Shift Permutation Invariance in Linear Random Factor Models

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Abstract

The objective of this paper is to consider shift invariance of random factors in linear models. Marginally shift invariant interaction factors are treated. The random factors are described via their covariance matrices and it is shown that shift invariance implies Toeplitz covariance matrices and marginally shift invariance implies block Toeplitz covariance matrices. In order to get interpretable linear models reparameterization is taken place and it is shown that by putting restrictions on the spectrum of the Toeplitz matrices natural reparameterization conditions are obtained.

Keywords: Block Toeplitz matrix, covariance structures, eigenspace, invariance, K-way tables, marginal permutations, reparameterization, shift invariance, spectrum, Toeplitz matrix.

AMS 2000 subject classifications. Primary: 62F30; Secondary: 62J10, 62F99.

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1 Introduction

This paper is a follow up paper of Nahtman (2005). In that paper random factors in linear models were considered under the condition that the factors were permutation invariant. The main idea is to fully couple the experimental design to the modelling part, which among others includes knowledge of how to incorporate designs which are invariant under some kind of permutations. Concerning estimation MLEs are since long time available (e.g. see Andersson (1975)). A commonly applied design is a design which is invariant under the exchange of factor levels. Moreover, besides the design being exchangeable we often have some linear restrictions on the factor. For example, the restriction which puts the sum of factor levels to 0, which among others does not violate the assumption of exchangeability. However, one factor is fairly straight-forward to study but our aim is to study interactions. We will limit the study to $K-$way tables which immediately leads to that we are going to study marginal permutations (see Nahtman (2005)).

The best way to describe invariance properties of random factors, including interactions, is via their covariance matrices. Because of invariance it appears that the natural quantities to study are the eigenvalues and eigenvectors. It is easy to imagine that restrictions on the factor levels will lead to singular covariance matrices with eigenvalues equal to 0. The corresponding eigenvectors then tell us what kind of restrictions can be imposed on the factors.

In the present paper we are going to study shift invariance. This leads to covariance matrices with Toeplitz structures. Statistical inference in linear models under Toeplitz structured covariance matrices has previously been considered by Olkin and Press (1969). In particular shift invariance implies that covariance matrices are build up with the help of Kronecker products, i.e. have block Toeplitz structures. It is interesting to note that in practise shift invariance is natural but that this property is not always taken into account when modelling data. Eigenvalues and eigenvectors of Toeplitz matrices are known. We start with this observation. Later results are extended to the study of higher order interactions of factors and block Toeplitz structures. In Section 2 spectral properties of symmetric Toeplitz matrices are given, Section 3 connects shift invariance with Toeplitz covariance matrices, Section 4 considers the reparametrization of factors and in particular we present detailed results for $n = 4, 5, 6, 7, 8$, where the size of the covariance matrix is $n \times n$, in Section 5 the most general results are given and finally in Section 6 t-shift invariance is briefly considered. The whole area is new. To connect shift invariance with Toeplitz covariance matrices, which spectrum will guide us what kind of restrictions can be assumed to hold, has not been studied before. Therefore, in particular in Section 4 as well as in the appendices we present many details.

2 Preliminaries and definitions

Some definitions and useful results from matrix theory are outlined.

An $n \times n$ matrix T of the form

$$T = \begin{pmatrix} t_0 & t_1 & t_2 & \cdots & t_1 \\ t_1 & t_0 & t_1 & \cdots & t_2 \\ t_2 & t_1 & t_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & t_1 \\ t_1 & t_2 & \cdots & t_1 & t_0 \end{pmatrix} = \mathrm{Toep}(t_0, t_1, t_2, \ldots, t_1) \tag{2.1}$$

is called a *symmetric circular Toeplitz matrix.* The matrix T depends on $[n/2] + 1$ parameters, where $[\bullet]$ stands for the integer part, and $t_{i,j} = t_{|i-j|}$, $i, j = 1, \ldots, n$.

A *symmetric circular matrix* $\mathrm{SC}(n, k)$ is defined in the following way:

$$\mathrm{SC}(n,k) = \mathrm{Toep}(\overbrace{\underbrace{0, \ldots, 0}_{k}, 1, 0, \ldots, 0, 1, \underbrace{0, \ldots, 0}_{k-1}}^{n}), \tag{2.2}$$

where $k \in \{1, \ldots, [n/2]\}$. For notational convenience denote $\mathrm{SC}(n, 0) = I_n$.

The matrix $\mathrm{SC}(n, k)$ has components (i,j) which equal 1 if $|i - j| = k$ or $|i - j| = n - k$, $k = 1, \ldots, [n/2]$. Notice that

$$a_0 I_n + \sum_{i=0}^{[n/2]} a_i \mathrm{SC}(n, i) = 0, \tag{2.3}$$

implies that $a_0 = \ldots = a_{[n/2]} = 0$, i.e. $I_n, \mathrm{SC}(n, 1), \ldots, \mathrm{SC}(n, [n/2])$ are linearly independent. Lemma 2.1, given below, establishes the known fact that these matrices commute. It is easy to see that

$$\mathrm{Toep}(t_0, t_1, t_2, \ldots, t_1) = \sum_{i=0}^{[n/2]} t_i \mathrm{SC}(n, i). \tag{2.4}$$

The spectral properties of symmetric circular Toeplitz matrices can be found in Davis (1979) or Basilevsky (1983). We present some additional results concerning multiplicities of the eigenvalues of such matrices.

Let λ_h, $h = 1, \ldots, n$, be an eigenvalue of the matrix $T : n \times n$. The following lemma gives the spectral property of the matrix T.

Lemma 2.1 *Let T: $n \times n$ be symmetric Toeplitz matrix with elements as in* (2.1). *If n is odd*

$$\lambda_h = t_0 + 2\sum_{j=1}^{[n/2]} t_j \cos(2\pi hj/n). \tag{2.5}$$

There is only one eigenvalue λ_n which has multiplicity 1 *and all other eigenvalues are of multiplicity* 2.
If n is even

$$\lambda_h = t_0 + 2\sum_{j=1}^{n/2-1} t_j \cos(2\pi hj/n) + t_{n/2}\cos(\pi h). \tag{2.6}$$

There are only two eigenvalues $\lambda_n, \lambda_{n/2}$ which have multiplicity 1 *and all others eigenvalues are of multiplicity* 2.

The eigenvectors corresponding to the eigenvalues $\lambda_1, \dots, \lambda_n$ are

$$v_h = n^{-1/2}(v_{h1}, \dots, v_{hn})' \tag{2.7}$$

with

$$v_{hi} = \cos(2\pi ih/n) + \sin(2\pi ih/n),\ i = 1, \dots, n. \tag{2.8}$$

Proof. For derivation of the eigenvalues and eigenvectors we refer the reader to Basilevsky (1983). If n is odd we can see that $\lambda_h = \lambda_{n-h}$, $h = 1, \dots, n-1$, and $\lambda_n = t_0 + 2\sum_{j=1}^{(n-1)/2} t_j$. If n is even, then for $h \neq n, n/2 : \lambda_h = \lambda_{n-h}$. However, the eigenvalues

$$\lambda_n = t_0 + 2\sum_{j=1}^{n/2-1} t_j \cos(2\pi j) + t_{n/2}\cos(\pi n),$$
$$\lambda_{n/2} = t_0 + 2\sum_{j=1}^{n/2-1} t_j \cos(\pi j) + t_{n/2}\cos(\pi n/2)$$

are distinct. □

It is worth observing that from (2.2) it follows that Lemma 2.1 immediately gives eigenvalues and eigenvectors for SC(n, k). Moreover, eigenvectors given in (2.7) do not depend on the elements in (2.1). One important consequence of this result is that any pair of two different symmetric circular Toeplitz matrices of the same size always commute.

3 Shift permutation invariance, Toeplitz covariance matrices

An orthogonal matrix $P = (p_{ij}) : n \times n$ is a *shift permutation matrix* if

$$p_{ij} = \begin{cases} 1, & \text{if } j = i + 1 - nI_{(i>n-1)} \\ 0, & \text{otherwise} \end{cases} , \tag{3.1}$$

where

$$I_{(a>b)} = \begin{cases} 1, & \text{if } a > b \\ 0, & \text{otherwise} \end{cases} . \tag{3.2}$$

Definition 3.1 *The covariance matrix $D(\xi)$ of a factor ξ is called invariant with respect to a shift permutation matrix P if $D(\xi) = D(P\xi)$ or, equivalently, if $PD(\xi)P' = D(\xi)$.*

Suppose that we have observations $Y_{i_1,i_2,\ldots,i_k}$ for which we assume a model consisting of k random factors, i.e. the observations $Y_{i_1,i_2,\ldots,i_k}$ form a $K - way$ table. A crucial assumption will be that if we permute the levels of one factor, the others will not be affected. This leads to the concept of *marginal permutations*. For $k = 2$ we have $Y_{i_1 i_2}$, i.e. a matrix $Y = (Y_{ij})$. Invariance implies that we can premultiply Y by a shift matrix $P^{(1)}$ and $P^{(1)}Y$ will have the same distribution as Y. Observe that $P^{(1)}$ affects the index i in Y_{ij} and if $E(Y) = 0$ invariance means $D(P^{(1)}Y) = D(Y)$. If we want to permute the j-index, we look at $YP^{(2)}$. Furthermore, if we intend to permute the indices i and j independently of each other we study $P^{(1)}YP^{(2)}$, or equivalently $(P^{(2)} \otimes P^{(1)})vecY$, where *vec* is the usual *vec*-operator. In the case of several factors we can repeat the arguments and obtain the next theorem.

Theorem 3.2 *In the K-way table the structure of the shift permutation matrix P_k equals*

$$P_k = P^{(k)} \otimes \cdots \otimes P^{(1)}, \tag{3.3}$$

where $P^{(h)}$ are shift permutation matrices, $h = 1, \ldots, k$.

The matrix P_k defined in Theorem 3.2 is called a *marginally shift permutation matrix of order k*.

In the proof, we are not going to discuss the vector of observations Y but instead study the underlying random factors. Based on our results for factors we can immediately consider observations but this is a trivial exercise. For example, for

$$Y_{ijk} = \xi_i^1 + \xi_j^2 + \gamma_{ij}^{(2)} + \varepsilon_{ijk},$$

where $\xi^1=(\xi^1_i) \sim N(0,\Sigma_{\xi^1})$, $\xi^2=(\xi^2_j) \sim N(0,\Sigma_{\xi^2})$, $\gamma^{(2)}=(\gamma^{(2)}_{ij}) \sim N(0,\Sigma_{\gamma^{(2)}})$, $\varepsilon=(\varepsilon_{ijk}) \sim N(0,\Sigma_\varepsilon)$ are independent, results are obtained when we have knowledge about the factors ξ^1, ξ^2, $\gamma^{(2)}$ and ε. Here $\gamma^{(2)}$ is a second order interaction factor. In the subsequent we are going to study an s-order interaction factor $\gamma^{(s)}$ with $D(\gamma^{(s)}) = \Sigma_s$. Let levels of the factor $\gamma^{(s)}$ be ordered lexicographically. The next theorems show that invariance has strong implications on the structure of the covariance matrix. We first present two special cases which are of interest in applications but also serve as a basis in an induction proof which will be used for proving the general statement.

Theorem 3.3 *The covariance matrix* Σ: $n_1 \times n_1$ *of the factor* ξ *is shift permutation invariant if and only if it is a symmetric circular Toeplitz matrix:*

$$\Sigma = \mathrm{Toep}(\tau_0, \tau_1, \tau_2, \ldots, \tau_1) = \sum_{i=0}^{[n_1/2]} \tau_i \mathrm{SC}(n_1, i), \tag{3.4}$$

where the matrices $\mathrm{SC}(n_1,i)$, $i = 0, \ldots, [n_1/2]$, *are given by* (2.2).

Proof. Let e_h be the h-th column of the identity matrix I_{n_1}, $h = 1, \ldots, n_1$. Then we can express $\Sigma = (\sigma_{ij})$ in the following way:

$$\Sigma = \sum_{i=1}^{n_1}\sum_{j=1}^{n_1} \sigma_{ij} e_i e_j' = \sum_{i}^{n_1} \sigma_{ii} e_i e_i' + \sum_{k=1}^{[n_1/2]} \sum_{\substack{i,j \\ |i-j|= \\ k, n_1-k}} \sigma_{ij} e_i e_j'. \tag{3.5}$$

Since by invariance, i.e. $P_1\gamma^{(1)}$ and $\gamma^{(1)}$ have the same covariance matrix, we study when $P_1 \Sigma P_1' = \Sigma$. Now,

$$P_1 \Sigma P_1' = \sum_{i=1}^{n_1} \sigma_{ii} (P_1 e_i e_i' P_1') + \sum_{k=1}^{[n_1/2]} \sum_{\substack{i,j \\ |i-j|= \\ k, n_1-k}} \sigma_{ij} (P_1 e_i e_j' P_1') \tag{3.6}$$

equals Σ for all P_1, if and only if

$$\begin{aligned} \sigma_{11} &= \sigma_{22} = \ldots = \sigma_{n_1 n_1}, \\ \sigma_{12} &= \sigma_{23} = \ldots = \sigma_{n_1-1,n_1} = \sigma_{n_1,1}, \\ \sigma_{13} &= \sigma_{24} = \ldots = \sigma_{n_1-2,n_1} = \sigma_{n_1,2}, \\ &\vdots \end{aligned} \tag{3.7}$$

By using τ_k instead of σ_{ij}, where $|i-j|=k$ or $|i-j|=n_1-k$, we obtain

$$\begin{aligned}\Sigma &= \sum_{i=1}^{n_1}\tau_0 e_i e_i' + \sum_{k=1}^{[n_1/2]}\tau_k \sum_{\substack{i,j\\|i-j|=k,n_1-k}} e_i e_j' = \tau_0 I_{n_1} + \sum_{k=1}^{[n_1/2]}\tau_k \mathrm{SC}(n_1,k)\\ &= \sum_{k=0}^{[n_1/2]}\tau_k \mathrm{SC}(n_1,k) = \mathrm{Toep}(\tau_0,\tau_1,\tau_2,\ldots,\tau_1).\end{aligned}$$

□

For the second order interactions we have

Theorem 3.4 *The covariance matrix $\Sigma_2 : n\times n$ of $\gamma^{(2)}$ is shift permutation invariant if and only if*

$$\Sigma_2 = \sum_{k_2=0}^{[n_2/2]}\sum_{k_1=0}^{[n_1/2]}\tau_k \mathrm{SC}(n_2,k_2)\otimes \mathrm{SC}(n_1,k_1), \tag{3.8}$$

where $\gamma^{(2)}$ represents the interaction between a factor with n_1 levels and a factor with n_2 levels, $n=n_1n_2$, the matrices $\mathrm{SC}(i,j)$ are given by (2.2), and

$$k = ([\tfrac{n_1}{2}]+1)k_2 + k_1. \tag{3.9}$$

Proof. Observe, that we may write

$$\Sigma_2 = \sum_{r,s}\sigma_{rs}e_r e_s' = \sum_{i_2,j_2=1}^{n_2}\sum_{i_1,j_1=1}^{n_1}\sigma_{(i_2i_1)(j_2j_1)}(e_{2i_2}e_{2j_2}')\otimes(e_{1i_1}e_{1j_1}'), \tag{3.10}$$

where $e_r,\ e_s$ are the r-th and the s-th columns of the identity matrix I_n, respectively, e_{hi_h} is the i_h-th column of the identity matrix I_{n_h}, $h=1,2$, $\sigma_{(i_2i_1)(j_2j_1)} = Cov(\gamma^{(2)}_{i_2i_1},\gamma^{(2)}_{j_2j_1})$ is the element of Σ_2 in the r-th row and the s-th column,

$$r=(i_2-1)n_1+i_1, \qquad s=(j_2-1)n_1+j_1,$$

and

$$e_r = e_{2i_2}\otimes e_{1i_1}, \qquad e_s = e_{2j_2}\otimes e_{1j_1}.$$

We apply the proof of Theorem 3.3, i.e. inquiring the condition

$$P_2\Sigma_2P_2' = \Sigma_2,$$

for all P_2, where $P_2 = P^{(2)} \otimes P^{(1)}$ is the marginally shift permutation matrix defined in (3.3). It follows that

$$\Sigma_2 = \sum_{k_2=0}^{[n_2/2]} \sum_{i_1,j_1=1}^{n_1} \sigma_{(k_2 i_1)(k_2 j_1)} \mathrm{SC}(n_2, k_2) \otimes P^{(1)}(e_{1i_1} e'_{1j_1}) P^{(1)'}$$

which implies that the theorem is true. □

Now we can formulate the result in the case of s-order interactions which is one of the main results in this paper.

Theorem 3.5 *The covariance matrix $\Sigma_s : n \times n$ of $\gamma^{(s)}$ is shift permutation invariant if and only if*

$$\Sigma_s = \sum_{k_s=0}^{[n_s/2]} \cdots \sum_{k_1=0}^{[n_1/2]} \tau_k \mathrm{SC}(n_s, k_s) \otimes \cdots \otimes \mathrm{SC}(n_1, k_1), \tag{3.11}$$

where $\gamma^{(s)}$ represents the interaction between s factors, the matrices $\mathrm{SC}(n_i, k_i)$*, $i = 1, \ldots, s$, are given by* (2.2)*, τ_k are constants, and*

$$k = \sum_{h=2}^{s} \prod_{i=1}^{h-1} \left(\left[\tfrac{n_i}{2}\right] + 1\right) k_h + k_1. \tag{3.12}$$

Proof. We only prove (3.12) since (3.11) is a straightforward consequence of (3.12) and the proof of Theorem 3.3. From Theorem 3.3 and Theorem 3.4 it follows that (3.12) is true for $s = 1, 2$. Suppose that (3.12) holds for $s - 1$, i.e. holds for $\Sigma_{s-1} : N_{s-1} \times N_{s-1}$, where $N_{s-1} = n_1 \times \cdots \times n_{s-1}$. However, the $s-1$ factors can be viewed as one factor with an index defined via $k_1, \ldots, k_{s-1}$:

$$\sum_{h=2}^{s-1} \prod_{i=1}^{h-1} \left(\left[\tfrac{n_i}{2}\right] + 1\right) k_h + k_1. \tag{3.13}$$

Let the index of the s factor be given by k_s. Then, by using (3.9) in Theorem 3.4 for two factors

$$\begin{aligned} k &= \prod_{i=1}^{s-1} \left(\left[\tfrac{n_i}{2}\right] + 1\right) k_s + \left(\sum_{h=2}^{s-1} \prod_{i=1}^{h-1} \left(\left[\tfrac{n_i}{2}\right] + 1\right) k_h + k_1 \right) \\ &= \sum_{h=2}^{s} \prod_{i=1}^{h-1} \left(\left[\tfrac{n_i}{2}\right] + 1\right) k_h + k_1, \end{aligned} \tag{3.14}$$

and thus (3.12) has been proved. □

4 Reparameterization of factors and shift permutation invariance

One can usually put an infinite number of constraints on factor levels. However under invariance there exist only some few possibilities. This will be studied in detail in this chapter. Moreover, it is worth observing that under permutation invariance there is only one reparameterization constraint, i.e. the sum-to-zero condition, whereas shift permutation invariance will give additional reparameterization possibilities.

We are going to examine the covariance matrices of order $n = 4, 5, 6, 7, 8$, satisfying dihedral block symmetry Perlman (1987). In particular we study the interpretation of τ_k in (3.11) and reparameterizations. The results are important because they guide us how to design interpretable experiments. There is a significant difference in the interpretation of the designs (with reparameterization) for various n, i.e. the number of factor levels. For example one should think about if n is odd or even, if $nk = 360$, or if $n = 2^k$, for some k. Therefore we present a detailed treatment of $n = 4, 5, 6, 7, 8$.

When $n = 4$

$$\begin{aligned}\Sigma &= \left(\begin{array}{cc|cc} \tau_0 & \tau_1 & \tau_2 & \tau_1 \\ \tau_1 & \tau_0 & \tau_1 & \tau_2 \\ \hline \tau_2 & \tau_1 & \tau_0 & \tau_1 \\ \tau_1 & \tau_2 & \tau_1 & \tau_0 \end{array}\right) = I_2 \otimes A + (J_2 - I_2) \otimes B \\ &= I_2 \otimes (\tau_0 I_2 + \tau_1(J_2 - I_2)) + (J_2 - I_2) \otimes (\tau_2 I_2 + \tau_1(J_2 - I_2)), \quad (4.1)\end{aligned}$$

where

$$cov(\xi_i, \xi_j) = \begin{cases} \tau_0, & i = j, \\ \tau_1, & |i - j| \in \{1, 3\}, \\ \tau_2, & |i - j| = 2, \end{cases} \quad (4.2)$$

and $i, j = 1, \ldots, 4$.

When $n = 5$

$$\Sigma = \begin{pmatrix} \tau_0 & \tau_1 & \tau_2 & \tau_2 & \tau_1 \\ \tau_1 & \tau_0 & \tau_1 & \tau_2 & \tau_2 \\ \tau_2 & \tau_1 & \tau_0 & \tau_1 & \tau_2 \\ \tau_2 & \tau_2 & \tau_1 & \tau_0 & \tau_1 \\ \tau_1 & \tau_2 & \tau_2 & \tau_1 & \tau_0 \end{pmatrix}, \quad (4.3)$$

where for $i, j = 1, \ldots, 5$,

$$cov(\xi_i, \xi_j) = \begin{cases} \tau_0, & i = j, \\ \tau_1, & |i-j| \in \{1, 4\}, \\ \tau_2, & |i-j| \in \{2, 3\}. \end{cases} \tag{4.4}$$

Comparing $n = 4$ and $n = 5$ it appears that it is much easier to discover the underlying symmetry in (4.1) compared to (4.3). Moreover, for $n = 6$, $n = 7$ and $n = 8$ we respectively have:

$$\Sigma = \left(\begin{array}{ccc|ccc} \tau_0 & \tau_1 & \tau_2 & \tau_3 & \tau_2 & \tau_1 \\ \tau_1 & \tau_0 & \tau_1 & \tau_2 & \tau_3 & \tau_2 \\ \tau_2 & \tau_1 & \tau_0 & \tau_1 & \tau_2 & \tau_3 \\ \hline \tau_3 & \tau_2 & \tau_1 & \tau_0 & \tau_1 & \tau_2 \\ \tau_2 & \tau_3 & \tau_2 & \tau_1 & \tau_0 & \tau_1 \\ \tau_1 & \tau_2 & \tau_3 & \tau_2 & \tau_1 & \tau_0 \end{array}\right), \tag{4.5}$$

and for $i, j = 1, \ldots, 6$,

$$cov(\xi_i, \xi_j) = \begin{cases} \tau_0, & i = j, \\ \tau_1, & |i-j| \in \{1, 5\}, \\ \tau_2, & |i-j| \in \{2, 4\}, \\ \tau_3, & |i-j| = 3; \end{cases}$$

if $n = 7$

$$\Sigma = \begin{pmatrix} \tau_0 & \tau_1 & \tau_2 & \tau_3 & \tau_3 & \tau_2 & \tau_1 \\ \tau_1 & \tau_0 & \tau_1 & \tau_2 & \tau_3 & \tau_3 & \tau_2 \\ \tau_2 & \tau_1 & \tau_0 & \tau_1 & \tau_2 & \tau_3 & \tau_3 \\ \tau_3 & \tau_2 & \tau_1 & \tau_0 & \tau_1 & \tau_2 & \tau_3 \\ \tau_3 & \tau_3 & \tau_2 & \tau_1 & \tau_0 & \tau_1 & \tau_2 \\ \tau_2 & \tau_3 & \tau_3 & \tau_2 & \tau_1 & \tau_0 & \tau_1 \\ \tau_1 & \tau_2 & \tau_3 & \tau_3 & \tau_2 & \tau_1 & \tau_0 \end{pmatrix}, \tag{4.6}$$

with elements

$$cov(\xi_i, \xi_j) = \begin{cases} \tau_0, & i = j, \\ \tau_1, & |i-j| \in \{1, 6\}, \\ \tau_2, & |i-j| \in \{2, 5\}, \\ \tau_3, & |i-j| \in \{3, 4\}, \end{cases}$$

where $i, j = 1, \ldots, 7$; and finally for $n = 8$ we once again have a fairly symmetric structure

$$\Sigma = \left(\begin{array}{cc|cc|cc|cc} \tau_0 & \tau_1 & \tau_2 & \tau_3 & \tau_4 & \tau_3 & \tau_2 & \tau_1 \\ \tau_1 & \tau_0 & \tau_1 & \tau_2 & \tau_3 & \tau_4 & \tau_3 & \tau_2 \\ \hline \tau_2 & \tau_1 & \tau_0 & \tau_1 & \tau_2 & \tau_3 & \tau_4 & \tau_3 \\ \tau_3 & \tau_2 & \tau_1 & \tau_0 & \tau_1 & \tau_2 & \tau_3 & \tau_4 \\ \hline \tau_4 & \tau_3 & \tau_2 & \tau_1 & \tau_0 & \tau_1 & \tau_2 & \tau_3 \\ \tau_3 & \tau_4 & \tau_3 & \tau_2 & \tau_1 & \tau_0 & \tau_1 & \tau_2 \\ \hline \tau_2 & \tau_3 & \tau_4 & \tau_3 & \tau_2 & \tau_1 & \tau_0 & \tau_1 \\ \tau_1 & \tau_2 & \tau_3 & \tau_4 & \tau_3 & \tau_2 & \tau_1 & \tau_0 \end{array}\right), \tag{4.7}$$

with elements $(i, j = 1, \ldots, 8)$

$$cov(\xi_i, \xi_j) = \begin{cases} \tau_0, & i = j, \\ \tau_1, & |i-j| \in \{1, 7\}, \\ \tau_2, & |i-j| \in \{2, 6\}, \\ \tau_3, & |i-j| \in \{3, 5\}, \\ \tau_4, & |i-j| = 4. \end{cases}$$

In the rest of this section we shall put different constraints on the spectrum of the shift permutation invariant covariance matrix and study in detail specific circular covariance structures and implications of reparameterization constraints. The results are based on Lemma 2.1.

<u>The case $n = 4$:</u>

The spectrum of $\Sigma : 4 \times 4$ of the factor ξ is the following:

$$\begin{aligned} \lambda_1 = \lambda_3 &= \tau_0 - \tau_2, \\ \lambda_2 &= \tau_0 - 2\tau_1 + \tau_2, \\ \lambda_4 &= \tau_0 + 2\tau_1 + \tau_2. \end{aligned} \tag{4.8}$$

Using the linear relationships among eigenvalues $\lambda_1, \lambda_2, \lambda_3$ and parameters τ_0, τ_1, τ_2 gives

$$\begin{aligned} \tau_0 &= \tfrac{1}{4}(2\lambda_1 + \lambda_2 + \lambda_4), \\ \tau_1 &= \tfrac{1}{4}(-\lambda_2 + \lambda_4), \\ \tau_2 &= \tfrac{1}{4}(-2\lambda_1 + \lambda_2 + \lambda_4), \end{aligned}$$

and we can express Σ given by (4.1) in the following way:

$$\begin{aligned}\Sigma &= \tfrac{1}{4}I_2 \otimes [(2\lambda_1+\lambda_2+\lambda_4)I_2 + (J_2-I_2)(-\lambda_2+\lambda_4)] \\ &+ \tfrac{1}{4}(J_2-I_2)\otimes[(-2\lambda_1+\lambda_2+\lambda_4)I_2+(J_2-I_2)(-\lambda_2+\lambda_4)].\end{aligned}$$

We also assume the natural condition $\xi_i \neq \xi_j$ for all $i \neq j,\ i,j = 1,\ldots,4$, in ξ because if two levels are equal it does not make sense to model both. Therefore this situation will not be considered.

Let us look at how the structure of Σ will change if it is singular, i.e. exists at least one $\lambda_i = 0,\ i = 1,\ldots,4$. To model data with singular covariance matrices we refer to Rao (1973) in the general Gauss-Markov setup and to Srivastava and von Rosen (2002) with an unknown Σ. In the present paper we study the problem from a design of experiment point of view.

(i) $\lambda_4 = 0$: In this case

$$\begin{aligned}\lambda_1 &= -2(\tau_1+\tau_2)\\ \lambda_2 &= -4\tau_1,\\ \tau_0 &= -2\tau_1-\tau_2, \quad \text{and } \tau_1<0, \tau_2<-\tau_1.\end{aligned}$$

Hence,

$$\begin{aligned}\Sigma &= \begin{pmatrix} -2\tau_1-\tau_2 & \tau_1 & \tau_2 & \tau_1\\ \tau_1 & -2\tau_1-\tau_2 & \tau_1 & \tau_2\\ \tau_2 & \tau_1 & -2\tau_1-\tau_2 & \tau_1\\ \tau_1 & \tau_2 & \tau_1 & -2\tau_1-\tau_2\end{pmatrix}\\ &= I_2\otimes(-(2\tau_1+\tau_2)I_2+\tau_1(J_2-I_2))+(J_2-I_2)\otimes(\tau_2 I_2+\tau_1(J_2-I_2))\\ &= \tfrac{1}{4}I_2\otimes[(2\lambda_1+\lambda_2)I_2-(J_2-I_2)\lambda_2]\\ &\qquad\qquad + \tfrac{1}{4}(J_2-I_2)\otimes[(-2\lambda_1+\lambda_2)I_2-(J_2-I_2)\lambda_2].\end{aligned}$$

The corresponding eigenvector of $\lambda_4 = 0$ is $v_4 = (1,1,1,1)' = \mathbf{1_4}$. Since

$$E(v_4'\xi) = 0,\ D(v_4'\xi) = 0,$$

we have $\mathbf{1}_4'\xi = 0$ a.s. which is a “sum-to-zero” reparameterization constraint. Hence we clearly see what model should be assumed under the assumption of shift invariance together with the commonly applied standardization condition $\mathbf{1}_4'\xi = 0$. This type of knowledge is usually not implemented in the data analysis which then will lead to an inefficient and sometimes erroneous analysis. For example, to have a wrong covariance model will lead to that confidence intervals will not be correctly constructed.

(ii) $\lambda_2 = 0$: In this case,

$$\begin{aligned} \lambda_1 &= 2(\tau_0 - \tau_1), \\ \lambda_4 &= 4\tau_1, \\ \tau_2 &= 2\tau_1 - \tau_0, \ \tau_0 > \tau_1 > 0. \end{aligned}$$

The corresponding covariance matrix equals

$$\begin{aligned} \Sigma &= \begin{pmatrix} \tau_0 & \tau_1 & 2\tau_1 - \tau_0 & \tau_1 \\ \tau_1 & \tau_0 & \tau_1 & 2\tau_1 - \tau_0 \\ 2\tau_1 - \tau_0 & \tau_1 & \tau_0 & \tau_1 \\ \tau_1 & 2\tau_1 - \tau_0 & \tau_1 & \tau_0 \end{pmatrix} \\ &= I_2 \otimes (\tau_0 I_2 + \tau_1(J_2 - I_2)) + (J_2 - I_2) \otimes ((2\tau_1 - \tau_0)I_2 + \tau_1(J_2 - I_2)) \\ &= \tfrac{1}{4} I_2 \otimes [(2\lambda_1 + \lambda_4)I_2 + (J_2 - I_2)\lambda_4] \\ &\qquad + \tfrac{1}{4}(J_2 - I_2) \otimes [(-2\lambda_1 + \lambda_4)I_2 + (J_2 - I_2)\lambda_4]. \end{aligned}$$

The eigenvector corresponding to $\lambda_2 = 0$ is $v_2 = (1, -1, 1, -1)'$. In this case, since $E(v_2'\xi) = 0$, $D(v_2'\xi) = 0$ we have $\xi_1 - \xi_2 + \xi_3 - \xi_4 = 0$ a.s. which also is a natural reparameterization constraint in many data sets.

(iii) The assumption $\xi_i \neq \xi_j, \ i \neq j$ a.s. makes it impossible that $\lambda_1 = 0$ or $\lambda_3 = 0$ holds.

(iv) $\lambda_4 = \lambda_2 = 0$: In this case, $\lambda_1 = 2\tau_0$ and $\Sigma = 2\tau_0(I_2 - \frac{1}{2}J_2) \otimes I_2$.

The eigenvectors corresponding to $\lambda_4 = \lambda_2 = 0$ are $v_4 = (1, 1, 1, 1)'$ and $v_2 = (1, -1, 1, -1)'$. Taking into account that $E(v_4'\xi) = E(v_2'\xi) = 0$ and $D(v_4'\xi) = D(v_2'\xi) = 0$ we get $\xi_1 = -\xi_3$ and $\xi_2 = -\xi_4$ a.s. which is a new and natural type of reparameterization constraint. However, if ξ has a symmetric distribution this case is excluded.

<u>THE CASE $n = 5$:</u>

The spectrum of $\Sigma : 5 \times 5$ is the following:

$$\begin{aligned} \lambda_1 = \lambda_4 &= \tau_0 + \tfrac{1}{2}(\sqrt{5} - 1)\tau_1 - \tfrac{1}{2}(\sqrt{5} + 1)\tau_2, \\ \lambda_2 = \lambda_3 &= \tau_0 - \tfrac{1}{2}(\sqrt{5} + 1)\tau_1 + \tfrac{1}{2}(\sqrt{5} - 1)\tau_2, \\ \lambda_5 &= \tau_0 + 2\tau_1 + 2\tau_2. \end{aligned}$$

The corresponding eigenvectors are

$$
\begin{aligned}
v_1 &= (-1, \tfrac{1}{2}(1-\sqrt{5}), -\tfrac{1}{2}(1-\sqrt{5}), 1, 0)', \\
v_2 &= (-1, \tfrac{1}{2}(\sqrt{5}+1), -\tfrac{1}{2}(\sqrt{5}+1), 1, 0)', \\
v_3 &= (-\tfrac{1}{2}(\sqrt{5}+1), \tfrac{1}{2}(\sqrt{5}+1), -1, 0, 1)', \\
v_4 &= (-\tfrac{1}{2}(1-\sqrt{5}), \tfrac{1}{2}(1-\sqrt{5}), -1, 0, 1)', \\
v_5 &= (1, 1, 1, 1, 1)'.
\end{aligned}
$$

The relationships between the eigenvalues $\lambda_1, \lambda_2, \lambda_3, \lambda_4$ and parameters τ_0, τ_1, τ_2 equal

$$
\begin{aligned}
\tau_0 &= \tfrac{1}{5}(2\lambda_1 + 2\lambda_2 + \lambda_5), \\
\tau_1 &= -\tfrac{\sqrt{5}}{50}(\sqrt{5}-5)\lambda_1 - \tfrac{\sqrt{5}}{50}(\sqrt{5}+5)\lambda_2 + \tfrac{1}{5}\lambda_5, \\
\tau_2 &= -\tfrac{\sqrt{5}}{50}(\sqrt{5}+5)\lambda_1 - \tfrac{\sqrt{5}}{50}(\sqrt{5}-5)\lambda_2 + \tfrac{1}{5}\lambda_5.
\end{aligned}
$$

In a similar manner to the case $n = 4$ we shall study the change of structure when $\Sigma : 5\times5$ becomes singular due to putting eigenvalues equal to zero. Then we find out what kind of different constraints are induced by this procedure.

However, we shall in some detail only consider the case when the singularity of Σ is caused by setting $\lambda_5 = 0$. In this case, $\tau_0 = -2(\tau_1 + \tau_2)$, and

$$
\begin{aligned}
\lambda_1 &= \tfrac{1}{2}(\sqrt{5}-5)\tau_1 - \tfrac{1}{2}(\sqrt{5}+5)\tau_2, \\
\lambda_2 &= -\tfrac{1}{2}(\sqrt{5}+5)\tau_1 + \tfrac{1}{2}(\sqrt{5}-5)\tau_2, \\
\tau_1 &< -(3+\sqrt{5})\tau_2/2.
\end{aligned}
$$

The covariance matrix Σ has in this case the following structure which unfortunately cannot be simplified more.

$$
\Sigma : 5\times5 = \begin{pmatrix}
-2(\tau_1+\tau_2) & \tau_1 & \tau_2 & \tau_2 & \tau_1 \\
\tau_1 & -2(\tau_1+\tau_2) & \tau_1 & \tau_2 & \tau_2 \\
\tau_2 & \tau_1 & -2(\tau_1+\tau_2) & \tau_1 & \tau_2 \\
\tau_2 & \tau_2 & \tau_1 & -2(\tau_1+\tau_2) & \tau_1 \\
\tau_1 & \tau_2 & \tau_2 & \tau_1 & -2(\tau_1+\tau_2)
\end{pmatrix}.
$$

The eigenvector corresponding to $\lambda_5 = 0$ is $v_5 = (1,1,1,1,1)'$. Since $E(v_5'\xi) = 0$ and $D(v_5'\xi) = 0$ we get a "sum-to-zero" reparameterization constraint, i.e. $\mathbf{1}_5'\xi = 0$ a.s.

Other types of constraints which are possible are $\lambda_2 = \lambda_3 = 0$, $\lambda_1 = \lambda_4 = 0$, $\lambda_1 = \lambda_4 = \lambda_5 = 0$, $\lambda_2 = \lambda_4 = \lambda_5 = 0$. The effects of these are shown in Appendix 1.

THE CASE $n = 6$:

The spectrum of $\Sigma : 6 \times 6$ is given by

$$\begin{aligned}
\lambda_1 = \lambda_5 &= \tau_0 + \tau_1 - \tau_2 - \tau_3, \\
\lambda_2 = \lambda_4 &= \tau_0 - \tau_1 - \tau_2 + \tau_3, \\
\lambda_3 &= \tau_0 - 2\tau_1 + 2\tau_2 - \tau_3, \\
\lambda_6 &= \tau_0 + 2\tau_1 + 2\tau_2 + \tau_3.
\end{aligned}$$

The eigenvectors of the corresponding eigenvalues equal:

$$\begin{aligned}
v_1 &= (\tfrac{1}{2}(1+\sqrt{3}), -\tfrac{1}{2}(1-\sqrt{3}), -1, -\tfrac{1}{2}(1+\sqrt{3}), \tfrac{1}{2}(1-\sqrt{3}), 1)' \\
v_2 &= (-\tfrac{1}{2}(1-\sqrt{3}), -\tfrac{1}{2}(1+\sqrt{3}), 1, -\tfrac{1}{2}(1-\sqrt{3}), -\tfrac{1}{2}(1+\sqrt{3}), 1)', \\
v_3 &= (-1, 1, -1, 1, -1, 1)', \\
v_4 &= (-\tfrac{1}{2}(1+\sqrt{3}), -\tfrac{1}{2}(1-\sqrt{3}), 1, -\tfrac{1}{2}(1+\sqrt{3}), -\tfrac{1}{2}(1-\sqrt{3}), 1)', \\
v_5 &= (\tfrac{1}{2}(1-\sqrt{3}), -\tfrac{1}{2}(1+\sqrt{3}), -1, -\tfrac{1}{2}(1-\sqrt{3}), \tfrac{1}{2}(1+\sqrt{3}), 1)', \\
v_6 &= (1, 1, 1, 1, 1, 1)'.
\end{aligned}$$

We can use the following relationships among τs and λs:

$$\begin{aligned}
\tau_0 &= \tfrac{1}{6}(2\lambda_1 + \lambda_2 + 2\lambda_3 + \lambda_6), \\
\tau_1 &= \tfrac{1}{6}(\lambda_1 - \lambda_2 - \lambda_3 + \lambda_6), \\
\tau_2 &= \tfrac{1}{6}(-\lambda_1 - \lambda_2 + \lambda_3 + \lambda_6), \\
\tau_3 &= \tfrac{1}{6}(-2\lambda_1 + 2\lambda_2 - \lambda_3 + \lambda_6),
\end{aligned}$$

to represent Σ via its spectrum.

The case $\lambda_3 = 0$. Then it follows from v_3 that $\xi_1 + \xi_3 + \xi_5 = \xi_2 + \xi_4 + \xi_6$.

The case $\lambda_6 = 0$. From v_6 it follows that we immediately can state that the sum to zero condition holds: $\xi_1 + \xi_2 + \xi_3 + \xi_4 + \xi_5 + \xi_6 = 0$. Other cases are presented in Appendix 2.

THE CASE $n = 7$:

For the case $n = 7$ we can just refer to Lemma 2.1 in order to find the eigenvalues and eigenvectors. However, it is difficult to present interpretable details. One reason for this is that the designs we are studying are connected to circularity. Since, for example 360/7 is not an integer we run into problems with the interpretations. The same also applies when putting eigenvalues to 0 and if we then want to see what kind of conditions are imposed on the factor levels.

<u>THE CASE $n = 8$:</u>

The spectrum of $\Sigma : 8 \times 8$ is the following:

$$\begin{aligned}
\lambda_1 = \lambda_7 &= \tau_0 + \sqrt{2}\tau_1 - \sqrt{2}\tau_3 - \tau_4, \\
\lambda_2 = \lambda_6 &= \tau_0 - 2\tau_2 + \tau_4, \\
\lambda_3 = \lambda_5 &= \tau_0 - \sqrt{2}\tau_1 + \sqrt{2}\tau_3 - \tau_4, \qquad (4.9) \\
\lambda_4 &= \tau_0 - 2\tau_1 + 2\tau_2 - 2\tau_3 + \tau_4, \\
\lambda_8 &= \tau_0 + 2\tau_1 + 2\tau_2 + 2\tau_3 + \tau_4.
\end{aligned}$$

The columns of the matrix

$$V = \begin{pmatrix}
\sqrt{2} & 1 & 0 & -1 & -\sqrt{2} & -1 & 0 & 1 \\
1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\
0 & -1 & \sqrt{2} & -1 & 0 & 1 & -\sqrt{2} & 1 \\
-1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\
-\sqrt{2} & 1 & 0 & -1 & \sqrt{2} & -1 & 0 & 1 \\
-1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\
0 & -1 & -\sqrt{2} & -1 & 0 & 1 & \sqrt{2} & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1
\end{pmatrix}$$

are the eigenvectors corresponding to the eigenvalues $\lambda_1, \ldots, \lambda_8$. We can express $\Sigma : 8 \times 8$ via its spectrum using the relationships among eigenvalues $\lambda_1, \ldots, \lambda_8$ in (4.9) and parameters $\tau_0, \ldots, \tau_4$

$$\begin{aligned}
\tau_0 &= \tfrac{1}{8}(2\lambda_1 + 2\lambda_2 + 2\lambda_3 + \lambda_4 + \lambda_8), \\
\tau_1 &= \tfrac{1}{8}(\sqrt{2}\lambda_1 - \sqrt{2}\lambda_3 - \lambda_4 + \lambda_8), \\
\tau_2 &= \tfrac{1}{8}(-2\lambda_2 + \lambda_4 + \lambda_8), \\
\tau_3 &= \tfrac{1}{8}(-\sqrt{2}\lambda_1 + \sqrt{2}\lambda_3 - \lambda_4 + \lambda_8, \\
\tau_4 &= \tfrac{1}{8}(-2\lambda_1 + 2\lambda_2 - 2\lambda_3 + \lambda_4 + \lambda_8).
\end{aligned}$$

Let us study how the structure of Σ will change in the case it is singular, i.e. exists at least one $\lambda_i = 0$, $i = 1, \ldots, 8$, and what kind of dependencies arise among factor levels, i.e. how the corresponding factor is reparameterized.

In the case $\lambda_8 = 0$,

$$\begin{aligned}
\lambda_1 &= (\sqrt{2}-2)\tau_1 - 2\tau_2 - (\sqrt{2}+2)\tau_3 - 2\tau_4, \\
\lambda_2 &= -2\tau_1 - 4\tau_2 - 2\tau_3, \\
\lambda_3 &= -(\sqrt{2}+2)\tau_1 - 2\tau_2 + (\sqrt{2}-2)\tau_3 - 2\tau_4, \\
\lambda_4 &= -4\tau_1 - 4\tau_3.
\end{aligned}$$

The eigenvector corresponding to λ_8 is a vector with all elements equal to one, i.e. $v_8 = \mathbf{1}_8'$. Since $E(\mathbf{1}_8'\xi) = 0$ and $D(\mathbf{1}_8'\xi) = 0$ we get "sum-to-zero" reparameterization constraint, i.e. $\mathbf{1}_8'\xi = 0$ a.s.

We can see that the "sum-to-zero" constraints on factor levels are only connected to the last eigenvalue of the covariance matrix λ_n which equals to the sum of row (or column) elements of this matrix. Other types of constraints can be found in Appendix 3.

In the case when two or three eigenvalues are zeros, one gets more restrictions on the components of a random factor, i.e. not just the sum over factor levels equals zero but some linear combination of them. Consider, for example, the case when $\lambda_4 = \lambda_8 = 0$. In this case the singularity of the covariance matrix means that $\xi_2 + \xi_4 + \xi_6 + \xi_8 = 0$ and $\xi_1 + \xi_3 + \xi_5 + \xi_7 = 0$.

5 Interactions

Suppose now that in our model besides main effects there are also second order interactions

$$\begin{aligned}
Y &= (\mathbf{1}_{n_1} \otimes \mathbf{1}_{n_2} \otimes \mathbf{1}_n)\mu + (I_{n_1} \otimes \mathbf{1}_{n_2} \otimes \mathbf{1}_n)\xi^1 \\
&\quad + (\mathbf{1}_{n_1} \otimes I_{n_2} \otimes \mathbf{1}_n)\xi^2 + (I_{n_1} \otimes I_{n_2} \otimes \mathbf{1}_n)\gamma^{(2)} \\
&\quad + (I_{n_1} \otimes I_{n_2} \otimes I_n)\varepsilon, \qquad (5.1)
\end{aligned}$$

where $\gamma^{(2)}$ represent second order interaction effects between factors ξ^1 with n_1 levels and factor ξ^2 with n_2 levels, ε is a random error.

Let Σ_2 denote the covariance matrix of $\gamma^{(2)}$. Due to marginal shift permutation invariance Σ_2 has a specific structure which can be described by a block Toeplitz matrix:

$$\Sigma_2 = \begin{pmatrix}
A_0 & A_1 & A_2 & \dots & A_2 & A_1 \\
A_1 & A_0 & A_1 & \dots & A_3 & A_2 \\
A_2 & A_1 & A_0 & \dots & A_4 & A_3 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
A_2 & A_3 & A_4 & \dots & A_0 & A_1 \\
A_1 & A_2 & A_3 & \dots & A_1 & A_0
\end{pmatrix}. \qquad (5.2)$$

Here every matrix A_i is a symmetric circular Toeplitz matrix with $[n_2/2]+1$ parameters, $i=0,\ldots,[n_1/2]$. Hence, the matrix Σ_2 is defined by $([n_1/2]+1)([n_2/2]+1)$ parameters.

Notice that Σ_2 can be written as a Kronecker product of two matrices

$$\Sigma_2 \quad = \quad \Sigma^{(1)} \otimes \Sigma^{(2)}, \tag{5.3}$$

where both $\Sigma^{(1)}$ and $\Sigma^{(2)}$ are symmetric circular Toeplitz matrices, as defined in (2.1), i.e. $\Sigma^{(1)} = \mathrm{Toep}(t_0, t_1, t_2, \ldots, t_1)$ and $\Sigma^{(2)} = \mathrm{Toep}(s_0, s_1, s_2, \ldots, s_1)$.

Let $\lambda_1^{(k)}, \ldots, \lambda_{[n_k/2]+1}^{(k)}$ be the distinct eigenvalues of $\Sigma^{(k)}$ with multiplicities $m_1, \ldots, m_{[n_k/2]+1}$, respectively, $k=1,2$. Because of the Kronecker product structure the distinct eigenvalues of Σ_2 are $\lambda_i^{(1)}\lambda_j^{(2)}$ of multiplicity $m_i m_j$, $i=1,\ldots,[n_1/2]+1$ and $j=1,\ldots,[n_2/2]+1$.

If we look at the presentation of Σ_2 in (5.2) and (5.3), it follows from Theorem 3.4 that the blocks in (5.2) are the following

$$A_i \quad = \quad t_i \Sigma_2 = \mathrm{Toep}(\tau_{i_0}, \tau_{i_1}, \tau_{i_2}, \ldots, \tau_{i_2}, \tau_{i_1}),$$

where

$$i_k = i([\tfrac{n_2}{2}]+1)+k, \qquad i=0,\ldots,[\tfrac{n_1}{2}], \quad k=0,\ldots,[\tfrac{n_2}{2}].$$

For example, $A_0 = t_0\Sigma_2 = \mathrm{Toep}(\tau_0, \tau_1, \tau_2, \ldots, \tau_2, \tau_1)$.

Now one can find the eigenvalues of Σ_2 directly using the expression for the eigenvalues of a symmetric circular Toeplitz matrix, given in Lemma 2.1.

Theorem 5.1 *Let $\omega_i^{(k)}$, $i=1,\ldots,[n_2/2]+1$, $k=0,\ldots,[n_1/2]$, be the distinct eigenvalues of block A_k in (5.2) of multiplicities m_i, respectively. Then the eigenvalues of Σ_2 in (5.2) are the following:*

If n_1 is odd,

$$\lambda_{h,i} = \omega_i^{(0)} + 2\sum_{j=1}^{[\frac{n_1}{2}]} \omega_i^{(j)} \cos(2\pi hj/n_1), \quad h=1,\ldots,n_1.$$

The multiplicity of $\lambda_{n_1,i}$ is m_i and all other eigenvalues are of multiplicity $2m_i$.

If n_1 is even,

$$\lambda_{h,i} = \omega_i^{(0)} + 2\sum_{j=1}^{\frac{n_1}{2}-1} \omega_i^{(j)} \cos(2\pi hj/n_1) + \omega_i^{(\frac{n_1}{2})} \cos(\pi h), \quad h=1,\ldots,n_1.$$

Only the eigenvalues $\lambda_{n_1,i}$ and $\lambda_{n_1/2,i}$ are of multiplicity m_i and all others eigenvalues are of multiplicity $2m_i$.

Proof. Notice first that Σ_2 in (5.2) can be written as

$$\Sigma_2 = \sum_{k_1=0}^{[\frac{n_1}{2}]} \mathrm{SC}(n_1, k_1) \otimes A_{k_1},$$

where

$$\begin{aligned} A_{k_1} &= \sum_{k_2=0}^{[\frac{n_2}{2}]} \tau_k \mathrm{SC}(n_2, k_2), \\ k &= k_1([\tfrac{n_2}{2}] + 1) + k_2. \end{aligned}$$

Since $\mathrm{SC}(n_i, k_i)$ are symmetric circular matrices, $k_i = 0, \ldots, [n_i/2]$, we know that they commute. Thus, there exists an orthogonal matrix V_i, $i = 1, 2$, such that

$$V_i' \mathrm{SC}(n_i, k_i) V_i = \Lambda_{k_i},$$

where Λ_{k_i} is a diagonal matrix where the diagonal elements are the eigenvalues of $\mathrm{SC}(n_i, k_i)$ given via Lemma 2.1. Let $V = V_1 \otimes V_2$. Then

$$V' \Sigma_2 V = \sum_{k_1=0}^{[\frac{n_1}{2}]} \Lambda_{k_1} \otimes \Lambda_{A,k_1},$$

where Λ_{A,k_1} is a diagonal matrix with diagonal elements equal to the eigenvalues of A_{k_1}, given in Lemma 2.1. Thus, the proof is complete. □

It is of interest to formulate the result in the case of s-order interactions and to present the eigenvalues of Σ_s in a recursive form. The next theorem presents Σ_s in a recursive way.

Theorem 5.2 *Let Σ_s be as in Theorem 3.5. Then*

$$\Sigma_s = \sum_{k_s=0}^{[n_s/2]} \mathrm{SC}(n_s, k_s) \otimes \Sigma_{s-1}^{(k_s)}, \tag{5.4}$$

where

$$\begin{aligned}
\Sigma_0^{(k)} &= \tau_k, &(5.5)\\
k &= 0,\ldots,N_{(s)}-1,\ N_{(s)}=\prod_{i=1}^{s}([\tfrac{n_i}{2}]+1),\\
\Sigma_h^{(k_{h+1}^*)} &= \sum_{k_h=0}^{[n_h/2]} \mathrm{SC}(n_h,k_h)\otimes\Sigma_{h-1}^{(k_{h+1}^*([\frac{n_h}{2}]+1)+k_h)}, &(5.6)\\
k_{h+1}^* &= 0,\ldots,N_{(s\backslash h)}-1,\ h=1,\ldots,s-1,\\
N_{(s\backslash h)} &= \prod_{i=h+1}^{s}([\tfrac{n_i}{2}]+1).
\end{aligned}$$

Proof. The proof is an immediate consequence of Theorem 3.5 if we observe that k in (3.12) can be obtained recursively via $k_{h+1}^*([n_h/2]+1)+k_h$:

$$\begin{aligned}
k &= \sum_{h=2}^{s}\prod_{i=1}^{h-1}\big([\tfrac{n_i}{2}]+1\big)\,k_h+k_1=\underbrace{(\sum_{h=3}^{s}\prod_{i=1}^{h-1}\big([\tfrac{n_i}{2}]+1\big)\,k_h+k_2)}_{k_2^*}([\tfrac{n_1}{2}]+1)+k_1\\
&= [\underbrace{[\sum_{h=4}^{s}\prod_{i=1}^{h-1}\big([\tfrac{n_i}{2}]+1\big)\,k_h+k_3]}_{k_3^*}([\tfrac{n_2}{2}]+1)+k_2]([\tfrac{n_1}{2}]+1)+k_1\\
&\ \vdots\\
&= [\cdots[\underbrace{[\prod_{i=1}^{s-1}\big([\tfrac{n_i}{2}]+1\big)\,k_s+k_{s-1}]}_{k_{s-1}^*}([\tfrac{n_{s-2}}{2}]+1)+k_{s-2}]\times\cdots\\
&\qquad\cdots+k_2]([\tfrac{n_1}{2}]+1)+k_1.
\end{aligned}$$

Thus,

$$\begin{aligned}
\Sigma_s &= \sum_{k_s=0}^{[n_s/2]}\cdots\sum_{k_2=0}^{[n_2/2]}\mathrm{SC}(n_s,k_s)\otimes\cdots\otimes\mathrm{SC}(n_2,k_2)\otimes\sum_{k_1=0}^{[n_1/2]}\mathrm{SC}(n_1,k_1)\Sigma_0^{k_2^*([\frac{n_1}{2}]+1)+k_1}\\
&= \sum_{k_s=0}^{[n_s/2]}\cdots\sum_{k_3=0}^{[n_3/2]}\mathrm{SC}(n_s,k_s)\otimes\cdots\otimes\mathrm{SC}(n_3,k_3)\otimes\sum_{k_2=0}^{[n_2/2]}\mathrm{SC}(n_2,k_2)\Sigma_1^{k_3^*([\frac{n_2}{2}]+1)+k_2}
\end{aligned}$$

If we continue applying (5.6) in a similar way, we get (5.4). □

From Lemma 2.1 it follows that the eigenvalues for SC(n,l) are given by

$$\lambda_k = \begin{cases} 2\cos(2\pi kl/n), & \text{if } l \leq [\frac{n}{2}], \quad n \text{ odd}, \\ 2\cos(2\pi kl/n), & \text{if } l \leq \frac{n}{2}-1, \quad n \text{ even}, \\ \cos(\pi k), & \text{if } l = \frac{n}{2}, \quad n \text{ even}, \end{cases}$$

and $k = 1, 2, \ldots, n$. Since SC(n_s, k_s), $k_s = 0, \ldots, [n_s/2]$ commute, it follows that all terms in the sum (3.11) commute. Thus, they have a common eigenspace. Let $\Lambda(n,l)$ denote the diagonal matrix of eigenvalues of SC(n,l). The next theorem is based on Theorem 3.5.

Theorem 5.3 *The diagonal matrix Λ_s of the eigenvalues to Σ_s in Theorem 3.5 is given by*

$$\Lambda_s = \sum_{k_s=0}^{[n_s/2]} \cdots \sum_{k_1=0}^{[n_1/2]} \tau_k \Lambda(n_s, k_s) \otimes \cdots \otimes \Lambda(n_1, k_1),$$

where k is given in (3.12).

From here one can in principle study multiplicities of eigenvalues. However, one has to take into account if n_i is odd or even and therefore no general formula will be presented. Alternatively using Theorem (5.4) we can state

$$\Lambda_s = \sum_{k_s=0}^{[n_s/2]} \Lambda(n_s, k_s) \otimes \Lambda_{s-1}^{(k_s)},$$

where

$$\begin{aligned}
\Lambda_0^{(k)} &= \tau_k, \\
k &= 0, \ldots, N_{(s)} - 1, \; N_{(s)} = \prod_{i=1}^{s} ([\tfrac{n_i}{2}] + 1), \\
\Lambda_h^{(k^*_{h+1})} &= \sum_{k_h=0}^{[n_h/2]} \Lambda(n_h, k_h) \otimes \Lambda_{h-1}^{(k^*_{h+1}([\frac{n_h}{2}]+1)+k_h)}, \\
k^*_{h+1} &= 0, \ldots, N_{(s\backslash h)} - 1, \; h = 1, \ldots, s-1, \\
N_{(s\backslash h)} &= \prod_{i=h+1}^{s} ([\tfrac{n_i}{2}] + 1).
\end{aligned}$$

6 Possible generalizations

Up to know we have been focusing on one step shift permutation invariance. However we will briefly consider what happens if we suppose t-shift permutation invariance. An orthogonal matrix $P(t): n \times n$ is a *t-shift permutation matrix*, $t = 2, \ldots, n-1$, if

$$p_{ij} = \begin{cases} 1, & \text{if } j = i + t - nI_{(i>n-t)} \\ 0, & \text{otherwise .} \end{cases} \tag{6.1}$$

It follows that $P(t)$ equals the product of t 1-shift matrices given in (3.1). Thus, we can start to copy the proofs given in Theorem 3.3. However, it is clear that some criteria of irreducibility should be included. Furthermore, one should consider the “smallest t”. Consider the following sequence: $n = 6$; $2 \to 4 \to 6 \to 2$, $1 \to 3 \to 5 \to 1$ which consists of two “independent” sequences. However, if $n = 7$ then $2 \to 4 \to 6 \to 1 \to 3 \to 5 \to 7 \to 2$ which is one sequence. Hence, it has been shown that the effect of t-shift invariance really depends on the size n of Σ.

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Appendix 1. Reparameterization constraints in the case $n = 5$

This appendix is a continuation of Section 4 when $n = 5$.

(ii) $\lambda_2 = \lambda_3 = 0$. In this case $\tau_0 = \frac{1}{2}(\sqrt{5}+1)\tau_1 - \frac{1}{2}(\sqrt{5}-1)\tau_2$ and

$$\begin{aligned}\lambda_1 &= \sqrt{5}(\tau_1 - \tau_2),\\ \lambda_5 &= \tfrac{1}{2}(\sqrt{5}+5)\tau_1 - \tfrac{1}{2}(\sqrt{5}-5)\tau_2.\end{aligned}$$

The eigenvectors corresponding to zero eigenvalues are

$$\begin{aligned}v_2 &= (-1, \tfrac{1}{2}(\sqrt{5}+1), -\tfrac{1}{2}(\sqrt{5}+1), 1, 0)',\\ v_3 &= (-\tfrac{1}{2}(\sqrt{5}+1), \tfrac{1}{2}(\sqrt{5}+1), -1, 0, 1)'.\end{aligned}$$

Because $E(v_i'\xi) = 0$ and $D(v_i'\xi) = 0$, $i = 2, 3$, we get as reparameterization constraints

$$\begin{aligned}&-\xi_1 + \tfrac{1}{2}(\sqrt{5}+1)\xi_2 - \tfrac{1}{2}(\sqrt{5}+1)\xi_3 + \xi_4 = 0,\\ &-\tfrac{1}{2}(\sqrt{5}+1)\xi_1 + \tfrac{1}{2}(\sqrt{5}+1)\xi_2 - \xi_3 + \xi_5 = 0.\end{aligned}$$

(iii) $\lambda_1 = \lambda_4 = 0$. In this case $\tau_0 = -\frac{1}{2}(\sqrt{5}-1)\tau_1 + \frac{1}{2}(\sqrt{5}+1)\tau_2$,

$$\begin{aligned}\lambda_2 &= -\sqrt{5}(\tau_1 - \tau_2),\\ \lambda_5 &= -\tfrac{1}{2}(\sqrt{5}-5)\tau_1 + \tfrac{1}{2}(\sqrt{5}+5)\tau_2\end{aligned}$$

and

$$\begin{aligned}v_1 &= (-1, \tfrac{1}{2}(1-\sqrt{5}), -\tfrac{1}{2}(1-\sqrt{5}), 1, 0)',\\ v_4 &= (-\tfrac{1}{2}(1-\sqrt{5}), \tfrac{1}{2}(1-\sqrt{5}), -1, 0, 1)'\end{aligned}$$

are eigenvectors corresponding to the zero eigenvalues, leading to the constraints

$$\begin{aligned}&-\xi_1 + \tfrac{1}{2}(1-\sqrt{5})\xi_2 - \tfrac{1}{2}(1-\sqrt{5})\xi_3 + \xi_4 = 0,\\ &-\tfrac{1}{2}(1-\sqrt{5})\xi_1 + \tfrac{1}{2}(1-\sqrt{5})\xi_2 - \xi_3 + \xi_5 = 0.\end{aligned}$$

(iv) $\lambda_1 = \lambda_4 = \lambda_5 = 0$. In this case $\tau_0 = (1-\sqrt{5})\tau_1$, $\tau_2 = \frac{1}{2}(\sqrt{5}-3)\tau_1$ and thus

$$\lambda_2 = \tfrac{5}{2}(1-\sqrt{5})\tau_1.$$

The eigenvectors corresponding to the zero eigenvalues are

$$\begin{aligned} v_1 &= (-1, \tfrac{1}{2}(1-\sqrt{5}), -\tfrac{1}{2}(1-\sqrt{5}), 1, 0)', \\ v_2 &= (-1, \tfrac{1}{2}(1+\sqrt{5}), -\tfrac{1}{2}(1+\sqrt{5}), 1, 0)', \\ v_5 &= (1, 1, 1, 1, 1)', \end{aligned}$$

Thus the elements of ξ satisfy

$$\begin{aligned} &-\xi_1 + \tfrac{1}{2}(1-\sqrt{5})\xi_2 - \tfrac{1}{2}(1-\sqrt{5})\xi_3 + \xi_4 = 0, \\ &-\xi_1 - \tfrac{1}{2}(1+\sqrt{5})\xi_2 1\tfrac{1}{2}(1+\sqrt{5})\xi_3 + \xi_4 = 0, \\ &\xi_1 + \xi_2 + \xi_3 + \xi_4 + \xi_5 = 0. \end{aligned}$$

(v) $\lambda_2 = \lambda_3 = \lambda_5 = 0$. In this case $\tau_0 = (1+\sqrt{5})\tau_1$, $\tau_2 = -\frac{1}{2}(\sqrt{5}+3)\tau_1$ and

$$\lambda_1 = \tfrac{5}{2}(1+\sqrt{5})\tau_1.$$

Moreover,

$$\begin{aligned} v_2 &= (-1, \tfrac{1}{2}(\sqrt{5}+1), -\tfrac{1}{2}(\sqrt{5}+1), 1, 0)', \\ v_3 &= (-\tfrac{1}{2}(\sqrt{5}+1), \tfrac{1}{2}(\sqrt{5}+1), -1, 0, 1)', \\ v_5 &= (1, 1, 1, 1, 1)' \end{aligned}$$

are the eigenvectors corresponding to zero eigenvalues. Thus,

$$\begin{aligned} &-\xi_1 + \tfrac{1}{2}(1+\sqrt{5})\xi_2 - \tfrac{1}{2}(1+\sqrt{5})\xi_3 + \xi_4 = 0, \\ &-\tfrac{1}{2}(\sqrt{5}+1)\xi_1 + \tfrac{1}{2}(\sqrt{5}+1)\xi_2 - \xi_3 + \xi_5 = 0, \\ &\xi_1 + \xi_2 + \xi_3 + \xi_4 + \xi_5 = 0. \end{aligned}$$

(vi) $\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = 0$. In this case $\tau_0 = 2\tau_1$, $\tau_2 = \sqrt{5}\tau_1$. Hence,

$$\lambda_5 = 2(2+\sqrt{5})\tau_1.$$

The eigenvectors $v_1, \ldots, v_4$, give the reparametrization conditions which in this case leads to that the vector of factor levels should be proportional to v_5 which implies that $\xi_i \neq \xi_j$, $i \neq j$, can not hold.

Appendix 2. Reparameterization constraints in the case $n = 6$

As in Appendix 1 we present the effect on factor levels if introducing various restrictions on the eigenvalues, i.e. put eigenvalues equal to 0.

(i) $\lambda_1 = \lambda_5 = \lambda_2 = \lambda_4 = 0$. The eigenvectors corresponding to the zero eigenvalues equal

$$\begin{aligned} v_1 &= (\tfrac{1}{2}(\sqrt{3}+1), \tfrac{1}{2}(\sqrt{3}-1), -1, -\tfrac{1}{2}(\sqrt{3}+1), -\tfrac{1}{2}(\sqrt{3}-1), 1)', \\ v_2 &= (\tfrac{1}{2}(\sqrt{3}-1), -\tfrac{1}{2}(\sqrt{3}+1), 1, \tfrac{1}{2}(\sqrt{3}-1), -\tfrac{1}{2}(\sqrt{3}+1), 1)', \\ v_4 &= (-\tfrac{1}{2}(\sqrt{3}+1), \tfrac{1}{2}(\sqrt{3}-1), 1, -\tfrac{1}{2}(\sqrt{3}+1), \tfrac{1}{2}(\sqrt{3}-1), 1)', \\ v_5 &= (-\tfrac{1}{2}(\sqrt{3}-1), -\tfrac{1}{2}(\sqrt{3}+1), -1, \tfrac{1}{2}(\sqrt{3}-1), \tfrac{1}{2}(\sqrt{3}+1), 1)'. \end{aligned}$$

As a result, $\xi = (\xi_1, \xi_2, \xi_1, \xi_2, \xi_1, \xi_2)'$.

(ii) $\lambda_1 = \lambda_5 = \lambda_3 = 0$. The corresponding eigenvectors are

$$\begin{aligned} v_1 &= (\tfrac{1}{2}(\sqrt{3}+1), \tfrac{1}{2}(\sqrt{3}-1), -1, -\tfrac{1}{2}(\sqrt{3}+1), -\tfrac{1}{2}(\sqrt{3}-1), 1)', \\ v_5 &= (-\tfrac{1}{2}(\sqrt{3}-1), -\tfrac{1}{2}(\sqrt{3}+1), -1, \tfrac{1}{2}(\sqrt{3}-1), \tfrac{1}{2}(\sqrt{3}+1), 1)', \\ v_3 &= (-1, 1, -1, 1, -1, 1)'. \end{aligned}$$

As a result we get, $\xi = (\xi_1, \xi_2, \xi_3, \xi_1, \xi_2, \xi_3)'$.

(iii) $\lambda_1 = \lambda_5 = \lambda_6 = 0$. In this case the corresponding eigenvectors are

$$\begin{aligned} v_1 &= (\tfrac{1}{2}(\sqrt{3}+1), \tfrac{1}{2}(\sqrt{3}-1), -1, -\tfrac{1}{2}(\sqrt{3}+1), -\tfrac{1}{2}(\sqrt{3}-1), 1)', \\ v_5 &= (-\tfrac{1}{2}(\sqrt{3}-1), -\tfrac{1}{2}(\sqrt{3}+1), -1, \tfrac{1}{2}(\sqrt{3}-1), \tfrac{1}{2}(\sqrt{3}+1), 1)', \\ v_6 &= (1, 1, 1, 1, 1, 1)'. \end{aligned}$$

This leads to that, $\xi_1 + \frac{3}{2}\xi_2 + \xi_3 - \frac{1}{2}\xi_5 = 0$, $\xi_1 + \xi_2 - \xi_4 - \xi_5 = 0$ and $\xi_1 + \frac{1}{2}\xi_2 + \frac{1}{2}\xi_5 + \xi_6 = 0$.

(iv) $\lambda_2 = \lambda_4 = \lambda_3 = 0$. In this case the corresponding eigenvectors are

$$\begin{aligned} v_2 &= (\tfrac{1}{2}(\sqrt{3}-1), -\tfrac{1}{2}(\sqrt{3}+1), 1, \tfrac{1}{2}(\sqrt{3}-1), -\tfrac{1}{2}(\sqrt{3}+1), 1)', \\ v_4 &= (-\tfrac{1}{2}(\sqrt{3}+1), \tfrac{1}{2}(\sqrt{3}-1), 1, -\tfrac{1}{2}(\sqrt{3}+1), \tfrac{1}{2}(\sqrt{3}-1), 1)', \\ v_3 &= (-1, 1, -1, 1, -1, 1)', \end{aligned}$$

and $2\xi_1 - 2\xi_2 + \xi_3 - \xi_6 = 0$, $3\xi_1 - 2\xi_2 + \xi_4 - 2\xi_6 = 0$ and $2\xi_1 - \xi_2 + \xi_5 - 2\xi_6 = 0$.

(v) $\lambda_2 = \lambda_4 = \lambda_6 = 0$. In this case the corresponding eigenvectors are

$$\begin{aligned} v_2 &= (\tfrac{1}{2}(\sqrt{3}-1), -\tfrac{1}{2}(\sqrt{3}+1), 1, \tfrac{1}{2}(\sqrt{3}-1), -\tfrac{1}{2}(\sqrt{3}+1), 1)', \\ v_4 &= (-\tfrac{1}{2}(\sqrt{3}+1), \tfrac{1}{2}(\sqrt{3}-1), 1, -\tfrac{1}{2}(\sqrt{3}+1), \tfrac{1}{2}(\sqrt{3}-1), 1)', \\ v_6 &= (1,1,1,1,1,1)'. \end{aligned}$$

As result, $\xi = (\xi_1, \xi_2, \xi_3, -\xi_1, -\xi_2, -\xi_3)'$.

(vi) $\lambda_3 = \lambda_6 = 0$. To these two eigenvalues the corresponding eigenvectors are

$$\begin{aligned} v_3 &= (-1,1,-1,1,-1,1)', \\ v_6 &= (1,1,1,1,1,1)'. \end{aligned}$$

Hence, $\xi_1 + \xi_3 + \xi_5 = 0$ and $\xi_2 + \xi_4 + \xi_6 = 0$.

(vii) $\lambda_1 = \lambda_5 = \lambda_2 = \lambda_4 = \lambda_3 = 0$. In this case $\xi = (\xi_5, \xi_5, \xi_5, \xi_5, \xi_5, \xi_5)'$.

(viii) $\lambda_1 = \lambda_5 = \lambda_3 = \lambda_6 = 0$. In this case $\xi = (-\xi_5 - \xi_6, \xi_5, \xi_6, -\xi_5 - \xi_6, \xi_5, \xi_6)'$.

(ix) $\lambda_2 = \lambda_4 = \lambda_3 = \lambda_6 = 0$. Then, $\xi = (\xi_1, \xi_1 - \xi_6, -\xi_6, -\xi_1 + \xi_6, \xi_6)'$.

(x) $\lambda_1 = \lambda_5 = \lambda_2 = \lambda_4 = \lambda_6 = 0$. In this case $\xi = (\xi_1, -\xi_1, \xi_1, -\xi_1, \xi_1, -\xi_1)'$.

Appendix 3. Reparameterization constraints in the case $n = 8$

(i) $\lambda_1 = \lambda_7 = 0$. In this case

$$\begin{aligned} \lambda_2 = \lambda_6 &= -\sqrt{2}\tau_1 - 2\tau_2 + \sqrt{2}\tau_3 + 2\tau_4, \\ \lambda_3 = \lambda_5 &= -2\sqrt{2}\tau_1 + 2\sqrt{2}\tau_3, \\ \lambda_4 &= -(\sqrt{2}+2)\tau_1 + 2\tau_2 - (2-\sqrt{2})\tau_3 + 2\tau_4, \\ \lambda_8 &= (2-\sqrt{2})\tau_1 + 2\tau_2 + (2+\sqrt{2})\tau_3 + 2\tau_4 \end{aligned}$$

and

$$\sqrt{2}\xi_1 + \xi_2 - \xi_4 - \sqrt{2}\xi_5 - \xi_6 + \xi_8 = 0, \quad (6.2)$$

$$-\xi_2 - \sqrt{2}\xi_3 - \xi_4 + \xi_6 + \sqrt{2}\xi_7 + \xi_8 = 0. \quad (6.3)$$

(ii) $\lambda_2 = \lambda_6 = 0$. In this case

$$\begin{aligned}
\lambda_1 = \lambda_7 &= \sqrt{2}\tau_1 + 2\tau_2 - \sqrt{2}\tau_3 - 2\tau_4, \\
\lambda_3 = \lambda_5 &= -\sqrt{2}\tau_1 + 2\tau_2 + \sqrt{2}\tau_3 - 2\tau_4, \\
\lambda_4 &= -2\tau_1 + 4\tau_2 - 2\tau_3, \\
\lambda_8 &= 2\tau_1 + 4\tau_2 + 2\tau_3
\end{aligned}$$

and

$$\xi_1 - \xi_2 - \xi_3 + \xi_4 + \xi_5 - \xi_6 - \xi_7 + \xi_8 = 0, \tag{6.4}$$
$$-\xi_1 - \xi_2 + \xi_3 + \xi_4 - \xi_5 - \xi_6 + \xi_7 + \xi_8 = 0. \tag{6.5}$$

(iii) $\lambda_3 = \lambda_5 = 0$. In this case

$$\begin{aligned}
\lambda_1 = \lambda_7 &= 2\sqrt{2}\tau_1 - 2\sqrt{2}\tau_3, \\
\lambda_2 = \lambda_6 &= \sqrt{2}\tau_1 - 2\tau_2 - \sqrt{2}\tau_3 + 2\tau_4, \\
\lambda_4 &= -(2 - \sqrt{2})\tau_1 + 2\tau_2 - (2 + \sqrt{2})\tau_3 + 2\tau_4, \\
\lambda_8 &= (2 + \sqrt{2})\tau_1 + 2\tau_2 + (2 - \sqrt{2})\tau_3 + 2\tau_4
\end{aligned}$$

and

$$-\xi_2 + \sqrt{2}\xi_3 - \xi_4 + \xi_6 - \sqrt{2}\xi_7 + \xi_8 = 0, \tag{6.6}$$
$$-\sqrt{2}\xi_1 + \xi_2 - \xi_4 + \sqrt{2}\xi_5 - \xi_6 + \xi_8 = 0. \tag{6.7}$$

(iv) $\lambda_4 = 0$. In this case

$$\begin{aligned}
\lambda_1 = \lambda_7 &= (2 + \sqrt{2})\tau_1 - 2\tau_2 + (2 - \sqrt{2})\tau_3 - 2\tau_4, \\
\lambda_2 = \lambda_6 &= 2\tau_1 - 4\tau_2 + 2\tau_3, \\
\lambda_3 = \lambda_5 &= (2 - \sqrt{2})\tau_1 - 2\tau_2 + (2 + \sqrt{2})\tau_3 - 2\tau_4, \\
\lambda_8 &= 4\tau_1 + 4\tau_3
\end{aligned}$$

and

$$-\xi_1 + \xi_2 - \xi_3 + \xi_4 - \xi_5 + \xi_6 - \xi_7 + \xi_8 = 0. \tag{6.8}$$

(v) $\lambda_1 = \lambda_7 = \lambda_8 = 0$, $\lambda_2 = \lambda_6 = \lambda_8 = 0$ or $\lambda_3 = \lambda_5 = \lambda_8 = 0$. In these cases the corresponding reparameterizations are given by (6.2), (6.3), (6.4), (6.5) and (6.6), (6.7), respectively, and additionally for all we must have

$$\xi_1 + \xi_2 + \xi_3 + \xi_4 + \xi_5 + \xi_6 + \xi_7 + \xi_8 = 0. \tag{6.9}$$

(vi) $\lambda_1 = \lambda_7 = \lambda_2 = \lambda_6 = \lambda_4 = 0$. In this case the reparameterization conditions are given by (6.2), (6.3), (6.4), (6.5) and (6.8).

(vii) $\lambda_1 = \lambda_7 = \lambda_2 = \lambda_6 = \lambda_8 = 0$. In this case the reparameterization conditions are given by (6.2), (6.3), (6.4), (6.5) and (6.9).

(viii) $\lambda_1 = \lambda_7 = \lambda_2 = \lambda_6 = \lambda_3 = \lambda_5 = 0$. In this case the reparameterization conditions are given by (6.2), (6.3), (6.4), (6.5), (6.6) and (6.7).