ij} = 0$, for all j, for the factor γ. □

3. Discussion

Advanced linear statistical analysis offers extremely wide possibilities for choosing underlying models and types of analysis. However, the increasing complexity and possibility to choose models make it necessary to even more precisely tune the model and hypotheses under testing. In the most difficult cases, the appropriateness of the whole statistical analysis must be tested by statistical modelling. This activity needs generation of various factor levels and their interactions with specific probability distributions including various reparameterizations. Hence it arises a motivation for searching new ways of characterizations of factors in mixed linear models. In the present paper we have proposed an approach that enables to consider reparameterization of second-order interaction effects in a common framework in mixed linear models. We have demonstrated that reparameterization of the factor under invariance is equivalent to imposing constraints on the covariance matrix of this factor.

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