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Ricardo Leiva
Departamento de Matemática
F.C.E., Universidad Nacional de Cuyo
5500 Mendoza, Argentina
Email: rleiva@fcemail.uncu.edu.ar

Anuradha Roy
Department of Management Science and Statistics
The University of Texas at San Antonio
San Antonio, TX 78249 USA
Email: Anuradha.Roy@utsa.edu

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Ricardo Leiva

Departamento de Matemática
F.C.E., Universidad Nacional de Cuyo
5500 Mendoza, Argentina
Email: rleiva@fcmail.uncu.edu.ar

Anuradha Roy

Department of Management Science and Statistics
The University of Texas at San Antonio
San Antonio, TX 78249 USA
Email: Anuradha.Roy@utsa.edu
Phone: +00-210-458-6343, Fax: +00-210-458-6350

Abstract

We study multi-level multivariate normal distribution with self similar compound symmetry covariance structure for k different levels of the multivariate data. Both maximum likelihood and unbiased estimates of the matrix parameters are obtained. The spectral decomposition of the new covariance structure are discussed and are demonstrated with a real dataset from medical studies.

Keywords: Eigenblock, eigenmatrix, k -level data, self similar compound symmetry covariance structure

Mathematics Subject Classification 62H12; 62H25.

1 Introduction

To understand why multi-level multivariate data analysis is indeed a need in the present era, we begin with an example of bone replacement surgery for elderly osteoporotic patients. Osteoporosis is a disease characterized by a reduced bone mass and a degeneration of the bone tissue; it leads to bone fragility, so to a higher risk of fractures. As the population ages, more patients with osteoporosis require orthopedic procedures, for example those with intraoperative fractures, periprosthetic osteolysis with implant migration, and postoperative periprosthetic fractures. In most cases, it brings relief and mobility after years of pain. Bone takes a long time to grow and repair, so treating serious damage or carrying out reconstructive procedures can be a slow and painstaking process. Up till now surgeons used to change the bone by highly polished strong metal, ceramic material or by polymers. However, after about 10

years of use, these artificial things often need to be replaced because of wear and fatigue-induced delamination of the polymeric component. Sometimes these foreign things induce allergic reactions as has been observed on occasion with some stainless steels, or they sometimes harbor bacteria. A shortcoming noted with ceramics used as standalone bone substitutes is the initial low resistance to impact and fracture. The ideal bone graft substitute should be osteogenic, biocompatible, bioabsorbable, able to provide structural support, easy to use clinically, and cost-effective. As a result scientists are now considering to use some organic structures. It is known that organic molecules mimic behavior of metals and thus could be used to repair the human body. Moreover, they do not have any adverse reactions and are tolerated well by the human body. To see which organic structure works best one needs to measure proliferation and viability of the organic structures along the circumference of the structure and at different depths of the structure. Furthermore, to see the effectiveness of these organic structures all these observations need to be measured repeatedly over time. Therefore, we see that this data is a four-level (proliferation and viability: Level 1, different points on circumference: Level 2, different depths: Level 3 and different time points: Level 4) dataset. As opposed to three-level data analysis showing the bone activities (proliferation and viability) of organic structure along circumference and at different depths, four-level data analysis can differentiate between the bone activities over time. The measurements at different points on circumference, at different depths as well as at different time points may have different measurement variations for the variables, and we must take these variations into account while analyzing these kinds of data. Examples of three-level data can be found in Leiva and Roy (2012) and examples of two-level data can be found in Roy (2006), Roy and Khattree (2007), and Roy and Leiva (2008).

Two-level data (two-dimensional arrays) is analyzed using a matrix-variate normal distribution, which is an extension of the traditional multivariate (vector-variate) normal distribution. Two-level data can also be analyzed vectorially with a 2-separable (Kronecker product) variance-covariance structure, or block exchangeable covariance structure. These covariance structures integrate the two-level information into the model. Whenever one has two or more levels of measurements collected within subjects (clusters), one has a data analysis situation that requires an assumption about the structure of a within-subject covariance matrix. One may choose to ignore it, but failing to understand how a covariance matrix works may influence the results. In the same way, multi-level data (multi-dimensional arrays) can be analyzed vectorially, however with some structured variance-covariance matrix which can incorporate multi-level information into the model, e.g., k -separable covariance structure (Leiva and Roy, 2014; Singull et al., 2012) for k -level data. Nonetheless, k -separable covariance structure

may not be suitable for all datasets; thus we explore some other structure for k -level data in this article. Our new structure can be utilized in situations where exchangeable feature is present at every level of the data.

Advancement of computer technology allows to store complex (e.g., multi-level) data more efficiently, inexpensively and instantly these days as compared to last century. Thus, appropriate methods need to be developed to analyze these multi-level data to draw right conclusion. Standard multivariate techniques with one big variance-covariance matrix do not work with these multi-level data, as these standard techniques cannot incorporate the multi-level information in the standard models, and thus would draw wrong conclusions (See Roy et al., 2015; Leiva and Roy, 2012).

A meaningful distinction between the multi-level normal and multivariate (vector-variate) normal distributions is the way in which their covariances are characterized. Treating a multi-level data as a vector-variate data with one big unstructured variance-covariance matrix fails to preserve certain intrinsic algebraic relationships among the response variables and their geometric relationships in which the response variables are measured. For example, algebraic operations e.g., decomposing the variance-covariance matrix into its eigenvalues and eigenvectors, performed on multi-level data are wrong when a multi-level data is treated as a vector-variate with the big unstructured variance-covariance matrix. One first needs to do the eigendecomposition of a suitable structured variance-covariance matrix for multi-level data to get the eigenblocks and eigenmatrices (Hao et al. (2015)), and a set of uncorrelated principal vectors with eigenblocks as their variance-covariance matrices. Then obtain the eigenvalues of each of the eigenblocks and the corresponding uncorrelated principal components which are linear combination of the components of the corresponding principal vector. Additionally, a big unstructured covariance matrix of the vectorial representation of the multi-level data offers no insights into the way the measurements of the experimental design are observed and affect their distribution. Sometimes the structure in multi-level data is simply implied by the organization (design in broad sense) of the experiment. Moreover, the computation of the parameters with the unstructured variance-covariance matrix is a real problem as the number of parameters multiply with the increase of the number of response variables and with the increase of the number of levels in the data. A multivariate analysis is not possible for these multi-level data in a small sample setting, and this necessitates a multi-level multivariate data analysis for these multi-level data.

Roy and Leiva (2007, 2011), and Leiva and Roy (2009, 2011, 2012) have written a series of articles for three-level data with different covariance structures. One of the structures they used is doubly exchangeable covariance structure. Roy and Fonseca (2012) studied linear models for three-level data

with doubly exchangeable covariance structure on errors. Doubly exchangeable covariance structure is a generalization of block exchangeable covariance structure or block compound symmetry covariance structure for two-level data, which in turn is a generalization of compound symmetry covariance structure for traditional multivariate (vector-variate) data. This article generalizes this compound symmetry covariance structure for k -level data, and we name it as “self similar compound symmetry” (SSCS) covariance structure; the connotation will be clear in Section 2 when we define the structure. A k -SSCS covariance structure, is a partitioned covariance matrix, consists of k unstructured covariance matrices for the k levels of the k -level data, and thus reduces the number of unknown parameters significantly. This is of critical importance to a variety of applied problems in medicine and engineering among many other fields with multi-level data. The major advantage, however is that this obviates some of the problems with small sample size. Multi-level data sets often contain many variables along with the number of levels of the data, and in most cases the total number of variables exceeds the sample size.

k -SSCS covariance structure for k -level data as opposed to unstructured covariance matrix is very interesting as it assumes different covariance matrices at each level and uses these k covariance matrices “cleverly” in the construction of the k -SSCS covariance matrix. In this paper we consider the balanced case of k -level data, where the same m_1 -dimensional vector of measurements is recorded for each combination $\mathbf{f} = (f_2, \dots, f_k)$ of $k - 1$ different levels (factors) with $f_t \in F_t = \{1, \dots, m_t\}$ at $t = 2, \dots, k$ for each individual (unit). We show through many examples throughout the article that our new k -SSCS covariance structure is indeed an extension of the compound symmetry covariance structure for multivariate data.

Let $\mathbf{x}_{r,\mathbf{f}}$ be a m_1 -variate vector of measurements on the r^{th} replicate (individual) at the \mathbf{f} factor combination. Let \mathbf{x} be the $p_{1,k} = \prod_{j=1}^k m_j$ -variate vector of all measurements corresponding to the r^{th} sample unit, that is, $\mathbf{x}_r = (x_{r,1,\dots,1}, \dots, x_{r,m_1,\dots,m_k})'$. The (arbitrary, but the same for all r) covariance matrix $\mathbf{\Gamma}_x$ has $q = p_{1,k}(p_{1,k} + 1)/2$ parameters. If the number of samples $n \leq p_{1,k}$, one cannot estimate the q unknown parameters. It is then necessary to assume some appropriate structure on $\mathbf{\Gamma}_x$ in order to reduce the number of unknown parameters. The number of parameters to be estimated in “ k -SSCS covariance matrix” is only $\frac{k}{2}m_1(m_1 + 1)$, which is much less than q , the number of unknown parameters in an unstructured variance-covariance matrix. Also, for this k -SSCS covariance structure the observations need not be of equally spaced. It is worth mentioning at this point that the total number of parameters in k -separable covariance structure is $\sum_{i=1}^k m_i(m_i + 1)/2$, but the total number of free parameters in k -separable covariance structure is $\sum_{i=1}^k (m_i(m_i + 1)/2) - (k - 1)$. For detail see Remark 3.1 in Leiva and Roy (2014). If m_1 is less than at least one of $\{m_2, m_3, \dots, m_k\}$, then the k -SSCS

covariance matrix is more parsimonious than the k -separable covariance structure.

The rest of the article is organized as follows. We introduce the k -self-similar compound symmetry covariance matrix in Section 2. Some examples of SSCS covariance structure is given in Section 3. Maximum likelihood estimators (MLEs) and unbiased estimators of the matrix parameters of k -SSCS covariance structure are derived in Section 4. Spectral decompositions of the k -SSCS covariance structure is obtained in Section 5. An example of a real data set is given in Section 6. Finally, Section 7 concludes with several comments and the scope for future research. Technical derivation of MLEs of all unknown parameters and other derivations are presented in the Appendix.

2 Self-Similar compound symmetry covariance matrix

Let m_h , for $h = 1, \dots, k$, be fixed positive integer numbers, that is, $m_h \in \mathbb{N}$, for $h = 1, \dots, k$. Let $p_{i,j}$ be the product $p_{i,j} = \prod_{h=i}^j m_h$, for $i \leq j = 1, \dots, k$, with $p_{i+1,i} = 1$, $p_{i+2,i} = 0$ and let \mathbf{x}_r be a $(p_{1,k} \times 1)$ -dimensional random vector, and it will be considered as a partitioned vector formed by $p_{1,j} \times 1$ -subvectors, that is, $\mathbf{x}_r = (\mathbf{x}'_{r;p_{1,j};1}, \dots, \mathbf{x}'_{r;p_{1,j};p_{j+1,k}})'$. Under symmetry conditions like the one imposed by the self-similar compound symmetry covariance matrix (defined later) these conditions can be stated (without loss of generality) to be “the first component of $\boldsymbol{\mu}_h$ is equal to 1, for $h = 2, \dots, k$ ”.

Definition 1 We define \mathbf{x}_r to have a k -self-similar compound symmetry covariance matrix (k -SSCS covariance matrix) if $\boldsymbol{\Gamma}_{\mathbf{x}_r} = \text{Cov}[\mathbf{x}_r]$ is of the form

$$\boldsymbol{\Gamma}_{\mathbf{x}_r} = \sum_{j=1}^k \left(\bigotimes_{h=1}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k:j,h}} \right) \otimes (\mathbf{U}_{k,j} - \mathbf{U}_{k,j+1}), \quad (1)$$

where $\mathbf{U}_{k,j}$, for $j = 1, \dots, k$, are symmetric $m_1 \times m_1$ -matrices, with $\mathbf{U}_{k,1}$ positive definite, $\mathbf{U}_{k,k+1} = \mathbf{0}_{m_1 \times m_1}$ and

$$\mathbf{i}_{k:j} = (i_{k:j,1}, \dots, i_{k:j,k-1}) = \begin{cases} \mathbf{0}_{1 \times (k-1)} & \text{if } j = 1 \\ \left(\mathbf{0}_{1 \times k-j}, \mathbf{1}'_{j-1} \right) & \text{if } j = 2, \dots, k-1 \\ \mathbf{1}'_{k-1} & \text{if } j = k \end{cases}, \quad (2)$$

with $\mathbf{1}_h$ denoting the $(h \times 1)$ -dimensional vector of ones, $\mathbf{J}_h = \mathbf{1}_h \mathbf{1}'_h$, and $\mathbf{J}_h^0 = \mathbf{I}_h$ the $(h \times h)$ -dimensional identity matrix. The matrices $\mathbf{U}_{k,j}$, $j = 1, \dots, k$, are called SSCS-component matrices.

The $m_1 \times m_1$ diagonal blocks $\mathbf{U}_{k,1}$ represent the variance-covariance matrix of the m_1 response variables at any of the k levels, whereas $m_1 \times m_1$ off-diagonal blocks $\mathbf{U}_{k,j}$, $j = 2, \dots, k$ represent the covariance matrix of the m_1 response variables at any two different levels (same or different). In particular, when

$p_{1,k} \times 1$ - random vectors \mathbf{x}_r and $E[\mathbf{x}_r] = \boldsymbol{\mu}_{\mathbf{x}_r}$ are partitioned in $m_1 \times 1$ - subvectors as

$$\mathbf{x}_r = (\mathbf{x}'_{r;f_2,f_3,\dots,f_k} : f_j \in F_j = \{1, \dots, m_j\}, \text{ for } j = 2, \dots, k)',$$

where $\mathbf{x}_{r;f_2,f_3,\dots,f_k} \in \mathbb{R}^{m_1}$ is an $m_1 \times 1$ subvector, and

$$\boldsymbol{\mu}_{\mathbf{x}_r} = (\boldsymbol{\mu}'_{f_2,f_3,\dots,f_k} : f_j \in F_j = \{1, \dots, m_j\}, \text{ for } j = 2, \dots, k)',$$

where $\boldsymbol{\mu}_{f_2,f_3,\dots,f_k} \in \mathbb{R}^{m_1}$ is an $m_1 \times 1$ subvector independent of r , that is,

$$\begin{aligned} \mathbf{x}_r = & (\mathbf{x}'_{r;1,1,\dots,1}, \dots, \mathbf{x}'_{r;m_2,1,\dots,1}, \mathbf{x}'_{r;1,2,\dots,1}, \dots, \mathbf{x}'_{r;m_2,2,\dots,1}, \dots, \mathbf{x}'_{r;1,m_3,\dots,1}, \dots, \mathbf{x}'_{r;m_2,m_3,\dots,1}, \\ & \dots, \mathbf{x}'_{r;1,1,\dots,2}, \dots, \mathbf{x}'_{r;m_2,1,\dots,2}, \mathbf{x}'_{r;1,2,\dots,2}, \dots, \mathbf{x}'_{r;m_2,2,\dots,2}, \dots, \mathbf{x}'_{r;1,m_3,\dots,m_k}, \dots, \mathbf{x}'_{r;m_2,m_3,\dots,m_k})', \end{aligned}$$

and

$$\begin{aligned} \boldsymbol{\mu}_{\mathbf{x}_r} = & (\boldsymbol{\mu}'_{1,1,\dots,1}, \dots, \boldsymbol{\mu}'_{m_2,1,\dots,1}, \boldsymbol{\mu}'_{1,2,\dots,1}, \dots, \boldsymbol{\mu}'_{m_2,2,\dots,1}, \dots, \boldsymbol{\mu}'_{1,m_3,\dots,1}, \dots, \boldsymbol{\mu}'_{m_2,m_3,\dots,1}, \\ & \dots, \boldsymbol{\mu}'_{1,1,\dots,2}, \dots, \boldsymbol{\mu}'_{m_2,1,\dots,2}, \boldsymbol{\mu}'_{1,2,\dots,2}, \dots, \boldsymbol{\mu}'_{m_2,2,\dots,2}, \dots, \boldsymbol{\mu}'_{1,m_3,\dots,m_k}, \dots, \boldsymbol{\mu}'_{m_2,m_3,\dots,m_k})', \end{aligned}$$

then

$$\begin{aligned} & E \left[(\mathbf{x}_{r;f_2,f_3,\dots,f_k} - \boldsymbol{\mu}_{f_2,f_3,\dots,f_k}) (\mathbf{x}_{r;f_2^*,f_3^*,\dots,f_k^*} - \boldsymbol{\mu}_{f_2^*,f_3^*,\dots,f_k^*})' \right] \\ & = \begin{cases} \mathbf{U}_{k,1} & \text{if } f_{j+h} = f_{j+h}^* : h = 1, \dots, k-j \quad \text{for } j = 1 \\ \mathbf{U}_{k,j} & \text{if } f_j \neq f_j^* \quad f_{j+h} = f_{j+h}^* : h = 1, \dots, k-j \quad \text{for } j = 2, \dots, k \end{cases} \end{aligned} \quad (3)$$

We believe that this k -SSCS structure described in such a manner can capture the data structure in a longitudinal study in all k levels, and therefore offer more information about the true association of the data. We now examine how the k -SSCS variance-covariance matrices look like for some particular values of k and m in the following examples.

3 Some useful examples of SCS structures

Example 1 If $k = 2$, and $m_1 = 1$, then $\mathbf{U}_{2,j}$, $j = 1, 2$, are real numbers and the $(m_2 \times 1)$ -dimensional random vector \mathbf{x}_r has the covariance matrix

$$\begin{aligned} \boldsymbol{\Gamma}_{\mathbf{x}} & = \sum_{j=1}^2 \left(\bigotimes_{h=1}^1 \mathbf{J}_{m_{k+1-h}}^{i_{2;j,h}} \right) \otimes (\mathbf{U}_{2,j} - \mathbf{U}_{2,j+1}) \\ & = \mathbf{I}_{m_2} \otimes (\mathbf{U}_{2,1} - \mathbf{U}_{2,2}) + \mathbf{J}_{m_2} \otimes \mathbf{U}_{2,2} \\ & = (\mathbf{U}_{2,1} - \mathbf{U}_{2,2}) \mathbf{I}_{m_2} + \mathbf{U}_{2,2} \mathbf{J}_{m_2}, \end{aligned}$$

which is a $m_2 \times m_2$ compound symmetry, equicorrelated or exchangeable covariance matrix.

Example 2 If $k = 2$, and $m_1 > 1$, then the $(m_1 m_2 \times 1)$ -dimensional random vector \mathbf{x}_r has the covariance matrix

$$\begin{aligned}\Gamma_{\mathbf{x}} &= \sum_{j=1}^2 \left(\bigotimes_{h=1}^1 \mathbf{J}_{m_{k+1-h}}^{i_{2;j,h}} \right) \otimes (\mathbf{U}_{2,j} - \mathbf{U}_{2,j+1}) \\ &= \mathbf{I}_{m_2} \otimes (\mathbf{U}_{2,1} - \mathbf{U}_{2,2}) + \mathbf{J}_{m_2} \otimes \mathbf{U}_{2,2},\end{aligned}$$

which is the equicorrelated covariance matrix (Leiva, 2007) or block exchangeable covariance matrix.

Example 3 If $k = 3$, the $(m_1 m_2 m_3 \times 1)$ -dimensional random vector \mathbf{x}_r has the covariance matrix

$$\begin{aligned}\Gamma_{\mathbf{x}} &= \sum_{j=1}^3 \left(\bigotimes_{h=1}^2 \mathbf{J}_{m_{k+1-h}}^{i_{3;j,h}} \right) \otimes (\mathbf{U}_{3,j} - \mathbf{U}_{3,j+1}) \\ &= \mathbf{I}_{m_3 m_2} \otimes (\mathbf{U}_{3,1} - \mathbf{U}_{3,2}) + \mathbf{I}_{m_3} \otimes \mathbf{J}_{m_2} \otimes (\mathbf{U}_{3,2} - \mathbf{U}_{3,3}) + \mathbf{J}_{m_3 m_2} \otimes \mathbf{U}_{3,3},\end{aligned}$$

which is the jointly equicorrelated covariance matrix (Roy and Leiva, 2007) or doubly exchangeable covariance matrix. Note that

$$\begin{aligned}\Gamma_{\mathbf{x}} &= \mathbf{I}_{m_3 m_2} \otimes (\mathbf{U}_{3,1} - \mathbf{U}_{3,2}) + \mathbf{I}_{m_3} \otimes \mathbf{J}_{m_2} \otimes (\mathbf{U}_{3,2} - \mathbf{U}_{3,3}) + \mathbf{J}_{m_3 m_2} \otimes \mathbf{U}_{3,3} \\ &= \mathbf{I}_{m_3} \otimes \{ [\mathbf{I}_{m_2} \otimes (\mathbf{U}_{3,1} - \mathbf{U}_{3,2}) + \mathbf{J}_{m_2} \otimes \mathbf{U}_{3,2}] - \mathbf{J}_{m_2} \otimes \mathbf{U}_{3,3} \} + \mathbf{J}_{m_3} \otimes (\mathbf{J}_{m_2} \otimes \mathbf{U}_{3,3}) \\ &= \mathbf{I}_{m_3} \otimes \{ \mathbf{V}_3 - \mathbf{W}_3 \} + \mathbf{J}_{m_3} \otimes (\mathbf{W}_3),\end{aligned}$$

where $\mathbf{V}_3 = \mathbf{I}_{m_2} \otimes (\mathbf{U}_{3,1} - \mathbf{U}_{3,2}) + \mathbf{J}_{m_2} \otimes \mathbf{U}_{3,2}$ is a 2-SSCS covariance matrix and $\mathbf{W}_3 = \mathbf{J}_{m_2} \otimes \mathbf{U}_{3,3}$. Therefore, we see that 2-SSCS covariance matrix is nested in 3-SSCS covariance matrix.

Example 4 If $k = 4$, the $(m_1 m_2 m_3 m_4 \times 1)$ -dimensional random vector \mathbf{x}_r has the covariance matrix

$$\begin{aligned}\Gamma_{\mathbf{x}} &= \sum_{j=1}^4 \left(\bigotimes_{h=1}^3 \mathbf{J}_{m_{k+1-h}}^{i_{4;j,h}} \right) \otimes (\mathbf{U}_{4,j} - \mathbf{U}_{4,j+1}) \\ &= \mathbf{I}_{m_4 m_3 m_2} \otimes (\mathbf{U}_{4,1} - \mathbf{U}_{4,2}) + \mathbf{I}_{m_4 m_3} \otimes \mathbf{J}_{m_2} \otimes (\mathbf{U}_{4,2} - \mathbf{U}_{4,3}) \\ &\quad + \mathbf{I}_{m_4} \otimes \mathbf{J}_{m_3 m_2} \otimes (\mathbf{U}_{4,3} - \mathbf{U}_{4,4}) + \mathbf{J}_{m_4 m_3 m_2} \otimes \mathbf{U}_{4,4}.\end{aligned}$$

This case has not been treated in the literature, even though there are cases in the experimental research where the obtained data (e.g., the organic structure data described in the Introduction) could be analyzed using this covariance structure.

Note again that

$$\begin{aligned}
\mathbf{\Gamma}_x &= \mathbf{I}_{m_4 m_3 m_2} \otimes (\mathbf{U}_{4,1} - \mathbf{U}_{4,2}) + \mathbf{I}_{m_4 m_3} \otimes \mathbf{J}_{m_2} \otimes (\mathbf{U}_{4,2} - \mathbf{U}_{4,3}) \\
&\quad + \mathbf{I}_{m_4} \otimes \mathbf{J}_{m_3 m_2} \otimes (\mathbf{U}_{4,3} - \mathbf{U}_{4,4}) + \mathbf{J}_{m_4 m_3 m_2} \otimes \mathbf{U}_{4,4} \\
&= \mathbf{I}_{m_4} \{ \mathbf{I}_{m_3 m_2} \otimes (\mathbf{U}_{4,1} - \mathbf{U}_{4,2}) + \mathbf{I}_{m_3} \otimes \mathbf{J}_{m_2} \otimes (\mathbf{U}_{4,2} - \mathbf{U}_{4,3}) + \mathbf{J}_{m_3 m_2} \otimes (\mathbf{U}_{4,3} - \mathbf{U}_{4,4}) \} \\
&\quad + \mathbf{J}_{m_4} \otimes (\mathbf{J}_{m_3 m_2} \otimes \mathbf{U}_{4,4}) \\
&= \mathbf{I}_{m_4} \otimes \{ \mathbf{V}_4 - \mathbf{W}_4 \} + \mathbf{J}_{m_4} \otimes (\mathbf{W}_4),
\end{aligned}$$

where $\mathbf{V}_4 = \mathbf{I}_{m_3 m_2} \otimes (\mathbf{U}_{4,1} - \mathbf{U}_{4,2}) + \mathbf{I}_{m_3} \otimes \mathbf{J}_{m_2} \otimes (\mathbf{U}_{4,2} - \mathbf{U}_{4,3}) + \mathbf{J}_{m_3 m_2} \otimes \mathbf{U}_{4,3}$ is a 3-SSCS covariance matrix and $\mathbf{W}_4 = \mathbf{J}_{m_3 m_2} \otimes \mathbf{U}_{4,4}$. Therefore, in this example we see that 3-SSCS covariance matrix is nested in 4-SSCS covariance matrix.

So, combining Examples 3 and 4 we find that 2-SSCS covariance matrix is nested in 3-SSCS covariance matrix; and 3-SSCS covariance matrix is nested in 4-SSCS covariance matrix. We now prove that this property is true for general k . From (1) $\mathbf{\Gamma}_x$ can be written as

$$\begin{aligned}
\mathbf{\Gamma}_x &= \left\{ \sum_{j=1}^{k-1} \left(\bigotimes_{h=1}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k:j,h}} \right) \otimes (\mathbf{U}_{k,j} - \mathbf{U}_{k,j+1}) \right\} + \left(\bigotimes_{h=1}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k:k,h}} \right) \otimes \mathbf{U}_{k,k} \\
&= \mathbf{I}_{m_k} \otimes \left\{ \sum_{j=1}^{k-1} \left(\bigotimes_{h=2}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k-1:j,h}} \right) \otimes (\mathbf{U}_{k,j} - \mathbf{U}_{k,j+1}) \right\} + \mathbf{J}_{m_k} \otimes \left(\bigotimes_{h=2}^{k-1} \mathbf{J}_{m_{k+1-h}} \right) \otimes \mathbf{U}_{k,k} \\
&= \mathbf{I}_{m_k} \otimes \left\{ \left[\sum_{j=1}^{k-2} \left(\bigotimes_{h=2}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k-1:j,h}} \right) \otimes (\mathbf{U}_{k,j} - \mathbf{U}_{k,j+1}) \right] + \left(\bigotimes_{h=2}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k-1:k-1,h}} \right) \otimes (\mathbf{U}_{k,k-1} - \mathbf{U}_{k,k}) \right\} \\
&\quad + \mathbf{J}_{m_k} \otimes \left(\bigotimes_{h=2}^{k-1} \mathbf{J}_{m_{k+1-h}} \right) \otimes \mathbf{U}_k \\
&= \mathbf{I}_{m_k} \otimes \left\{ \left[\sum_{j=1}^{k-2} \left(\bigotimes_{h=2}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k-1:j,h}} \right) \otimes (\mathbf{U}_{k,j} - \mathbf{U}_{k,j+1}) + \left(\bigotimes_{h=2}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k-1:k-1,h}} \right) \otimes \mathbf{U}_{k,k-1} \right] \right. \\
&\quad \left. - \left(\bigotimes_{h=2}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k-1:k-1,h}} \right) \otimes \mathbf{U}_{k,k} \right\} + \mathbf{J}_{m_k} \otimes \left(\bigotimes_{h=2}^{k-1} \mathbf{J}_{m_{k+1-h}} \right) \otimes \mathbf{U}_{k,k} \\
&= \mathbf{I}_{m_k} \otimes \{ \mathbf{V}_k - \mathbf{W}_k \} + \mathbf{J}_{m_k} \otimes \mathbf{W}_k,
\end{aligned}$$

where

$$\mathbf{V}_k = \sum_{j=1}^{k-2} \left(\bigotimes_{h=2}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k-1:j,h}} \right) \otimes (\mathbf{U}_{k,j} - \mathbf{U}_{k,j+1}) + \left(\bigotimes_{h=2}^{k-1} \mathbf{J}_{m_{k+1-h}} \right) \otimes \mathbf{U}_{k,k-1}$$

is a $(k-1)$ -SSCS variance-covariance matrix and

$$\mathbf{W}_k = \left(\bigotimes_{h=2}^{k-1} \mathbf{J}_{m_{k+1-h}} \right) \otimes \mathbf{U}_{k,k}.$$

Therefore, for general k , the above property justifies the name why the covariance matrix $\mathbf{\Gamma}_x$ is called self similar compound symmetry or exchangeable covariance matrix as it has a compound symmetry (structure) behavior at each of its k depth levels.

More precisely, if the $(p_{1,k} \times 1)$ -dimensional random vector \mathbf{x}_r is considered as a partitioned vector $\mathbf{x}_r = (\mathbf{x}'_{r,p_{1,k-1};1}, \dots, \mathbf{x}'_{r,p_{1,k-1};m_k})'$, then its partitioned covariance matrix $\mathbf{\Gamma}_x$ in its first depth level has the form

$$\begin{aligned} \mathbf{\Gamma}_x &= \mathbf{V}_{k+1} = \begin{bmatrix} \mathbf{V}_k & \mathbf{W}_k & \cdots & \mathbf{W}_k \\ \mathbf{W}_k & \mathbf{V}_k & \cdots & \mathbf{W}_k \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{W}_k & \mathbf{W}_k & \cdots & \mathbf{V}_k \end{bmatrix} \\ &= \mathbf{I}_{m_k} \otimes (\mathbf{V}_k - \mathbf{W}_k) + \mathbf{J}_{m_k} \otimes \mathbf{W}_k, \end{aligned}$$

where \mathbf{V}_k and \mathbf{W}_k are $(p_{1,k-1} \times p_{1,k-1})$ matrices such that $\mathbf{V}_k = \text{cov} [\mathbf{x}'_{r,p_{1,k-1};t}]$, $t = 1, \dots, m_k$ and $\mathbf{W}_k = \mathbf{J}_{p_{2,k-1}} \otimes \mathbf{U}_{k,k}$.

In the second depth level when we consider \mathbf{V}_k is partitioned into $(p_{1,k-2} \times p_{1,k-2})$ matrices, it turns out to be also of the form

$$\begin{aligned} \mathbf{V}_k &= \begin{bmatrix} \mathbf{V}_{k-1} & \mathbf{W}_{k-1} & \cdots & \mathbf{W}_{k-1} \\ \mathbf{W}_{k-1} & \mathbf{V}_{k-1} & \cdots & \mathbf{W}_{k-1} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{W}_{k-1} & \mathbf{W}_{k-1} & \cdots & \mathbf{V}_{k-1} \end{bmatrix} \\ &= \mathbf{I}_{m_{k-1}} \otimes (\mathbf{V}_{k-1} - \mathbf{W}_{k-1}) + \mathbf{J}_{m_{k-1}} \otimes \mathbf{W}_{k-1}, \end{aligned}$$

where \mathbf{V}_{k-1} and \mathbf{W}_{k-1} are $(p_{1,k-2} \times p_{1,k-2})$ matrices such that $\mathbf{V}_{k-1} = \text{Cov} [\mathbf{x}'_{r,p_{1,k-2};t}]$, for $t = 1, \dots, m_{k-1}m_k = p_{k-1,k}$, and $\mathbf{W}_{k-1} = \mathbf{J}_{p_{2,k-2}} \otimes \mathbf{U}_{k,k-1}$.

The same phenomenon happens for each $j = 0, 1, \dots, k-2$, in the $j+1$ depth level when we consider \mathbf{V}_{k-j} is partitioned into $(p_{1,k-j-2} \times p_{1,k-j-2})$ matrices it turns out to be of the form

$$\begin{aligned} \mathbf{V}_{k+1-j} &= \begin{bmatrix} \mathbf{V}_{k-j} & \mathbf{W}_{k-j} & \cdots & \mathbf{W}_{k-j} \\ \mathbf{W}_{k-j} & \mathbf{V}_{k-j} & \cdots & \mathbf{W}_{k-j} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{W}_{k-j} & \mathbf{W}_{k-j} & \cdots & \mathbf{V}_{k-j} \end{bmatrix} \\ &= \mathbf{I}_{m_{k-j}} \otimes (\mathbf{V}_{k-j} - \mathbf{W}_{k-j}) + \mathbf{J}_{m_{k-j}} \otimes \mathbf{W}_{k-j}, \end{aligned} \tag{4}$$

where \mathbf{V}_{k-j} and \mathbf{W}_{k-j} are $(p_{1,k-j-1} \times p_{1,k-j-1})$ matrices such that $\mathbf{V}_{k-j} = \text{Cov} [\mathbf{x}'_{r,p_{1,k-j-1};t}]$, for $t = 1, \dots, p_{k-j,k}$, and $\mathbf{W}_{k-j} = \mathbf{J}_{p_{2,k-j-1}} \otimes \mathbf{U}_{k,k-j}$. We use this self similar property of $\mathbf{\Gamma}_x$ to find out the inverse and the determinants of $\mathbf{\Gamma}_x$ in the following two lemmas. In both lemmas, matrices

$$\Delta_{k,j} = \sum_{i=1}^j p_{2,i} (\mathbf{U}_{k,i} - \mathbf{U}_{k,i+1}), \quad \text{for } j = 1, \dots, k, \tag{5}$$

play an important role. These matrices can also be expressed using the $\mathbf{i}_{k:j} = (i_{k:j,h} : h = 1, \dots, k-1)$ notation given in (2), that is,

$$\Delta_{k,j} = \sum_{j^*=1}^j \left(\prod_{h=k-j^*+1}^{k-1} m_{k+1-h}^{i_{k:j^*,h}} \right) (\mathbf{U}_{k,j^*} - \mathbf{U}_{k,j^*+1}), \quad (6)$$

since

$$\begin{aligned} \prod_{h=1}^{k-1} m_{k+1-h}^{i_{k:j^*,h}} &= \prod_{h=k-j^*+1}^{k-1} m_{k+1-h}^{i_{k:j^*,h}} \\ &= \prod_{h=k-j^*+1}^{k-1} m_{k+1-h} = p_{2,j^*}, \end{aligned} \quad (7)$$

because $\mathbf{i}_{k:j^*} = (i_{k:j^*,h} : h = 1, \dots, k-1)$ with

$$i_{k:j^*,h} = \begin{cases} 0 & \text{if } h = 1, \dots, k-j^* \\ 1 & \text{if } h = k-(j^*-1), \dots, k-1. \end{cases}$$

Lemma 1 *Let $\mathbf{\Gamma}_x$ be a k -SSCS variance-covariance matrix as in equation (1) of Definition 1. It can be proved that if $\Delta_{k,j}$, for $j = 1, \dots, k$, are all non singular matrices, then*

$$\mathbf{\Gamma}_{x_r}^{-1} = \sum_{j=1}^k \left(\bigotimes_{h=1}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k:j,h}} \right) \otimes \frac{1}{p_{2,j}} (\Delta_{k,j}^{-1} - \Delta_{k,j-1}^{-1}), \quad (8)$$

where the symbol $\Delta_{k,0}^{-1}$ indicates the $(m_1 \times m_1)$ zero matrix ($\Delta_{k,0}^{-1} = \mathbf{0}_{m_1 \times m_1}$). Notice that when $\mathbf{U}_{k,j} = \mathbf{U}_{k+1,j}$ for $j = 1, \dots, k$, then $\Delta_{k+1,j} = \Delta_{k,j}$, for $j = 1, \dots, k-1$, but $\Delta_{k+1,k} = \Delta_{k,k} - p_{2,k} \mathbf{U}_{k+1,k+1}$.

The proof of this lemma is given in Appendix A.1. It is worthwhile to note that the form of $\mathbf{\Gamma}_{x_r}^{-1}$ is the same as the form of $\mathbf{\Gamma}_{x_r}$. Therefore, the SSCS covariance structure is invariant with respect to the inverse. Furthermore, SSCS covariance structure is invariant with respect to addition. Using similar inductive arguments as above we can prove the following lemma.

Lemma 2 *Let $\mathbf{\Gamma}_x$ be a k -SSCS variance-covariance matrix as in equation (1) of Definition 1. Let $p_{k+1,k} = 1$ and $p_{k+2,k} = 0$. Then, it can be proved that*

$$|\mathbf{\Gamma}_{x_r}| = |\mathbf{V}_{k+1}| = \prod_{j=1}^k |\Delta_j|^{p_{j+1,k} - p_{j+2,k}}, \quad (9)$$

The proof of this lemma is given in Appendix A.2.

4 Estimation

To carry out any statistical analysis with multi-level data we need to estimate the k -SSCS covariance matrix $\mathbf{\Gamma}_x$. We obtain MLEs of $\mathbf{\Gamma}_x$ and its component matrices in the following Section 4.1. However, for the derivation of many statistics for testing purposes we need the unbiased estimates of the k -SSCS covariance matrix $\mathbf{\Gamma}_x$ and its component matrices, which are derived in Section 4.2.

4.1 Maximum likelihood estimators of the k -SSCS covariance matrix $\mathbf{\Gamma}_x$

Theorem 1 *If $\mathbf{x}_1, \dots, \mathbf{x}_n$ is a random sample of size n from a population with distribution $N_{p_{1,k}}(\boldsymbol{\mu}_x; \mathbf{\Gamma}_x)$, where $\mathbf{\Gamma}_x$ is a positive definite k -SSCS covariance matrix, then the MLE of $\boldsymbol{\mu}_x$ is $\hat{\boldsymbol{\mu}}_x = \bar{\mathbf{x}}$, where*

$$\bar{\mathbf{x}} = \frac{1}{n} \sum_{r=1}^n \mathbf{x}_r,$$

and the MLE $\hat{\mathbf{\Gamma}}_x$ of $\mathbf{\Gamma}_x$ is

$$\hat{\mathbf{\Gamma}}_x = \sum_{j=1}^k \left(\bigotimes_{h=1}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k:j,h}} \right) \otimes (\hat{\mathbf{U}}_{k,j} - \hat{\mathbf{U}}_{k,j+1}),$$

where $\hat{\mathbf{U}}_{k,h}$, for $j = 1, \dots, k$, and $h = 1, \dots, k-1$, are given in (A27).

The proof of this theorem which is straightforward but tedious is given in Appendix A.3.

Example 5 *If $k = 2$ (see Example 2) we have*

$$\hat{\mathbf{U}}_{2,1} = \mathbf{C}_{2,1} = \frac{\mathbf{B}_{2,1}}{n \cdot m_2} = \frac{1}{n \cdot m_2} \sum_{r=1}^n \sum_{f_2=1}^{m_2} (\mathbf{x}_{r,f_2} - \bar{\mathbf{x}}_{f_2}) (\mathbf{x}_{r,f_2} - \bar{\mathbf{x}}_{f_2})' \quad \text{and}$$

$$\hat{\mathbf{U}}_{2,2} = \mathbf{C}_{2,2} = \frac{\mathbf{B}_{2,2}}{n \cdot m_2 (m_2 - 1)} = \frac{1}{n \cdot m_2 (m_2 - 1)} \sum_{r=1}^n \sum_{f_2=1}^{m_2} \sum_{f_2^* \neq f_2}^{m_2} (\mathbf{x}_{r,f_2} - \bar{\mathbf{x}}_{f_2}) (\mathbf{x}_{r,f_2^*} - \bar{\mathbf{x}}_{f_2^*})'.$$

The same estimates are obtained by Leiva (2007).

Example 6 *If $k = 3$ (see Example 3) then*

$$\begin{aligned} \mathbf{B}_{3,1} &= \sum_{r=1}^n \sum_{f_2=1}^{m_2} \sum_{f_3=1}^{m_3} (\mathbf{x}_{r,f_2 f_3} - \bar{\mathbf{x}}_{f_2 f_3}) (\mathbf{x}_{r,f_2 f_3} - \bar{\mathbf{x}}_{f_2 f_3})' \\ \mathbf{B}_{3,2} &= \sum_{r=1}^n \sum_{f_2=1}^{m_2} \sum_{f_3=1}^{m_3} \sum_{f_3^* \neq f_3}^{m_3} (\mathbf{x}_{r,f_2 f_3} - \bar{\mathbf{x}}_{f_2 f_3}) (\mathbf{x}_{r,f_2 f_3^*} - \bar{\mathbf{x}}_{f_2 f_3^*})' \quad \text{and} \\ \mathbf{B}_{3,3} &= \sum_{r=1}^n \sum_{f_2=1}^{m_2} \sum_{f_2^* \neq f_2}^{m_2} \sum_{f_3=1}^{m_3} \sum_{f_3^*=1}^{m_3} (\mathbf{x}_{r,f_2 f_3} - \bar{\mathbf{x}}_{f_2 f_3}) (\mathbf{x}_{r,f_2^* f_3^*} - \bar{\mathbf{x}}_{f_2^* f_3^*})'. \end{aligned}$$

Therefore

$$\begin{aligned}\widehat{U}_{3,1} &= C_{3,1} = \frac{B_{3,1}}{n \cdot m_3 \cdot m_2} \\ \widehat{U}_{3,2} &= C_{3,2} = \frac{B_{3,2}}{n \cdot m_3 \cdot m_2 (m_2 - 1)} \quad \text{and} \\ \widehat{U}_{3,3} &= C_{3,3} = \frac{B_{3,3}}{n \cdot m_3 (m_3 - 1) \cdot m_2 m_2}.\end{aligned}$$

The same estimates are obtained by Roy and Leiva (2007).

Example 7 If $k = 4$ (see Example 4) then

$$\begin{aligned}B_{4,1} &= \sum_{r=1}^n \sum_{f_2=1}^{m_2} \sum_{f_3=1}^{m_3} \sum_{f_4=1}^{m_4} (\mathbf{x}_{r;f_2f_3f_4} - \bar{\mathbf{x}}_{f_2f_3f_4}) (\mathbf{x}_{r;f_2f_3f_4} - \bar{\mathbf{x}}_{f_2f_3f_4})', \\ B_{4,2} &= \sum_{r=1}^n \sum_{f_2=1}^{m_2} \sum_{f_3=1}^{m_3} \sum_{f_4=1}^{m_4} \sum_{f_4 \neq f_4^*=1}^{m_4} (\mathbf{x}_{r;f_2f_3f_4} - \bar{\mathbf{x}}_{f_2f_3f_4}) (\mathbf{x}_{r;f_2f_3f_4} - \bar{\mathbf{x}}_{f_2f_3f_4})', \\ B_{4,3} &= \sum_{r=1}^n \sum_{f_2=1}^{m_2} \sum_{f_3=1}^{m_3} \sum_{f_3 \neq f_3^*=1}^{m_3} \sum_{f_4=1}^{m_4} \sum_{f_4^*=1}^{m_4} (\mathbf{x}_{r;f_2f_3f_4} - \bar{\mathbf{x}}_{f_2f_3f_4}) (\mathbf{x}_{r;f_2f_3f_4} - \bar{\mathbf{x}}_{f_2f_3f_4})' \quad \text{and} \\ B_{4,4} &= \sum_{r=1}^n \sum_{f_2=1}^{m_2} \sum_{f_2 \neq f_2^*=1}^{m_2} \sum_{f_3=1}^{m_3} \sum_{f_3^*=1}^{m_3} \sum_{f_4=1}^{m_4} \sum_{f_4^*=1}^{m_4} (\mathbf{x}_{r;f_2f_3f_4} - \bar{\mathbf{x}}_{f_2f_3f_4}) (\mathbf{x}_{r;f_2f_3f_4} - \bar{\mathbf{x}}_{f_2f_3f_4})' .\end{aligned}$$

Therefore

$$\begin{aligned}\widehat{U}_{4,1} &= C_{4,1} = \frac{B_{4,1}}{n \cdot m_4 \cdot m_3 \cdot m_2} \\ \widehat{U}_{4,2} &= C_{4,2} = \frac{B_{4,2}}{n \cdot m_4 \cdot m_3 \cdot m_2 (m_2 - 1)} \\ \widehat{U}_{4,3} &= C_{4,3} = \frac{B_{4,3}}{n \cdot m_4 \cdot m_3 (m_3 - 1) \cdot m_2 m_2} \quad \text{and} \\ \widehat{U}_{4,4} &= C_{4,4} = \frac{B_{4,4}}{n \cdot m_4 (m_4 - 1) \cdot m_3 m_3 \cdot m_2 m_2}.\end{aligned}$$

4.2 Unbiased estimators of the k -SSCS covariance matrix $\Gamma_{\mathbf{x}}$

Theorem 2 An unbiased estimator of the k -SSCS covariance matrix $\Gamma_{\mathbf{x}}$ is given by

$$\tilde{\Gamma}_{\mathbf{x}} = \sum_{j=1}^k \left(\bigotimes_{h=1}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k;j,h}} \right) \otimes (\tilde{U}_{k,j} - \tilde{U}_{k,j+1}),$$

where an unbiased estimator of the component matrices $U_{k,j}$ for each $j = 1, \dots, k$ are given by

$$\tilde{U}_{k,j} = \frac{n}{n-1} C_{k,j} = \frac{B_{k,j}}{(n-1) q_{k,j}} = \frac{n}{n-1} \widehat{U}_{k,j}.$$

Under the Normal assumption of Theorem 1 of the previous Section 4.1 and using the partitioned $\bar{\mathbf{x}}$ into $m_1 \times 1$ subvectors given in (A20), we know that

$$\bar{\mathbf{x}} = \left(\bar{\mathbf{x}}'_{f_2, f_3, \dots, f_k} : f_j \in F_j = \{1, \dots, m_j\}, \text{ for } j = 2, \dots, k \right)' \sim N_{p_{1,k}} \left(\boldsymbol{\mu}_{\mathbf{x}}; \frac{1}{n} \boldsymbol{\Gamma}_{\mathbf{x}} \right), \quad (10)$$

where $\bar{\mathbf{x}}_{f_2, f_3, \dots, f_k} \in \mathbb{R}^{m_1}$ is given by (A21), where

$$\boldsymbol{\mu}_{\mathbf{x}} = \boldsymbol{\mu}_{\mathbf{x}_r} = \left(\boldsymbol{\mu}'_{f_2, f_3, \dots, f_k} : f_j \in F_j = \{1, \dots, m_j\}, \text{ for } j = 2, \dots, k \right)',$$

and $\boldsymbol{\Gamma}_{\mathbf{x}}$ is a k -SSCS positive definite covariance matrix given by (1).

By the definition $\boldsymbol{\Gamma}_{\mathbf{x}}$ is

$$E \left[\left(\mathbf{x}_{r; f_2^*, \dots, f_{j+1}^*, f_j, \dots, f_k} - \boldsymbol{\mu}_{f_2^*, \dots, f_{j+1}^*, f_j, \dots, f_k} \right) \left(\mathbf{x}_{r; f_2, f_3, \dots, f_k} - \boldsymbol{\mu}_{f_2, f_3, \dots, f_k} \right)' \right] = \mathbf{U}_{k,j}, \quad (11)$$

and from (10) we know that

$$E \left[\left(\bar{\mathbf{x}}_{f_2^*, \dots, f_{j+1}^*, f_j, \dots, f_k} - \boldsymbol{\mu}_{f_2^*, \dots, f_{j+1}^*, f_j, \dots, f_k} \right) \left(\bar{\mathbf{x}}_{f_2, f_3, \dots, f_k} - \boldsymbol{\mu}_{f_2, f_3, \dots, f_k} \right)' \right] = \frac{1}{n} \mathbf{U}_{k,j}. \quad (12)$$

Now from (A17) we have

$$\sum_{r=1}^n (\mathbf{x}_r - \bar{\mathbf{x}}) (\mathbf{x}_r - \bar{\mathbf{x}})' = \left[\sum_{r=1}^n (\mathbf{x}_r - \boldsymbol{\mu}_{\mathbf{x}}) (\mathbf{x}_r - \boldsymbol{\mu}_{\mathbf{x}})' \right] - n (\bar{\mathbf{x}} - \boldsymbol{\mu}_{\mathbf{x}}) (\bar{\mathbf{x}} - \boldsymbol{\mu}_{\mathbf{x}})',$$

and, in particular, using the notation $q_{k,j}$ given in (A26) we have

$$\begin{aligned} nq_{k,j} \mathbf{C}_{k,j} &= \sum_{r=1}^n \overbrace{\sum_{f_k \in F_k} \cdots \sum_{f_{j+1} \in F_{j+1}}}^{k-j \text{ sums}} \overbrace{\left(\sum_{f_j \in F_j} \sum_{f_j \neq f_j^* \in F_j} \right)}^{1 \text{ special sum pair}} \overbrace{\left(\sum_{f_{j-1} \in F_{j-1}} \sum_{f_{j-1}^* \in F_{j-1}} \right) \cdots \left(\sum_{f_2 \in F_k} \sum_{f_2^* \in F_k} \right)}^{j-2 \text{ sum pairs}} \\ &\quad \left(\mathbf{x}_{r; \mathbf{f}^*(i_{k:j})} - \bar{\mathbf{x}}_{\mathbf{f}^*(i_{k:j})} \right) \left(\mathbf{x}_{r; \mathbf{f}} - \bar{\mathbf{x}}_{\mathbf{f}} \right)' \\ &= \left[\sum_{r=1}^n \sum_{f_k \in F_k} \cdots \sum_{f_{j+1} \in F_{j+1}} \left(\sum_{f_j \in F_j} \sum_{f_j \neq f_j^* \in F_j} \right) \left(\sum_{f_{j-1} \in F_{j-1}} \sum_{f_{j-1}^* \in F_{j-1}} \right) \right. \\ &\quad \left. \cdots \left(\sum_{f_2 \in F_k} \sum_{f_2^* \in F_k} \right) \left(\mathbf{x}_{r; \mathbf{f}^*(i_{k:j})} - \boldsymbol{\mu}_{\mathbf{f}^*(i_{k:j})} \right) \left(\mathbf{x}_{r; \mathbf{f}} - \boldsymbol{\mu}_{\mathbf{f}} \right)' \right] \\ &\quad - \left[\sum_{f_k \in F_k} \cdots \sum_{f_{j+1} \in F_{j+1}} \left(\sum_{f_j \in F_j} \sum_{f_j \neq f_j^* \in F_j} \right) \left(\sum_{f_{j-1} \in F_{j-1}} \sum_{f_{j-1}^* \in F_{j-1}} \right) \right. \\ &\quad \left. \cdots \left(\sum_{f_2 \in F_k} \sum_{f_2^* \in F_k} \right) n \left(\bar{\mathbf{x}}_{\mathbf{f}^*(i_{k:j})} - \boldsymbol{\mu}_{\mathbf{f}^*(i_{k:j})} \right) \left(\bar{\mathbf{x}}_{\mathbf{f}} - \boldsymbol{\mu}_{\mathbf{f}} \right)' \right]. \end{aligned}$$

Therefore

$$\begin{aligned} E[nq_{k,j}\mathbf{C}_{k,j}] &= nq_{k,j}\mathbf{U}_{k,j} - q_{k,j}\mathbf{U}_{k,j} \\ &= (n-1)q_{k,j}\mathbf{U}_{k,j}, \end{aligned}$$

and thus,

$$E\left[\frac{n}{n-1}\mathbf{C}_{k,j}\right] = \mathbf{U}_{k,j}.$$

As a result

$$\tilde{\mathbf{U}}_{k,j} = \frac{n}{n-1}\mathbf{C}_{k,j} = \frac{\mathbf{B}_{k,j}}{(n-1)q_{k,j}} = \frac{n}{n-1}\hat{\mathbf{U}}_{k,j} \quad (13)$$

is an unbiased estimator of $\mathbf{U}_{k,j}$ for each $j = 1, \dots, k$. Therefore,

$$\tilde{\mathbf{\Gamma}}_{\mathbf{x}} = \sum_{j=1}^k \left(\bigotimes_{h=1}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k:j,h}} \right) \otimes (\tilde{\mathbf{U}}_{k,j} - \tilde{\mathbf{U}}_{k,j+1}) \quad (14)$$

is an unbiased estimator of the k -SSCS covariance matrix $\mathbf{\Gamma}_{\mathbf{x}}$.

5 Spectral decompositions of the k -SSCS covariance matrix

We perform spectral decompositions of the k -SSCS variance-covariance matrix. We get the eigenblocks $\mathbf{\Delta}_{k,k}, \mathbf{\Delta}_{k,k-1}, \dots, \mathbf{\Delta}_{k,1}$ and the corresponding eigenmatrices of the k -SSCS variance-covariance matrix $\mathbf{\Gamma}_{\mathbf{x}}$ in this section. Explicit unbiased estimators of the eigenblocks are given in Lemma 5.

5.1 Eigenblocks and eigenmatrices

Let us consider the following orthogonal matrices

$$\begin{aligned} \mathbf{\Gamma}^1 &= \mathbf{H}'_{m_k} \otimes \mathbf{I}_{m_1 \dots m_{k-1}} \\ \mathbf{\Gamma}^2 &= \mathbf{I}_{m_k} \otimes (\mathbf{H}'_{m_{k-1}} \otimes \mathbf{I}_{m_1 \dots m_{k-2}}) \\ &\vdots \\ \text{and } \mathbf{\Gamma}^{k-1} &= \mathbf{I}_{m_k} \otimes \mathbf{I}_{m_{k-1}} \otimes \dots \otimes \mathbf{I}_{m_3} \otimes (\mathbf{H}'_{m_2} \otimes \mathbf{I}_{m_1}) \end{aligned}$$

where for each $j = 2, \dots, k$, \mathbf{H}_{m_j} is $m_j \times m_j$ Helmert matrix, that is, an orthogonal matrix whose first column is proportional to $\mathbf{1}_{m_j}$, (note that $\mathbf{\Gamma}^1, \dots, \mathbf{\Gamma}^{k-1}$ are not function of neither \mathbf{U}_i 's). Since the product of orthogonal matrices is an orthogonal matrix,

$$\begin{aligned} \mathbf{L}'_k &= \mathbf{\Gamma}^{k-1} \dots \mathbf{\Gamma}^1 \\ &= [\mathbf{I}_{m_k} \otimes \mathbf{I}_{m_{k-1}} \otimes \dots \otimes \mathbf{I}_{m_3} \otimes (\mathbf{H}'_{m_2} \otimes \mathbf{I}_{m_1})] \dots (\mathbf{H}'_{m_k} \otimes \mathbf{I}_{m_1 \dots m_{k-1}}) \\ &= \mathbf{H}' \otimes \mathbf{I}_{m_1} \end{aligned}$$

is an orthogonal matrix where

$$\mathbf{H}_{p_{2,k} \times p_{2,k}} = \mathbf{H}_{m_k} \otimes \mathbf{H}_{m_{k-1}} \otimes \cdots \otimes \mathbf{H}_{m_2}.$$

This \mathbf{L}_k diagonalizes the SSCS matrix $\mathbf{\Gamma}_{\mathbf{x}}$. The following theorem present this result and it is proved using mathematical induction. To anticipate the idea of the inductive implication proof, let's consider the example where starting from the knowledge of the diagonalization of $\mathbf{\Gamma}_{\mathbf{x}} = \mathbf{V}_{k+1}$ for the case $k = 2$, then the case $k = 3$ is proved

Example 8 When $k = 2$ (see Example 2) the diagonalization of matrix

$$\begin{aligned} \mathbf{V}_{k+1} &= \mathbf{V}_3 = \mathbf{I}_{m_2} \otimes (\mathbf{V}_2 - \mathbf{W}_2) + \mathbf{J}_{m_1} \otimes \mathbf{W}_2 \\ &= \mathbf{I}_{m_2} \otimes (\mathbf{U}_1 - \mathbf{U}_2) + \mathbf{J}_{m_1} \otimes \mathbf{U}_2 \end{aligned} \quad (15)$$

is doing by pre and post multiplying \mathbf{V}_3 as follows (see Leiva 2007)

$$\begin{aligned} \mathbf{L}'_2 \mathbf{V}_3 \mathbf{L}_2 &= (\mathbf{H}'_{m_2} \otimes \mathbf{I}_{m_1}) \mathbf{V}_3 (\mathbf{H}_{m_2} \otimes \mathbf{I}_{m_1}) \\ &= \text{diag}\{\mathbf{U}_1 + (m_2 - 1)\mathbf{U}_2; \mathbf{I}_{m_2-1} \otimes (\mathbf{U}_1 - \mathbf{U}_2)\}, \end{aligned}$$

where

$$\begin{aligned} \Delta_{2,2} &= \mathbf{U}_1 + (m_2 - 1)\mathbf{U}_2 \quad \text{and} \\ \Delta_{2,1} &= \mathbf{U}_1 - \mathbf{U}_2, \end{aligned}$$

This result is assumed known (in the proof of Theorem 2 this will be replaced by the inductive hypothesis). We want to proof the corresponding result for the case $k = 3$, that is, for the 3-SSCS covariance matrix (see example 3)

$$\mathbf{V}_4 = \mathbf{I}_{m_3} \otimes \mathbf{I}_{m_2} \otimes (\mathbf{U}_1 - \mathbf{U}_2) + \mathbf{I}_{m_3} \otimes \mathbf{J}_{m_2} \otimes (\mathbf{U}_2 - \mathbf{U}_3) + \mathbf{J}_{m_3} \otimes \mathbf{J}_{m_2} \otimes \mathbf{U}_3,$$

that is, the result to be proved is

$$\begin{aligned} &\mathbf{L}'_3 \mathbf{V}_4 \mathbf{L}_3 \\ &= (\mathbf{H}'_{m_3} \otimes \mathbf{H}'_{m_2} \otimes \mathbf{I}_{m_1}) \mathbf{V}_4 (\mathbf{H}_{m_3} \otimes \mathbf{H}_{m_2} \otimes \mathbf{I}_{m_1}) \\ &= \text{diag}\{\Delta_{3,3}; \mathbf{I}_{m_2-1} \otimes \Delta_{3,1}; \mathbf{I}_{m_3-1} \otimes \text{diag}\{\Delta_{3,2}; \mathbf{I}_{m_2-1} \otimes \Delta_{3,1}\}\}, \end{aligned}$$

where

$$\begin{aligned} \Delta_{3,3} &= (\mathbf{U}_1 - \mathbf{U}_2) + m_2(\mathbf{U}_2 - \mathbf{U}_3) + m_2 m_3 \mathbf{U}_3 \\ \Delta_{3,2} &= (\mathbf{U}_1 - \mathbf{U}_2) + m_2(\mathbf{U}_2 - \mathbf{U}_3) \quad \text{and} \\ \Delta_{3,1} &= \mathbf{U}_1 - \mathbf{U}_2, \end{aligned}$$

For a proof see Lemma 3.1 in Roy and Fonseca (2012). However, we prove the result for $k = 3$ here as well, so that it would help the readers to follow the next theorem structurally. In the first step we write \mathbf{V}_4 as a $3 - 1 = 2$ -SSCS matrix of the form

$$\mathbf{V}_4 = \mathbf{I}_{m_3} \otimes (\mathbf{V}_3 - \mathbf{W}_3) + \mathbf{J}_{m_3} \otimes \mathbf{W}_3, \quad \begin{matrix} p_{1,3-1} \times p_{1,3-1} & p_{1,3-1} \times p_{1,3-1} \end{matrix},$$

where \mathbf{V}_3 is given in (15) and $\mathbf{W}_3 = \mathbf{J}_{m_2} \otimes \mathbf{U}_3$. Then using the known result for the case $k = 2$ diagonalize the matrix \mathbf{V}_4 using the orthogonal matrix $\mathbf{H}_{m_3} \otimes \mathbf{I}_{p_{1,2}}$

$$\begin{aligned} \mathbf{D}_3 &= (\mathbf{H}'_{m_3} \otimes \mathbf{I}_{m_1 m_2}) \mathbf{V}_4 (\mathbf{H}_{m_3} \otimes \mathbf{I}_{m_1 m_2}) \\ &= \text{diag} \{ \mathbf{V}_3 + (m_3 - 1) \mathbf{W}_3; \mathbf{I}_{m_3-1} \otimes (\mathbf{V}_3 - \mathbf{W}_3) \}. \end{aligned} \quad (16)$$

In the second step we realize that both $\mathbf{V}_3 + (m_3 - 1) \mathbf{W}_3$ and $\mathbf{V}_3 - \mathbf{W}_3$ are 2-SSCS matrix of the form

$$\begin{aligned} &\mathbf{V}_3 + (m_3 - 1) \mathbf{W}_3 \\ &= \mathbf{I}_{m_2} \otimes [(\mathbf{U}_1 + (m_3 - 1) \mathbf{U}_3) - (\mathbf{U}_2 + (m_3 - 1) \mathbf{U}_3)] + \mathbf{J}_{m_2} \otimes (\mathbf{U}_2 + (m_3 - 1) \mathbf{U}_3) \\ &\quad \begin{matrix} p_{1,2-1} \times p_{1,2-1} & p_{1,2-1} \times p_{1,2-1} \end{matrix} \\ &= \mathbf{I}_{m_2} \otimes (\mathbf{U}_1 - \mathbf{U}_2) + \mathbf{J}_{m_2} \otimes (\mathbf{U}_2 + (m_3 - 1) \mathbf{U}_3), \end{aligned}$$

and

$$\begin{aligned} \mathbf{V}_3 - \mathbf{W}_3 &= \mathbf{I}_{m_2} \otimes [(\mathbf{U}_1 - \mathbf{U}_3) - (\mathbf{U}_2 - \mathbf{U}_3)] + \mathbf{J}_{m_2} \otimes (\mathbf{U}_2 - \mathbf{U}_3) \\ &= \mathbf{I}_{m_2} \otimes (\mathbf{U}_1 - \mathbf{U}_2) + \mathbf{J}_{m_2} \otimes (\mathbf{U}_2 - \mathbf{U}_3), \end{aligned}$$

repectively, and consequently, both can be diagonalize using $\mathbf{H}_{m_2} \otimes \mathbf{I}_{p_{1,1}}$, that is,

$$\begin{aligned} \mathbf{D}_3^{**} &= (\mathbf{H}'_{m_2} \otimes \mathbf{I}_{p_{1,1}}) [\mathbf{V}_3 + (m_3 - 1) \mathbf{W}_3] (\mathbf{H}_{m_2} \otimes \mathbf{I}_{p_{1,1}}) \\ &= \text{diag} \{ (\mathbf{U}_1 - \mathbf{U}_2) + m_2 (\mathbf{U}_2 + (m_3 - 1) \mathbf{U}_3); \mathbf{I}_{m_2-1} \otimes (\mathbf{U}_1 - \mathbf{U}_2) \} \\ &= \text{diag} \{ (\mathbf{U}_1 - \mathbf{U}_2) + m_2 (\mathbf{U}_2 - \mathbf{U}_3) + m_2 m_3 \mathbf{U}_3; \mathbf{I}_{m_2-1} \otimes (\mathbf{U}_1 - \mathbf{U}_2) \} \end{aligned} \quad (17)$$

and

$$\begin{aligned} \mathbf{D}_3^* &= (\mathbf{H}'_{m_2} \otimes \mathbf{I}_{p_{1,1}}) (\mathbf{V}_3 - \mathbf{W}_3) (\mathbf{H}_{m_2} \otimes \mathbf{I}_{p_{1,1}}) \\ &= \text{diag} \{ (\mathbf{U}_1 - \mathbf{U}_2) + m_2 (\mathbf{U}_2 - \mathbf{U}_3); \mathbf{I}_{m_2-1} \otimes (\mathbf{U}_1 - \mathbf{U}_2) \}. \end{aligned} \quad (18)$$

The final step is to apply $\mathbf{I}_{m_3} \otimes \mathbf{H}_{m_2} \otimes \mathbf{I}_{p_{1,1}} = \text{diag} \{ \mathbf{H}_{m_2} \otimes \mathbf{I}_{p_{1,1}}, \mathbf{I}_{m_3-1} \otimes \mathbf{H}_{m_2} \otimes \mathbf{I}_{p_{1,1}} \}$ to diagonalize

Proof: Proof is given in Appendix A.4.

Finally, note that the diagonal blocks $\Delta_{k,j}$, $j = 1, \dots, k$ in the diagonal matrix $\mathbf{L}'_k \boldsymbol{\Gamma}_x \mathbf{L}_k$, are repeated, and not in order. One can cluster them together with the help of commutation matrix. Thus, we have the following corollary.

Corollary 1 *Multiplying the orthogonal matrix \mathbf{L}_k by an appropriate $(p_{1,k} \times p_{1,k})$ -dimensional permutation matrix (orthogonal) \mathbf{K}_k we have*

$$\mathbf{K}'_k \mathbf{L}'_k \boldsymbol{\Gamma}_x \mathbf{L}_k \mathbf{K}_k = \text{Diag} \left[\underbrace{\Delta_{k,k}; \Delta_{k,k-1}; \dots; \Delta_{k,k-1}}_{(m_k-1) \text{ times}}; \dots; \underbrace{\Delta_{k,1}; \dots; \Delta_{k,1}}_{m_3 \dots m_k (m_2-1) \text{ times}} \right].$$

We have

$$\begin{aligned} \boldsymbol{\Gamma}_x &= \mathbf{L}_k \mathbf{K}_k \text{Diag} \left[\underbrace{\Delta_{k,k}; \Delta_{k,k-1}; \dots; \Delta_{k,k-1}}_{(m_k-1) \text{ times}}; \dots; \underbrace{\Delta_{k,1}; \dots; \Delta_{k,1}}_{m_3 \dots m_k (m_2-1) \text{ times}} \right] \mathbf{K}'_k \mathbf{L}'_k \\ &= \mathbf{L}_k \mathbf{K}_k \text{Diag} \left[\underbrace{\Delta_{k,k}; \Delta_{k,k-1}; \dots; \Delta_{k,k-1}}_{(p_{k,k}-1) \text{ times}}; \dots; \underbrace{\Delta_{k,1}; \dots; \Delta_{k,1}}_{p_{2,k}-p_{3,k} \text{ times}} \right] \mathbf{K}'_k \mathbf{L}'_k. \end{aligned}$$

We now partition (horizontal, side by side) the orthogonal matrix $\mathbf{L}_k \mathbf{K}_k$ as $p_{2,k}$ $p_{1,k} \times m_1$ blocks as $\mathbf{L}_k \mathbf{K}_k = [\mathbf{E}_1 : \dots : \mathbf{E}_{p_{2,k}}]$. So,

$$(\mathbf{L}_k \mathbf{K}_k)' = \begin{bmatrix} \mathbf{E}'_1 \\ \vdots \\ \mathbf{E}'_{p_{2,k}} \end{bmatrix}$$

Therefore,

$$\boldsymbol{\Gamma}_x = \mathbf{E}_1 \Delta_{k,k} \mathbf{E}'_1 + \sum_{i=2}^{p_{k,k}} \mathbf{E}_i \Delta_{k,k-1} \mathbf{E}'_i + \dots + \sum_{i=p_{3,k}+1}^{p_{2,k}} \mathbf{E}_i \Delta_{k,1} \mathbf{E}'_i,$$

where \mathbf{E}_1 is the eigenmatrix corresponding to eigenblock $\Delta_{k,k}$, \mathbf{E}_i , $i = 2, \dots, p_{k,k}$ is the eigenmatrices corresponding to eigenblock $\Delta_{k,k-1}$ and \mathbf{E}_i , $i = p_{3,k} + 1, \dots, p_{2,k}$ is the eigenmatrices corresponding to eigenblock $\Delta_{k,1}$. The eigenmatrices $[\mathbf{E}_1 : \dots : \mathbf{E}_{p_{2,k}}]$ are not functions of either of the SSCS-component matrices $\mathbf{U}_{k,j}$, $j = 1, \dots, k$.

Thus, SSCS covariance structure for k -level data has k distinct eigenblocks: $\Delta_{k,k}$, $\Delta_{k,k-1}$ with multiplicity $p_{k,k} - 1$, \dots , $\Delta_{k,1}$ with multiplicity $p_{2,k} - p_{3,k}$.

Now, since $L_k K_k$ is an orthogonal matrix

$$\begin{aligned}
\text{tr}(\Gamma_x) &= \text{tr}\left(L_k K_k \text{Diag}\left[\Delta_{k,k}; \underbrace{\Delta_{k,k-1}; \dots; \Delta_{k,k-1}}_{(p_{k,k}-1) \text{ times}}; \dots; \underbrace{\Delta_{k,1}; \dots; \Delta_{k,1}}_{p_{2,k}-p_{3,k} \text{ times}}\right] K_k' L_k'\right) \\
&= \text{tr}\left(\text{Diag}\left[\Delta_{k,k}; \underbrace{\Delta_{k,k-1}; \dots; \Delta_{k,k-1}}_{(p_{k,k}-1) \text{ times}}; \dots; \underbrace{\Delta_{k,1}; \dots; \Delta_{k,1}}_{p_{2,k}-p_{3,k} \text{ times}}\right] K_k' L_k' L_k K_k\right) \\
&= \text{tr}\left(\text{Diag}\left[\Delta_{k,k}; \underbrace{\Delta_{k,k-1}; \dots; \Delta_{k,k-1}}_{(p_{k,k}-1) \text{ times}}; \dots; \underbrace{\Delta_{k,1}; \dots; \Delta_{k,1}}_{p_{2,k}-p_{3,k} \text{ times}}\right]\right) \\
&= \text{tr}(\Delta_{k,k}) + (p_{k,k} - 1)\text{tr}(\Delta_{k,k-1}) + \dots + (p_{2,k} - p_{3,k})\text{tr}(\Delta_{k,1}). \tag{21}
\end{aligned}$$

Thus, the total population variance $\text{tr}(\Gamma_x) = \text{tr}(\Delta_{k,k}) + (p_{k,k} - 1)\text{tr}(\Delta_{k,k-1}) + \dots + (p_{2,k} - p_{3,k})\text{tr}(\Delta_{k,1})$. Therefore, the trace of the variance-covariance matrix of the data is the sum of the traces of the $(p_{2,k} - p_{3,k})$ eigenblocks.

Note that the variability of each eigenblock $\Delta_{k,j}$, $j = 1, \dots, k$ depends on the data set at hand. It depends on the interconnections or the correlation matrix of the variables between the levels. However, if one wants to arrange the diagonal matrix according to the variability of the eigenblocks, one needs to choose an appropriate commutation matrix K_k . Suppose for some 3–SSCS covariance structure it may happen $\text{tr}(\tilde{\Delta}_{3,2}) > \text{tr}(\tilde{\Delta}_{3,1})$, and for some other 3–SSCS covariance structure the relationship may be opposite. In the following example we show a commutation matrix K_3 for a dataset where $\text{tr}(\tilde{\Delta}_{3,2}) > \text{tr}(\tilde{\Delta}_{3,1})$.

Example 9 *If $k = 3$, then there exists an $m_3 m_2 m_1 \times m_3 m_2 m_1$ orthogonal matrix L_3 such that*

$$L_3' \Gamma_x L_3 = \text{Diag}\left[\Delta_{3,3}; \underbrace{\Delta_{3,1}; \dots; \Delta_{3,1}}_{m_2-1}; \Delta_{3,2}; \underbrace{\Delta_{3,1}; \dots; \Delta_{3,1}}_{m_2-1}; \dots; \Delta_{3,2}; \underbrace{\Delta_{3,1}; \dots; \Delta_{3,1}}_{m_2-1}\right], \tag{22}$$

where the $m_3 m_2 m_1 \times m_1$ eigenblocks $\Delta_{3,1}; \Delta_{3,2}; \Delta_{3,3}$ are given in (5), and $P_3 = P_{m_3} P_{m_2} I_{m_1}$.

Now, one can find an appropriate $m_3 m_2 m_1 \times m_3 m_2 m_1$ –dimensional permutation matrix (orthogonal) K_3 such that K_3 matrix looks as follows:

$$K_3 = \begin{bmatrix} I_{m_1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & I_{m_2-1} \otimes I_{m_1} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & I_{m_1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & I_{m_2-1} \otimes I_{m_1} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & I_{m_1} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & I_{m_2-1} \otimes I_{m_1} \end{bmatrix},$$

Now,

$$\mathbf{K}'_3 \mathbf{L}'_3 \boldsymbol{\Gamma}_x \mathbf{L}_3 \mathbf{K}_3 = \text{Diag} \left[\underbrace{\Delta_{3,3}; \Delta_{3,2}; \dots; \Delta_{3,2}}_{(m_3-1) \text{ times}}; \underbrace{\Delta_{3,1}; \dots; \Delta_{3,1}}_{m_3(m_2-1) \text{ times}} \right],$$

5.2 Principal vectors for k -SSCS covariance matrix

From Section we have \mathbf{E}_1 is the eigenmatrix corresponding to eigenblock $\Delta_{k,k}$, \mathbf{E}_i , $i = 2, \dots, p_{k,k}$ is the eigenmatrices corresponding to eigenblock $\Delta_{k,k-1}$ and \mathbf{E}_i , $i = p_{3,k} + 1, \dots, p_{2,k}$ is the eigenmatrices corresponding to eigenblock $\Delta_{k,1}$. Therefore the principal vectors are

$$\mathbf{y}_j = \mathbf{E}'_j \mathbf{x},$$

where $j = 1, \dots, (2, k)$, and these principal vectors are independent. The first principal vector \mathbf{y}_1 has variance $\Delta_{k,k}$, the second has variance $\Delta_{k,k-1}$, and the last one $\mathbf{y}_{2,k}$ has $\Delta_{k,1}$.

In the following section we derive the distributions of the unbiased estimates of the eigenblocks $\Delta_{k,j}$, $j = 1, \dots, k$. For this derivation we need the following definition.

Definition 2 Let the $(p_{1,k} \times p_{1,k})$ -dimensional matrix \mathbf{A} be partitioned in $(p_{1,k-j} \times p_{1,k-j})$ -dimensional submatrices, that is $\mathbf{A}_{p_{1,k} \times p_{1,k}} = \begin{pmatrix} \mathbf{A}_{h,h^*} \end{pmatrix}_{\substack{p_{1,k-j} \times p_{1,k-j} \\ h,h^*=1}}^{p_{k-j+1,k}}$, then the block operators $b \sum_{p_{1,k-j}} (\mathbf{A})$ and $bTr_{p_{1,k-j}} (\mathbf{A})$ are defined respectively by

$$b \sum_{p_{1,k-j}} (\mathbf{A}) = \sum_{h=1}^{p_{k-j+1,k}} \sum_{h^*=1}^{p_{k-j+1,k}} \mathbf{A}_{h,h^*}$$

and

$$bTr_{p_{1,k-j}} (\mathbf{A}) = \sum_{h=1}^{p_{k-j+1,k}} \mathbf{A}_{h,h},$$

where the subindex $p_{1,k-j}$ in both operators indicates that they apply to a matrix \mathbf{A} partitioned in $p_{1,k-j} \times p_{1,k-j}$ - submatrices, and consequently their results are also $p_{1,k-j} \times p_{1,k-j}$ - matrices.

Using these operators on the $SSCS$ -covariance matrix, the following properties hold

Lemma 3 Let $\boldsymbol{\Gamma}_x$ the k -SSCS variance covariance matrix (as in equation (1) of Definition 1) be partitioned in $p_{1,k-j} \times p_{1,k-j}$ - submatrices, then

1. $bTr_{p_{1,k-j}} (\boldsymbol{\Gamma}_x) = p_{k-(j-1),k} \mathbf{V}_{k+1-j}$, where \mathbf{V}_{k+1-j} is given in (4).
2. $bTr_{p_{1,k-j}} (\boldsymbol{\Gamma}_x) = bTr_{p_{1,k-j}} (bTr_{p_{1,k-i}} \boldsymbol{\Gamma}_x)$, for $i < j = 1, \dots, k-1$.
3. $\mathbf{U}_{k,k-j} = \frac{bSum_{p_{1,1}} (\mathbf{W}_{k-j})}{p_{2,k-(j+1)}^2} = \frac{bSum_{p_{1,1}} (\mathbf{J}_{p_{2,k-(j+1)}} \otimes \mathbf{U}_{k,k-j})}{p_{2,k-(j+1)}^2}$, for $j = 0, \dots, k-2$.

$$\begin{aligned}
4. \mathbf{W}_{k-j} &= \frac{bSum_{p_1, k-(j+1)}(\mathbf{V}_{k+1-j}) - bTr_{p_1, k-(j+1)}(\mathbf{V}_{k+1-j})}{m_{k-j} \cdot (m_{k-j} - 1)} = \frac{bSum_{p_1, k-(j+1)}(bTr_{p_1, k-j}(\mathbf{\Gamma}_x)) - bTr_{p_1, k-(j+1)}(\mathbf{\Gamma}_x)}{p_{k-(j-1), k} \cdot m_{k-j} \cdot (m_{k-j} - 1)} \\
5. \mathbf{U}_{k, k-j} &= \frac{bSum_{p_1, 1} \left(\left[bSum_{p_1, k-(j+1)}(bTr_{p_1, k-j}(\mathbf{\Gamma}_x)) - bTr_{p_1, k-(j+1)}(\mathbf{\Gamma}_x) \right] \right)}{p_{k-(j-1), k} \cdot [m_{k-j} \cdot (m_{k-j} - 1)] \cdot p_{2, k-(j+1)}^2}, \text{ for } j = 0, \dots, k-2. \text{ and } \mathbf{U}_{k, 1} = \\
&\frac{bTr_{p_1, 1}(\mathbf{V}_k)}{p_{2, k-1}} = \frac{bTr_{p_1, 1}(\mathbf{\Gamma}_x)}{p_{2, k}}.
\end{aligned}$$

Proof: Proof is straightforward

Note that if one has a good unbiased estimator $\tilde{\mathbf{\Gamma}}_x$ of $\mathbf{\Gamma}_x$, then using property (5) of Lemma 3 it is easy to see that

$$\tilde{\mathbf{U}}_{k, 1} = \frac{bTr_{p_1, 1}(\tilde{\mathbf{\Gamma}}_x)}{p_{2, k}} \quad (23)$$

and

$$\tilde{\mathbf{U}}_{k, k-j} = \frac{bSum_{p_1, 1} \left(\left[bSum_{p_1, k-(j+1)}(bTr_{p_1, k-j}(\tilde{\mathbf{\Gamma}}_x)) - bTr_{p_1, k-(j+1)}(\tilde{\mathbf{\Gamma}}_x) \right] \right)}{p_{k-(j-1), k} \cdot [m_{k-j} \cdot (m_{k-j} - 1)] \cdot p_{2, k-(j+1)}^2}, \quad (24)$$

for $j = 0, \dots, k-2$, are estimators of the corresponding $\mathbf{U}_{k, k-j}$, for $j = 0, \dots, k-1$.

In the following Lemma we give an interesting property using the $\mathbf{\Delta}_{k, j} = \sum_{i=1}^j p_{2, i} (\mathbf{U}_{k, i} - \mathbf{U}_{k, i+1})$, for $j = 1, \dots, k$, given by (6). Consider the mutually orthogonal projector matrices $\mathbf{P}_{m_i} = \frac{1}{m_i} \mathbf{J}_{m_i}$ and $\mathbf{Q}_{m_i} = \mathbf{I}_{m_i} - \mathbf{P}_{m_i}$ and noting that these projector matrices are idempotent, we have

$$\begin{aligned}
\mathbf{P}_{m_i}^2 &= \mathbf{P}_{m_i}, \\
\mathbf{P}_{m_i} \mathbf{J}_{m_i} \mathbf{P}_{m_i} &= m_i \mathbf{P}_{m_i}, \\
\mathbf{Q}_{m_i}^2 &= \mathbf{Q}_{m_i} \\
\mathbf{Q}_{m_i} \mathbf{J}_{m_i} \mathbf{Q}_{m_i} &= \mathbf{0}.
\end{aligned} \quad (25)$$

We now define the matrices $\mathbf{Q}_{k, j} : j = 1, \dots, k-1$, by

$$\begin{aligned}
\mathbf{Q}_{k, 1} &= \mathbf{P}_{m_k} \otimes \mathbf{P}_{m_{k-1}} \otimes \dots \otimes \mathbf{P}_{m_2} \otimes \mathbf{I}_{m_1} = \left(\bigotimes_{h=1}^{k-1} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{I}_{m_1} = \mathbf{Q}_{k, 1}^* \otimes \mathbf{I}_{m_1} \\
\mathbf{Q}_{k, j} &= \left(\bigotimes_{h=1}^{k-j} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{Q}_{m_j} \otimes \left(\bigotimes_{h=k-(j-2)}^{k-1} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{I}_{m_1} \\
&= \mathbf{Q}_{k, j}^* \otimes \mathbf{I}_{m_1}, \text{ for } j = 2, \dots, k,
\end{aligned} \quad (26)$$

where

$$\begin{aligned}\mathbf{Q}_{k,1}^* &= \bigotimes_{h=1}^{k-1} \mathbf{P}_{m_{k+1-h}} \\ \mathbf{Q}_{k,j}^* &= \left(\bigotimes_{h=1}^{k-j} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{Q}_{m_j} \otimes \left(\bigotimes_{h=k-(j-2)}^{k-1} \mathbf{P}_{m_{k+1-h}} \right).\end{aligned}$$

Lemma 4 Let $\mathbf{\Gamma}_x$ the k -SSCS variance covariance matrix (as in equation (1) of Definition 1).

1. Let $\Delta_{k,j}$, for $j = 1, \dots, k$, be given by (5), that is, $\Delta_{k,j} = \sum_{i=1}^j p_{2,i} (\mathbf{U}_{k,i} - \mathbf{U}_{k,i+1})$, then

$$\Delta_{k,1} = \frac{m_2 \cdot bTr_{p_{1,1}}(\mathbf{\Gamma}_x) - bSum_{p_{1,1}} [bTr_{p_{1,2}}(\mathbf{\Gamma}_x)]}{p_{2,k} (m_2 - 1)},$$

$$\begin{aligned}\Delta_{k,k} &= \frac{1}{p_{2,k}} \left\{ bSum_{p_{1,1}} [bTr_{p_{1,2}}(\mathbf{\Gamma}_x)] + \sum_{i=2}^{k-1} [bSum_{p_{1,1}} [bSum_{p_{1,i}} (bTr_{p_{1,i+1}}(\mathbf{\Gamma}_x))] - bTr_{p_{1,i}}(\mathbf{\Gamma}_x)] \right\},\end{aligned}$$

and

$$\begin{aligned}\Delta_{k,j} &= \frac{1}{p_{2,k}} \left\{ bSum_{p_{1,1}} [bTr_{p_{1,2}}(\mathbf{\Gamma}_x)] + \sum_{i=2}^{j-1} [bSum_{p_{1,1}} [bSum_{p_{1,i}} (bTr_{p_{1,i+1}}(\mathbf{\Gamma}_x))] - bTr_{p_{1,i}}(\mathbf{\Gamma}_x)] \right. \\ &\quad \left. - \frac{1}{m_{j+1} - 1} [bSum_{p_{1,1}} [bSum_{p_{1,j}} (bTr_{p_{1,j+1}}(\mathbf{\Gamma}_x))] - bTr_{p_{1,j}}(\mathbf{\Gamma}_x)] \right\}, \quad \text{for } j = 2, \dots, k-1.\end{aligned}$$

2. Let the matrices $\mathbf{Q}_{k,j}$ be given by (26), then

$$\begin{aligned}\mathbf{Q}_{k,1} \mathbf{\Gamma}_x \mathbf{Q}_{k,1} &= \left(\bigotimes_{h=1}^{k-1} \mathbf{P}_{m_{k+1-h}} \right) \otimes \Delta_{k,k} \\ \mathbf{Q}_{k,j} \mathbf{\Gamma}_x \mathbf{Q}_{k,j} &= \left(\bigotimes_{h=1}^{k-j} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{Q}_{m_j} \otimes \left(\bigotimes_{h=k-(j-2)}^{k-1} \mathbf{P}_{m_{k+1-h}} \right) \otimes \Delta_{k,j-1}, \quad \text{for } j = 2, \dots, k.\end{aligned}$$

3.

$$\begin{aligned}\Delta_{k,k} &= bTr_{p_{1,1}}(\mathbf{Q}_{k,1} \mathbf{\Gamma}_x \mathbf{Q}_{k,1}) = \frac{1}{p_{2,k}} bSum_{p_{1,1}}(\mathbf{Q}_{k,1} \mathbf{\Gamma}_x \mathbf{Q}_{k,1}) \\ \Delta_{k,j-1} &= \frac{bTr_{p_{1,1}}(\mathbf{Q}_{k,j} \mathbf{\Gamma}_x \mathbf{Q}_{k,j})}{m_j - 1}, \quad \text{for } j = 2, \dots, k.\end{aligned}$$

Proof: The proof of Lemma 4 is given in Appendix A.5.

Now, using the unbiased estimate of $\mathbf{\Gamma}_x$ in (14), it can be easily proved the following result that corresponds to Lemma 4 using instead of $\mathbf{\Gamma}_x$ its unbiased estimator $\tilde{\mathbf{\Gamma}}_x = \frac{n}{n-1} \mathbf{S}$,

Lemma 5 Let $\Gamma_{\mathbf{x}}$ the k -SSCS variance covariance matrix (as in equation (1) of Definition 1), and let $\Delta_{k,j}$, for $j = 1, \dots, k$, be given by (5), then.

1. For each $j = 1, \dots, k$, the estimator $\tilde{\Delta}_{k,j}$ is given by

$$\tilde{\Delta}_{k,1} = \frac{n}{n-1} \frac{m_2 \cdot bTr_{p_{1,1}}(\mathbf{S}) - bSum_{p_{1,1}} [bTr_{p_{1,2}}(\mathbf{S})]}{p_{2,k}(m_2 - 1)},$$

$$\begin{aligned} & \tilde{\Delta}_{k,k} \\ = & \frac{n}{n-1} \frac{1}{p_{2,k}} \left\{ bSum_{p_{1,1}} [bTr_{p_{1,2}}(\mathbf{S})] + \sum_{i=2}^{k-1} [bSum_{p_{1,1}} [bSum_{p_{1,i}} (bTr_{p_{1,i+1}}(\mathbf{S}))]] - bTr_{p_{1,i}}(\mathbf{S}) \right\}, \end{aligned}$$

and

$$\begin{aligned} & \tilde{\Delta}_{k,j} \\ = & \frac{n}{n-1} \frac{1}{p_{2,k}} \left\{ bSum_{p_{1,1}} [bTr_{p_{1,2}}(\mathbf{S})] + \sum_{i=2}^{j-1} [bSum_{p_{1,1}} [bSum_{p_{1,i}} (bTr_{p_{1,i+1}}(\mathbf{S}))]] - bTr_{p_{1,i}}(\mathbf{S}) \right. \\ & \left. - \frac{1}{m_{j+1} - 1} [bSum_{p_{1,1}} [bSum_{p_{1,j}} (bTr_{p_{1,j+1}}(\mathbf{S}))]] - bTr_{p_{1,j}}(\mathbf{S}) \right\}, \text{ for } j = 2, \dots, k-1, \end{aligned}$$

is an unbiased estimator of the corresponding $\Delta_{k,j}$.

2. Let the matrices $\mathbf{Q}_{k,j}$ be given by (26), then

$$\begin{aligned} \mathbf{Q}_{k,1} \left(\frac{n}{n-1} \mathbf{S} \right) \mathbf{Q}_{k,1} &= \left(\bigotimes_{h=1}^{k-1} \mathbf{P}_{m_{k+1-h}} \right) \otimes \tilde{\Delta}_{k,k} \\ \mathbf{Q}_{k,j} \left(\frac{n}{n-1} \mathbf{S} \right) \mathbf{Q}_{k,j} &= \left(\bigotimes_{h=1}^{k-j} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{Q}_{m_j} \otimes \left(\bigotimes_{h=k-(j-2)}^{k-1} \mathbf{P}_{m_{k+1-h}} \right) \otimes \tilde{\Delta}_{k,j-1}, \end{aligned}$$

for $j = 2, \dots, k$.

3.

$$\begin{aligned} \tilde{\Delta}_{k,k} &= \frac{n}{n-1} \cdot bTr_{p_{1,1}}(\mathbf{Q}_{k,1} \cdot \mathbf{S} \cdot \mathbf{Q}_{k,1}) \\ &= \frac{n}{(n-1)p_{2,k}} \cdot bSum_{p_{1,1}}(\mathbf{Q}_{k,1} \cdot \mathbf{S} \cdot \mathbf{Q}_{k,1}) \\ \tilde{\Delta}_{k,j-1} &= \frac{n \cdot bTr_{p_{1,1}}(\mathbf{Q}_{k,j} \cdot \mathbf{S} \cdot \mathbf{Q}_{k,j})}{(n-1)(m_j - 1)}, \text{ for } j = 2, \dots, k. \end{aligned}$$

Proof: Proof is straightforward using Lemma 4.

6 A real data example

In this section we demonstrate our new methods with a real data set, where an investigator measured the mineral content of bones (radius, humerus and ulna) by photon absorptiometry to examine whether dietary supplements would slow bone loss in 25 older women. This data set is taken from Johnson and Wichern (2007, p. 43 and p. 353). Measurements were recorded for three bones on the dominant and nondominant sides Johnson and Wichern (2007, p. 43). The bone mineral contents for the first 24 women one year after their participation in an experimental program is given in Johnson and Wichern (2007, p. 353). Thus, for our analysis we take only first 24 women in the first data set. Thus, for our analysis we take only the first 24 women in the first data set, and combine these two data sets side by side into a new one, which we analyze in this article. Thus, this new three-level dataset has 3–SSCS covariance structure, with $m_3 = 2$, $m_2 = 2$ and $m_1 = 3$. We rearrange the variables in the new data set by grouping together the mineral content of the dominant sides of radius, humerus and ulna as the first three variables, that is, the variables in the dominant side and then the mineral contents for the non-dominant side of the same bones on the first year of the experiment; and do the same thing at the second year of the experiment. Let a typical sample of this data after rearranging by dominant and non-dominant sides, and then by time looks like

$$\mathbf{y} = (y_{11.1}, y_{11.2}, y_{11.3}, y_{12.1}, y_{12.2}, y_{12.3}, y_{21.1}, y_{21.2}, y_{21.3}, y_{22.1}, y_{22.2}, y_{22.3})',$$

where the first subscript from the right represents the variable. The second subscript: if it is 1, then it is the dominant side, and if it is 2, it is the non-dominant side. The third subscript represents the time: for example, if it is 1 then it is first year, and if 2, it represents the second year. The unbiased estimates $\tilde{\mathbf{U}}_{3,1}$, $\tilde{\mathbf{U}}_{3,2}$ and $\tilde{\mathbf{U}}_{3,3}$ of 3–SSCS covariance structure are

$$\tilde{\mathbf{U}}_{3,1} = \begin{bmatrix} 0.01297 & 0.02428 & 0.00900 \\ 0.02428 & 0.08587 & 0.01908 \\ 0.00900 & 0.01908 & 0.01115 \end{bmatrix}, \tilde{\mathbf{U}}_{3,2} = \begin{bmatrix} 0.01081 & 0.02164 & 0.00843 \\ 0.02164 & 0.07633 & 0.01726 \\ 0.00843 & 0.01726 & 0.00733 \end{bmatrix},$$

$$\text{and } \tilde{\mathbf{U}}_{3,3} = \begin{bmatrix} 0.01143 & 0.02255 & 0.00868 \\ 0.02255 & 0.07837 & 0.01829 \\ 0.00868 & 0.01829 & 0.00877 \end{bmatrix},$$

respectively, and the unbiased estimates of the eigenblocks $\tilde{\mathbf{\Delta}}_{3,1}$, $\tilde{\mathbf{\Delta}}_{3,2}$ and $\tilde{\mathbf{\Delta}}_{3,3}$ are

$$\tilde{\mathbf{\Delta}}_{3,1} = \begin{bmatrix} 0.00217 & 0.00264 & 0.00057 \\ 0.00264 & 0.00955 & 0.00182 \\ 0.00057 & 0.00182 & 0.00381 \end{bmatrix}, \tilde{\mathbf{\Delta}}_{3,2} = \begin{bmatrix} 0.00091 & 0.00083 & 0.00007 \\ 0.00083 & 0.00546 & -0.00024 \\ 0.00007 & -0.00024 & 0.00094 \end{bmatrix},$$

$$\text{and } \tilde{\Delta}_{3,3} = \begin{bmatrix} 0.04665 & 0.09101 & 0.03480 \\ 0.09101 & 0.31895 & 0.07293 \\ 0.03480 & 0.07293 & 0.03602 \end{bmatrix},$$

respectively. The 3–SSCS covariance matrix has a total of four eigenblocks: the eigenblocks $\Delta_{3,3}$ and $\Delta_{3,2}$ are with multiplicity one, and the eigenblock $\Delta_{3,1}$ is with multiplicity two. From Roy (2014) the four (3×1) –dimensional principal vectors of the 3–SSCS covariance structure are as follows:

$$\mathbf{y}_1 = \begin{bmatrix} ((y_{11.1} + y_{21.1}) + (y_{12.1} + y_{22.1}))/2 \\ ((y_{11.2} + y_{21.2}) + (y_{12.2} + y_{22.2}))/2 \\ ((y_{11.3} + y_{21.3}) + (y_{12.3} + y_{22.3}))/2 \end{bmatrix},$$

$$\mathbf{y}_2 = \begin{bmatrix} ((y_{11.1} - y_{21.1}) + (y_{12.1} - y_{22.1}))/2 \\ ((y_{11.2} - y_{21.2}) + (y_{12.2} - y_{22.2}))/2 \\ ((y_{11.3} - y_{21.3}) + (y_{12.3} - y_{22.3}))/2 \end{bmatrix},$$

$$\mathbf{y}_3 = \begin{bmatrix} ((y_{11.1} + y_{21.1} - (y_{12.1} + y_{22.1}))/2 \\ ((y_{11.2} + y_{21.2} - (y_{12.2} + y_{22.2}))/2 \\ ((y_{11.3} + y_{21.3} - (y_{12.3} + y_{22.3}))/2 \end{bmatrix},$$

and

$$\mathbf{y}_4 = \begin{bmatrix} ((y_{11.1} - y_{21.1}) - (y_{12.1} - y_{22.1}))/2 \\ ((y_{11.2} - y_{21.2}) - (y_{12.2} - y_{22.2}))/2 \\ ((y_{11.3} - y_{21.3}) - (y_{12.3} - y_{22.3}))/2 \end{bmatrix}.$$

The first principal vector \mathbf{y}_1 corresponding to eigenblock $\Delta_{3,3}$ represents the total grand midpoints of the variables over sides and time points. The second principal vector \mathbf{y}_2 corresponding to eigenblock $\Delta_{3,2}$ represents the difference between the two time points. For example $(y_{11.1} - y_{21.1})$ provides the difference between the first year and the second year of the first variable radius at the dominant side. And, $(y_{12.1} - y_{22.1})$ provides the difference between the first year and the second year of the first variable radius at the non-dominant side. So, $((y_{11.1} - y_{21.1}) + (y_{12.1} - y_{22.1}))/2$ represents the average difference between the first year and the second year of the first variable radius. Similarly, for the other two components of the second principal vector represent the average difference between the first year and the second year of the second and third variables humerus and ulna. The third and the fourth principal vectors \mathbf{y}_3 and \mathbf{y}_4 correspond to the same eigenblocks $\Delta_{3,1}$. And, these two principal vectors are independent. The average of these two blocks, which represents the difference between the dominant and non-dominant sides has the variance-covariance matrix $\Delta_{3,1}$.

We see that the variability in the first eigenblock is $\text{tr}(\tilde{\Delta}_{3,3}) = 0.4016149$, and the variabilities in the second and the third eigenblocks are $\text{tr}(\tilde{\Delta}_{3,2}) = 0.0073121$ and $\text{tr}(\tilde{\Delta}_{3,1}) = 0.0155271$ respectively.

Table 1: Trace(eigenblocks) and percent(%) trace(eigenblocks) of Mineral data.

Eigenblock	Trace(Eigenblock)	%Trace(Eigenblock)
$\Delta_{3,3}$	0.4016149	91.27999
$\Delta_{3,1}$	2×0.0155271	7.05807
$\Delta_{3,2}$	0.0073121	1.66191
Total	0.4399813	100.00

That is, in this data set $\text{tr}(\tilde{\Delta}_{3,1}) > \text{tr}(\tilde{\Delta}_{3,2})$. Therefore, from (21) the total variability in the data is

$$\begin{aligned} \text{tr}(\tilde{\Gamma}_{\mathbf{x}}) &= \text{tr}(\tilde{\Delta}_{3,3}) + 2\text{tr}(\tilde{\Delta}_{3,1}) + \text{tr}(\tilde{\Delta}_{3,2}) \\ &= 0.4016149 + 2(0.0155271) + 0.0073121 = 0.4399813. \end{aligned}$$

We see that the first eigenblock $\Delta_{3,3}$ accounts for the 91.27999% of the variability of the data. One can calculate the (3×3) first principal vector \mathbf{y}_1 corresponding to the first eigenblock $\Delta_{3,3}$, and then one can obtain the eigenvalues of $\Delta_{3,3}$ and the corresponding principal components, which are linear combination of the components of the first principal vector \mathbf{y}_1 (total grand midpoints of the variables over sides and time points) using any known software, e.g., SAS.

7 Conclusions

Multi-level data is present in almost every field these days, there are many interconnections among the k levels, but it takes time to see them. More and more Multi-level datasets are coming and will continue to come in future. So, it is important that we develop statistical tool to analyze these datasets. One can develop testing of mean vectors for one population/ two populations or paired populations when the populations have k -SSCS covariance structure; and obtain the classification rules with the derived estimates of the k -SSCS matrix parameters. One can also study the optimality properties of k -SSCS matrix parameters; we are currently working on these problems and report it in future publications. Optimality properties of 2-SSCS matrix parameters are studied by Roy et al. (2016). There may be some structure on mean vector too. One can study the k -SSCS covariance structure in this setting too.

A Appendix

A.1 Proof of Lemma 1

Proof: We use mathematical induction to prove that (8) is true for all natural numbers k . We know that expression (8) is valid for $k = 2$ and $k = 3$. See Leiva and Roy (2007). We assume that the inverse of any

$(k-1)$ -SSCS matrix is given by (8), and we will prove that (8) is true for an arbitrary k -SSCS matrix. Given $\mathbf{\Gamma}_{\mathbf{x}_r} = \mathbf{V}_{k+1}$ an arbitrary k -SSCS matrix with SSCS-component matrices $\mathbf{U}_{k,j}$, $j = 1, \dots, k$, it can be written as

$$\mathbf{V}_{k+1} = \mathbf{\Gamma}_{\mathbf{x}_r} = \mathbf{I}_{m_k} \otimes (\mathbf{V}_k - \mathbf{W}_k) + \mathbf{J}_{m_k} \otimes \mathbf{W}_k,$$

we know that

$$\mathbf{\Gamma}_{\mathbf{x}_r}^{-1} = \mathbf{I}_{m_k} \otimes (\mathbf{V}_k - \mathbf{W}_k)^{-1} + \mathbf{J}_{m_k} \otimes \frac{1}{m_k} \left[(\mathbf{V}_k + (m_k - 1)\mathbf{W}_k)^{-1} - (\mathbf{V}_k - \mathbf{W}_k)^{-1} \right]. \quad (\text{A1})$$

Noting $i_{k-1:k-1} = 1'_{k-2}$ and then

$$\mathbf{J}_{p_{2,k-1}} \otimes \mathbf{U}_{k,k} = \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:k-1},h} \right) \otimes \mathbf{U}_{k,k},$$

we prove that $\mathbf{V}_k - \mathbf{W}_k$ has $(k-1)$ -SSCS form. Now,

$$\begin{aligned} \mathbf{V}_k - \mathbf{W}_k &= \mathbf{V}_k - \mathbf{J}_{p_{2,k-1}} \otimes \mathbf{U}_{k,k} \\ &= \sum_{j=1}^{k-2} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k+1-h}}^{i_{k-1:j},h} \right) \otimes (\mathbf{U}_{k-1,j} - \mathbf{U}_{k-1,j+1}) \\ &\quad + \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k+1-h}}^{i_{k-1:k-1},h} \right) \otimes \mathbf{U}_{k-1,k-1} - \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:k-1},h} \right) \otimes \mathbf{U}_{k,k} \\ &= \sum_{j=1}^{k-2} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k+1-h}}^{i_{k-1:j},h} \right) \otimes [(\mathbf{U}_{k,j} - \mathbf{U}_{k,k}) - (\mathbf{U}_{k,j+1} - \mathbf{U}_{k,k})] \\ &\quad + \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k+1-h}}^{i_{k-1:k-1},h} \right) \otimes (\mathbf{U}_{k-1,k-1} - \mathbf{U}_{k,k}). \end{aligned}$$

Now, by defining the matrices $\mathbf{U}_{k-1,j}^*$ for $j = 1, \dots, k-1$

$$\mathbf{U}_{k-1,j}^* = \mathbf{U}_{k,j} - \mathbf{U}_{k,k}, \text{ for } j = 1, \dots, k-1, \quad (\text{A2})$$

and by denoting $\mathbf{U}_{k-1,k}^*$ as the null matrix, we have

$$\begin{aligned} \mathbf{V}_k - \mathbf{W}_k &= \sum_{j=1}^{k-1} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:j},h} \right) \otimes (\mathbf{U}_{k-1,j}^* - \mathbf{U}_{k-1,j+1}^*) \\ &= \sum_{j=1}^{k-2} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:j},h} \right) \otimes (\mathbf{U}_{k,j} - \mathbf{U}_{k,j+1}) + \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:k-1},h} \right) \otimes \mathbf{U}_{k,k-1}. \end{aligned} \quad (\text{A3})$$

Therefore, $\mathbf{V}_k - \mathbf{W}_k$ has the $(k-1)$ -SSCS form, and thus by the inductive hypothesis we get

$$\begin{aligned} (\mathbf{V}_k - \mathbf{W}_k)^{-1} &= \sum_{j=1}^{k-1} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:j},h} \right) \otimes \frac{1}{p_{2,j}} (\mathbf{\Delta}_{k-1,j}^{*-1} - \mathbf{\Delta}_{k-1,j-1}^{*-1}) \\ &= \sum_{j=1}^{k-1} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:j},h} \right) \otimes \frac{1}{p_{2,j}} (\mathbf{\Delta}_{k,j}^{-1} - \mathbf{\Delta}_{k,j-1}^{-1}), \end{aligned} \quad (\text{A4})$$

where for $j = 1, \dots, k-1$, we use

$$\begin{aligned}\Delta_{k-1,j}^* &= \sum_{i=1}^j p_{2,i} (\mathbf{U}_{k-1,i}^* - \mathbf{U}_{k-1,i+1}^*) \\ &= \sum_{i=1}^j p_{2,i} (\mathbf{U}_{k,i} - \mathbf{U}_{k,i+1}) = \Delta_{k,j}.\end{aligned}\tag{A5}$$

We now prove that $\mathbf{V}_k + (m_k - 1)\mathbf{W}_k$ also has $(k-1)$ -SSCS form. Now,

$$\begin{aligned}&\mathbf{V}_k + (m_k - 1)\mathbf{W}_k \\ &= \mathbf{V}_k + \mathbf{J}_{p_{2,k-1}} \otimes (m_k - 1)\mathbf{U}_{k,k} \\ &= \sum_{j=1}^{k-2} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k+1-h}}^{i_{k-1:j,h}} \right) \otimes (\mathbf{U}_{k-1,j} - \mathbf{U}_{k-1,j+1}) \\ &\quad + \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k+1-h}}^{i_{k-1:k-1,h}} \right) \otimes \mathbf{U}_{k-1,k-1} + \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:k-1,h}} \right) \otimes (m_k - 1)\mathbf{U}_{k,k} \\ &= \sum_{j=1}^{k-2} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k+1-h}}^{i_{k-1:j,h}} \right) \otimes \{[\mathbf{U}_{k-1,j} + (m_k - 1)\mathbf{U}_{k,k}] - [\mathbf{U}_{k-1,j+1} + (m_k - 1)\mathbf{U}_{k,k}]\} \\ &\quad + \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k+1-h}}^{i_{k-1:k-1,h}} \right) \otimes [\mathbf{U}_{k-1,k-1} + (m_k - 1)\mathbf{U}_{k,k}].\end{aligned}$$

Now, by defining the matrices $\mathbf{U}_{k-1,j}^{**}$ for $j = 1, \dots, k-1$

$$\mathbf{U}_{k-1,j}^{**} = \mathbf{U}_{k,j} + (m_k - 1)\mathbf{U}_{k,k}, \text{ for } j = 1, \dots, k-1,\tag{A6}$$

and denoting with $\mathbf{U}_{k-1,k}^{**}$ as the null matrix, we have

$$\begin{aligned}\mathbf{V}_k + (m_k - 1)\mathbf{W}_k &= \sum_{j=1}^{k-1} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:j,h}} \right) \otimes (\mathbf{U}_{k-1,j}^{**} - \mathbf{U}_{k-1,j+1}^{**}) \\ &= \left[\sum_{j=1}^{k-2} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:j,h}} \right) \otimes (\mathbf{U}_{k,j} - \mathbf{U}_{k,j+1}) \right] \\ &\quad + \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}} \right) \otimes (\mathbf{U}_{k,k-1} + (m_k - 1)\mathbf{U}_{k,k}).\end{aligned}\tag{A7}$$

Thus, $\mathbf{V}_k + (m_k - 1)\mathbf{W}_k$ has the $(k - 1)$ -SSCS form and by the inductive hypothesis we get

$$\begin{aligned}
(\mathbf{V}_k + (m_k - 1)\mathbf{W}_k)^{-1} &= \sum_{j=1}^{k-1} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:j,h}} \right) \otimes \frac{1}{p_{2,j}} \left(\Delta_{k-1,j}^{**,-1} - \Delta_{k-1,j-1}^{**,-1} \right) \\
&= \sum_{j=1}^{k-2} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:j,h}} \right) \otimes \frac{1}{p_{2,j}} \left(\Delta_{k,j}^{-1} - \Delta_{k,j-1}^{-1} \right) \\
&\quad + \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}} \right) \otimes \frac{1}{p_{2,k-1}} \left(\Delta_{k-1,k-1}^{**,-1} - \Delta_{k,k-2}^{-1} \right) \\
&= \sum_{j=1}^{k-2} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:j,h}} \right) \otimes \frac{1}{p_{2,j}} \left(\Delta_{k,j}^{-1} - \Delta_{k,j-1}^{-1} \right) \\
&\quad + \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}} \right) \otimes \frac{1}{p_{2,k-1}} \left(\Delta_{k,k}^{-1} - \Delta_{k,k-2}^{-1} \right), \tag{A8}
\end{aligned}$$

where for $j = 1, \dots, k - 2$, we use

$$\begin{aligned}
\Delta_{k-1,j}^{**} &= \sum_{i=1}^j p_{2,i} (\mathbf{U}_i^{**} - \mathbf{U}_{i+1}^{**}) \\
&= \sum_{i=i}^j p_{2,i} (\mathbf{U}_i - \mathbf{U}_{i+1}) = \Delta_{k,j}, \quad \text{and} \tag{A9}
\end{aligned}$$

$$\begin{aligned}
\Delta_{k-1,k-1}^{**} &= \sum_{i=1}^{k-2} p_{2,i} (\mathbf{U}_{k-1,i}^{**} - \mathbf{U}_{k-1,i+1}^{**}) + p_{2,k-1} \mathbf{U}_{k-1,k-1}^{**} \\
&= \sum_{i=1}^{k-1} p_{2,i} (\mathbf{U}_{k,i} - \mathbf{U}_{k,i+1}) + p_{2,k} \mathbf{U}_{k,k} = \Delta_{k,k}. \tag{A10}
\end{aligned}$$

Now,

$$\begin{aligned}
&(\mathbf{V}_k + (m_k - 1)\mathbf{W}_k)^{-1} - (\mathbf{V}_k - \mathbf{W}_k)^{-1} \\
&= \sum_{j=1}^{k-2} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:j,h}} \right) \otimes \frac{1}{p_{2,j}} \left(\Delta_{k,j}^{-1} - \Delta_{k,j-1}^{-1} \right) \\
&\quad + \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}} \right) \otimes \frac{1}{p_{2,k-1}} \left(\Delta_{k,k}^{-1} - \Delta_{k,k-2}^{-1} \right) \\
&\quad - \sum_{j=1}^{k-1} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:j,h}} \right) \otimes \frac{1}{p_{2,j}} \left(\Delta_{k,j}^{-1} - \Delta_{k,j-1}^{-1} \right) \\
&= \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}} \right) \otimes \frac{1}{p_{2,k-1}} \otimes \left(\Delta_{k,k}^{-1} - \Delta_{k,k-1}^{-1} \right). \tag{A11}
\end{aligned}$$

Now, substituting the values of $(\mathbf{V}_k - \mathbf{W}_k)^{-1}$ and $(\mathbf{V}_k + (m_k - 1)\mathbf{W}_k)^{-1} - (\mathbf{V}_k - \mathbf{W}_k)^{-1}$ from (A4) and (A11) in (A1) we obtain

$$\begin{aligned}
\Gamma_{\mathbf{x}_r}^{-1} &= \mathbf{I}_{m_k} \otimes (\mathbf{V}_k - \mathbf{W}_k)^{-1} + \mathbf{J}_{m_k} \otimes \frac{1}{m_k} \left[(\mathbf{V}_k + (m_k - 1)\mathbf{W}_k)^{-1} - (\mathbf{V}_k - \mathbf{W}_k)^{-1} \right] \\
&= \mathbf{I}_{m_k} \otimes \sum_{j=1}^{k-1} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1;j,h}} \right) \otimes \frac{1}{p_{2,j}} \left(\Delta_{k,j}^{-1} - \Delta_{k,j-1}^{-1} \right) \\
&\quad + \mathbf{J}_{m_k} \otimes \frac{1}{m_k} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}} \right) \otimes \frac{1}{p_{2,k-1}} \otimes \left(\Delta_{k,k}^{-1} - \Delta_{k,k-1}^{-1} \right) \\
&= \sum_{j=1}^k \left(\bigotimes_{h=1}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k;j,h}} \right) \otimes \frac{1}{p_{2,j}} \left(\Delta_{k,j}^{-1} - \Delta_{k,j-1}^{-1} \right).
\end{aligned}$$

This completes the proof of Lemma 1.

A.2 Proof of Lemma 2

Proof: We know that expression (9) is valid for $k = 2$ and $k = 3$. See Leiva (2007) and Roy and Leiva (2007). We assume that the determinant of any $(k - 1)$ -SSCS matrix is given by (9), and we will prove that (9) is true for an arbitrary k -SSCS matrix. Now,

$$\begin{aligned}
\sum_{j=1}^k (p_{j+1,k} - p_{j+2,k}) &= \left[\sum_{j=1}^{k-2} (p_{j+1,k} - p_{j+2,k}) \right] + m_k - 1 + 1 - 0 \\
&= (p_{2,k} - p_{k,k}) + m_k - 1 + 1 = p_{2,k}.
\end{aligned}$$

Noting that both $\mathbf{V}_k - \mathbf{W}_k$ and $\mathbf{V}_k + (m_k - 1)\mathbf{W}_k$ have the $(k - 1)$ -SSCS form, using (A5) and (A9) we get

$$\begin{aligned}
|\mathbf{V}_{k+1}| &= |\mathbf{V}_k - \mathbf{W}_k|^{m_k - 1} |\mathbf{V}_k + (m_k - 1)\mathbf{W}_k| \\
&= \left(\prod_{j=1}^{k-1} |\Delta_{k-1,j}^*|^{p_{j+1,k-1} - p_{j+2,k-1}} \right)^{m_k - 1} \prod_{j=1}^{k-1} |\Delta_{k-1,j}^{**}|^{p_{j+1,k-1} - p_{j+2,k-1}} \\
&= \prod_{j=1}^{k-1} |\Delta_{k,j}|^{(p_{j+1,k-1} - p_{j+2,k-1})(m_k - 1)} \prod_{j=1}^{k-2} |\Delta_{k,j}|^{p_{j+1,k-1} - p_{j+2,k-1}} |\Delta_{k,k}| \\
&= \left(\prod_{j=1}^{k-2} |\Delta_{k,j}|^{(p_{j+1,k-1} - p_{j+2,k-1})m_k} \right) |\Delta_{k,k-1}|^{(p_{k-1+1,k-1} - p_{k-1+2,k-1})(m_k - 1)} |\Delta_{k,k}| \\
&= \prod_{j=1}^k |\Delta_j|^{p_{j+1,k} - p_{j+2,k}}.
\end{aligned}$$

This completes the proof of Lemma 2.

A.3 Proof of Theorem 1

Proof: For $r = 1, \dots, n$, let \mathbf{x}_r be an $p_{1,k}$ -variate vector with mean $\boldsymbol{\mu}_{\mathbf{x}}$ and a k -SSCS covariance matrix $\boldsymbol{\Gamma}_{\mathbf{x}}$ with SSSS component matrices $\mathbf{U}_{k,j} : j = 1, \dots, k$. Assume $\mathbf{x}_1, \dots, \mathbf{x}_n$ is a random sample of size n of a population with distribution $N_{p_{1,k}}(\boldsymbol{\mu}_{\mathbf{x}}; \boldsymbol{\Gamma}_{\mathbf{x}})$, where $\boldsymbol{\Gamma}_{\mathbf{x}}$ is a positive definite k -SSCS covariance matrix. The likelihood function $L = L(\boldsymbol{\mu}_{\mathbf{x}}; \boldsymbol{\Gamma}_{\mathbf{x}})$ is given by

$$L(\boldsymbol{\mu}_{\mathbf{x}}, \boldsymbol{\Gamma}_{\mathbf{x}}) = \frac{\exp -\frac{1}{2} \sum_{r=1}^n (\mathbf{x}_r - \boldsymbol{\mu}_{\mathbf{x}})' \boldsymbol{\Gamma}_{\mathbf{x}}^{-1} (\mathbf{x}_r - \boldsymbol{\mu}_{\mathbf{x}})}{(2\pi)^{\frac{p_{1,k}}{2}} |\boldsymbol{\Gamma}_{\mathbf{x}}|^{\frac{n}{2}}},$$

or equivalently,

$$L(\boldsymbol{\mu}_{\mathbf{x}_*}, \boldsymbol{\Gamma}_{\mathbf{x}_*}) = \frac{\exp -\frac{1}{2} (\mathbf{x}_* - \boldsymbol{\mu}_{\mathbf{x}_*})' \boldsymbol{\Gamma}_{\mathbf{x}_*}^{-1} (\mathbf{x}_* - \boldsymbol{\mu}_{\mathbf{x}_*})}{(2\pi)^{\frac{p_{1,k}}{2}} |\boldsymbol{\Gamma}_{\mathbf{x}_*}|^{\frac{1}{2}}}, \quad (\text{A12})$$

where

$$\mathbf{x}_* = (\mathbf{x}'_1, \dots, \mathbf{x}'_n)', \quad \text{and}$$

$$\boldsymbol{\mu}_{\mathbf{x}_*} = \mathbf{1}_n \otimes \boldsymbol{\mu}_{\mathbf{x}} = \mathbf{1}_n \otimes (\boldsymbol{\mu}_{x_{r;1,\dots,1}}, \dots, \boldsymbol{\mu}_{x_{r;m_1,\dots,m_k}})',$$

with $\boldsymbol{\mu}_{x_{r;j_1,\dots,j_k}} \in \mathfrak{R}$, is the same for all $r = 1, \dots, n$, and

$$\boldsymbol{\Gamma}_{\mathbf{x}_*} = \mathbf{I}_n \otimes \boldsymbol{\Gamma}_{\mathbf{x}} = \mathbf{I}_n \otimes \sum_{j=1}^k \left(\bigotimes_{h=1}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k;j,h}} \right) \otimes (\mathbf{U}_{k,j} - \mathbf{U}_{k,j+1}),$$

where \mathbf{U}_j , for $j = 1, \dots, k$, are $m_1 \times m_1$ -matrices, where \mathbf{U}_{k+1} is the $m_1 \times m_1$ zero matrix ($\mathbf{U}_{k+1} = \mathbf{0}_{m_1 \times m_1}$). Thus, the log likelihood function is

$$\begin{aligned} \log(L) &= -\frac{np_{1,k}}{2} \log(2\pi) - \frac{n}{2} \log |\boldsymbol{\Gamma}_{\mathbf{x}}| - \frac{1}{2} \sum_{r=1}^n (\mathbf{x}_r - \boldsymbol{\mu}_{\mathbf{x}})' \boldsymbol{\Gamma}_{\mathbf{x}}^{-1} (\mathbf{x}_r - \boldsymbol{\mu}_{\mathbf{x}}) \\ &= -\frac{np_{1,k}}{2} \log(2\pi) - \frac{1}{2} \log |\boldsymbol{\Gamma}_{\mathbf{x}_*}| - \frac{1}{2} (\mathbf{x}_* - \boldsymbol{\mu}_{\mathbf{x}_*})' \boldsymbol{\Gamma}_{\mathbf{x}_*}^{-1} (\mathbf{x}_* - \boldsymbol{\mu}_{\mathbf{x}_*}). \end{aligned} \quad (\text{A13})$$

The matrix $\boldsymbol{\Gamma}_{\mathbf{x}}^{-1}$ in (A13) is by (8) of the form

$$\boldsymbol{\Gamma}_{\mathbf{x}}^{-1} = \sum_{j=1}^k \left(\bigotimes_{h=1}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k;j,h}} \right) \otimes \mathbf{A}_j,$$

with

$$\mathbf{A}_j = \frac{1}{p_{2,j}} \left(\boldsymbol{\Delta}_{k,j}^{-1} - \boldsymbol{\Delta}_{k,j-1}^{-1} \right), \quad (\text{A14})$$

for $j = 1, \dots, k$, where it is assumed that $\boldsymbol{\Delta}_{k,0}^{-1} = \mathbf{0}$, and where $\boldsymbol{\Delta}_{k,j}$, for $j = 1, \dots, k$, are given in (5) and with $p_{2,1} = 1$

Let $\dot{\mathbf{x}}_r = \mathbf{x}_r - \boldsymbol{\mu}_x$ be expressed as $\dot{\mathbf{x}}_r = \mathbf{x}_r - \boldsymbol{\mu}_x = (\mathbf{x}_r - \bar{\mathbf{x}}) + (\bar{\mathbf{x}} - \boldsymbol{\mu}_x)$, where $\bar{\mathbf{x}}$ is the global sample mean, that is,

$$\bar{\mathbf{x}} = \frac{1}{n} \sum_{r=1}^n \mathbf{x}_r. \quad (\text{A15})$$

The sum of quadratic forms in the exponent of (A13) is

$$\begin{aligned} Q(\mathbf{x}_* : \boldsymbol{\mu}_{\mathbf{x}_*}, \boldsymbol{\Gamma}_{\mathbf{x}_*}^{-1}) &= (\mathbf{x}_* - \boldsymbol{\mu}_{\mathbf{x}_*})' \boldsymbol{\Gamma}_{\mathbf{x}_*}^{-1} (\mathbf{x}_* - \boldsymbol{\mu}_{\mathbf{x}_*}) = \sum_{r=1}^n (\mathbf{x}_r - \boldsymbol{\mu}_x)' \boldsymbol{\Gamma}_x^{-1} (\mathbf{x}_r - \boldsymbol{\mu}_x) \\ &= \text{tr} \left[\boldsymbol{\Gamma}_x^{-1} \sum_{r=1}^n (\mathbf{x}_r - \boldsymbol{\mu}_x) (\mathbf{x}_r - \boldsymbol{\mu}_x)' \right] = \text{tr} [\boldsymbol{\Gamma}_x^{-1} \mathbf{R}], \end{aligned} \quad (\text{A16})$$

where

$$\begin{aligned} \mathbf{R} &= \sum_{r=1}^n (\mathbf{x}_r - \boldsymbol{\mu}_x) (\mathbf{x}_r - \boldsymbol{\mu}_x)' \\ &= \sum_{r=1}^n [(\mathbf{x}_r - \bar{\mathbf{x}}) + (\bar{\mathbf{x}} - \boldsymbol{\mu}_x)] [(\mathbf{x}_r - \bar{\mathbf{x}}) + (\bar{\mathbf{x}} - \boldsymbol{\mu}_x)]' \\ &= \sum_{r=1}^n (\mathbf{x}_r - \bar{\mathbf{x}}) (\mathbf{x}_r - \bar{\mathbf{x}})' + \sum_{r=1}^n (\bar{\mathbf{x}} - \boldsymbol{\mu}_x) (\bar{\mathbf{x}} - \boldsymbol{\mu}_x)' + 2 \left[\sum_{r=1}^n (\mathbf{x}_r - \bar{\mathbf{x}}) \right] (\bar{\mathbf{x}} - \boldsymbol{\mu}_x)' \\ &= \left[\sum_{r=1}^n (\mathbf{x}_r - \bar{\mathbf{x}}) (\mathbf{x}_r - \bar{\mathbf{x}})' \right] + n (\bar{\mathbf{x}} - \boldsymbol{\mu}_x) (\bar{\mathbf{x}} - \boldsymbol{\mu}_x)' = \mathbf{W} + \mathbf{Z}, \end{aligned} \quad (\text{A17})$$

with

$$\mathbf{W} = \sum_{r=1}^n (\mathbf{x}_r - \bar{\mathbf{x}}) (\mathbf{x}_r - \bar{\mathbf{x}})'$$

and

$$\mathbf{Z} = n (\bar{\mathbf{x}} - \boldsymbol{\mu}_x) (\bar{\mathbf{x}} - \boldsymbol{\mu}_x)'.$$

Then, $\log(L) = -\frac{np_{1,k}}{2} \log(2\pi) - \frac{n}{2} \log |\boldsymbol{\Gamma}_X| - \frac{1}{2} \sum_{r=1}^n (\mathbf{x}_r - \boldsymbol{\mu}_X)' \boldsymbol{\Gamma}_X^{-1} (\mathbf{x}_r - \boldsymbol{\mu}_X)$ can be written as

$$\log(L) = -\frac{np_{1,k}}{2} \log(2\pi) - \frac{n}{2} \log |\boldsymbol{\Gamma}_x| - \frac{1}{2} \text{tr} (\boldsymbol{\Gamma}_x^{-1} \mathbf{W}) - \frac{1}{2} \text{tr} (\boldsymbol{\Gamma}_x^{-1} \mathbf{Z}). \quad (\text{A18})$$

When the vector mean $\boldsymbol{\mu}_x$ is unstructured, that is,

$$\boldsymbol{\mu}_x = \boldsymbol{\mu}_{\mathbf{x}_r} = \left(\boldsymbol{\mu}_{x_{r;1,\dots,1}}, \dots, \boldsymbol{\mu}_{x_{r;m_1,\dots,m_k}} \right)',$$

with $\boldsymbol{\mu}_{x_{r;j_1,\dots,j_k}} \in \mathfrak{R}$, equation (A18) assures that MLE of $\boldsymbol{\mu}_x$ is $\hat{\boldsymbol{\mu}}_x = \bar{\mathbf{x}}$, given in (A15). Therefore, by replacing $\boldsymbol{\mu}_x$ by $\bar{\mathbf{x}}$ the log likelihood reduces to

$$\begin{aligned} \log(L) &= -\frac{np_{1,k}}{2} \log(2\pi) - \frac{n}{2} \log |\boldsymbol{\Gamma}_x| - \frac{1}{2} \text{tr} (\boldsymbol{\Gamma}_x^{-1} \mathbf{W}) \\ &= -\frac{np_{1,k}}{2} \log(2\pi) - \frac{n}{2} \log |\boldsymbol{\Gamma}_x| - \frac{1}{2} \text{tr} \left(\boldsymbol{\Gamma}_x^{-1} \sum_{r=1}^n (\mathbf{x}_r - \bar{\mathbf{x}}) (\mathbf{x}_r - \bar{\mathbf{x}})' \right). \end{aligned} \quad (\text{A19})$$

Let $\bar{\mathbf{x}}$ given in (A15) be partitioned in $m_1 \times 1$ subvectors as $\bar{\mathbf{x}} = \left(\bar{\mathbf{x}}'_{f_2, f_3, \dots, f_k} : f_j \in F_j = \{1, \dots, m_j\}, \text{ for } j = 2, \dots, k \right)$, where $\bar{\mathbf{x}}_{f_2, f_3, \dots, f_k} \in \mathbb{R}^{m_1}$, that is,

$$\begin{aligned} \bar{\mathbf{x}} = & \left(\bar{\mathbf{x}}'_{1,1,\dots,1}, \dots, \bar{\mathbf{x}}'_{m_2,1,\dots,1}, \bar{\mathbf{x}}'_{1,2,\dots,1}, \dots, \bar{\mathbf{x}}'_{m_2,2,\dots,1}, \dots, \bar{\mathbf{x}}'_{1,m_3,\dots,1}, \dots, \bar{\mathbf{x}}'_{m_2,m_3,\dots,1}, \right. \\ & \left. \dots, \bar{\mathbf{x}}'_{1,1,\dots,2}, \dots, \bar{\mathbf{x}}'_{m_2,1,\dots,2}, \bar{\mathbf{x}}'_{1,2,\dots,2}, \dots, \bar{\mathbf{x}}'_{m_2,2,\dots,2}, \dots, \bar{\mathbf{x}}'_{1,m_3,\dots,m_k}, \dots, \bar{\mathbf{x}}'_{m_2,m_3,\dots,m_k} \right)', \end{aligned} \quad (\text{A20})$$

with

$$\bar{\mathbf{x}}_{\mathbf{f}} = \bar{\mathbf{x}}_{f_2, f_3, \dots, f_k} = \frac{1}{n} \sum_{r=1}^n x_{r; f_2, f_3, \dots, f_k}, \quad (\text{A21})$$

for each $\mathbf{f} = (f_2, f_3, \dots, f_k)' \in F = \prod_{j=2}^k F_j$.

With this notation and using (8), we first find an appropriate expression for

$$\begin{aligned} Q(\mathbf{x}_* : \bar{\mathbf{x}}_*, \mathbf{\Gamma}_{\mathbf{x}_*}^{-1}) & \quad (\text{A22}) \\ = & \text{tr} \left[\mathbf{\Gamma}_{\mathbf{x}_*}^{-1} (\mathbf{x}_* - \bar{\mathbf{x}}_*) (\mathbf{x}_* - \bar{\mathbf{x}}_*)' \right] \\ = & \text{tr} \left(\mathbf{\Gamma}_{\mathbf{x}}^{-1} \sum_{r=1}^n (\mathbf{x}_r - \bar{\mathbf{x}}) (\mathbf{x}_r - \bar{\mathbf{x}})' \right), \end{aligned}$$

where

$$\begin{aligned} \mathbf{x}_* &= \left(\mathbf{x}'_1, \dots, \mathbf{x}'_n \right)', \quad \text{and} \\ \bar{\mathbf{x}}_* &= \mathbf{1}_n \otimes \bar{\mathbf{x}}. \end{aligned}$$

Since for the calculation of this *trace* of a product of this two matrices, both partitioned in $m_1 \times m_1$ we only need the product of a block row indicated by $\mathbf{f} = (f_2, f_3, \dots, f_k)$ in $\mathbf{\Gamma}_{\mathbf{x}}^{-1}$ by the corresponding $\mathbf{f} = (f_2, f_3, \dots, f_k)$ block column of $\sum_{r=1}^n (\mathbf{x}_r - \bar{\mathbf{x}}) (\mathbf{x}_r - \bar{\mathbf{x}})'$. The $\mathbf{f} = (f_2, f_3, \dots, f_k)$ block row of $\mathbf{\Gamma}_{\mathbf{x}}^{-1}$ is formed by the following $p_{2,k}$ blocks: $(f_k - 1) p_{2,k-1}$ blocks equal to \mathbf{A}_k , $(f_{k-1} - 1) p_{2,k-2}$ blocks equal to $\mathbf{A}_{k-1} + \mathbf{A}_k$, \dots , $(f_3 - 1) p_{2,2}$ blocks equal to $\mathbf{A}_3 + \dots + \mathbf{A}_k$, $(f_2 - 1)$ blocks equal to $\mathbf{A}_2 + \dots + \mathbf{A}_k$, one block equal to $\mathbf{A}_1 + \dots + \mathbf{A}_k$, $(m_2 - f_2)$ blocks equal to $\mathbf{A}_2 + \dots + \mathbf{A}_k$, $(m - f_3) p_{2,2}$ blocks equal to $\mathbf{A}_3 + \dots + \mathbf{A}_k$, \dots , $(m_{k-1} - f_{k-1}) p_{2,k-2}$ blocks equal to $\mathbf{A}_{k-1} + \mathbf{A}_k$ and $(m_k - f_k) p_{2,k-1}$ blocks

equal to \mathbf{A}_k . Note that

$$\begin{aligned}
\# \text{ of blocks} &= \left[\sum_{j=1}^{k-1} (f_{k+1-j} - 1) p_{2,k-j} \right] + 1 + \left[\sum_{j=1}^{k-1} (m_{k+1-j} - f_{k+1-j}) p_{2,k-j} \right] \\
&= \left[\sum_{j=1}^{k-1} (m_{k+1-j} - 1) p_{2,k-j} \right] + 1 = \left[\sum_{j=1}^{k-1} m_{k+1-j} p_{2,k-j} - \sum_{j=1}^{k-1} p_{2,k-j} \right] + 1 \\
&= \left[\sum_{j=1}^{k-1} p_{2,k+1-j} - \sum_{j=1}^{k-1} p_{2,k-j} \right] + 1 = \left[\sum_{j^*=0}^{k-2} p_{2,k-j^*} - \sum_{j=1}^{k-1} p_{2,k-j} \right] + 1 \\
&= p_{2,k} + \left[\sum_{j^*=1}^{k-2} p_{2,k-j^*} - \sum_{j=1}^{k-2} p_{2,k-j} \right] - p_{2,1} + 1 = p_{2,k}.
\end{aligned}$$

The product of the above row block with $\mathbf{f} = (f_2, f_3, \dots, f_k)$ block column of $\sum_{r=1}^n (\mathbf{x}_r - \bar{\mathbf{x}}) (\mathbf{x}_r - \bar{\mathbf{x}})'$ is

$$\begin{aligned}
&\mathbf{A}_k \sum_{f_k^*=1}^{f_k-1} \sum_{f_{k-1}^* \in F_{k-1}} \cdots \sum_{f_2^* \in F_2} \left(\mathbf{x}_{r;f_2^*, \dots, f_{k-1}^*, f_k^*} - \bar{\mathbf{x}}_{f_2^*, \dots, f_{k-1}^*, f_k^*} \right) \left(\mathbf{x}_{r;f_2, \dots, f_k} - \bar{\mathbf{x}}_{f_2, \dots, f_k} \right)' \\
&+ (\mathbf{A}_{k-1} + \mathbf{A}_k) \sum_{f_{k-1}^*=1}^{f_{k-1}-1} \sum_{f_{k-2}^* \in F_{k-2}} \cdots \sum_{f_2^* \in F_2} \left(\mathbf{x}_{r;f_2^*, \dots, f_{k-1}^*, f_k} - \bar{\mathbf{x}}_{f_2^*, \dots, f_{k-1}^*, f_k} \right) \left(\mathbf{x}_{r;f_2, \dots, f_k} - \bar{\mathbf{x}}_{f_2, \dots, f_k} \right)' \\
&\vdots \\
&+ (\mathbf{A}_{k-1} + \mathbf{A}_k) \sum_{f_{k-1}^*=f_{k-1}+1}^{m_{k-1}-1} \sum_{f_{k-2}^* \in F_{k-2}} \cdots \sum_{f_2^* \in F_2} \left(\mathbf{x}_{r;f_2^*, \dots, f_{k-1}^*, f_k} - \bar{\mathbf{x}}_{f_2^*, \dots, f_{k-1}^*, f_k} \right) \left(\mathbf{x}_{r;f_2, \dots, f_k} - \bar{\mathbf{x}}_{f_2, \dots, f_k} \right)' \\
&\mathbf{A}_k \sum_{f_k^*=f_k+1}^{m_k-1} \sum_{f_{k-1}^* \in F_{k-1}} \cdots \sum_{f_2^* \in F_2} \left(\mathbf{x}_{r;f_2^*, \dots, f_{k-1}^*, f_k^*} - \bar{\mathbf{x}}_{f_2^*, \dots, f_{k-1}^*, f_k^*} \right) \left(\mathbf{x}_{r;f_2, \dots, f_k} - \bar{\mathbf{x}}_{f_2, \dots, f_k} \right)'.
\end{aligned}$$

Then, denoting by $\mathbf{B}_{k,j}$, for each $j = 1, 2, \dots, k$, the $m_1 \times m_1$ matrix

$$\begin{aligned}
&\mathbf{B}_{k,j} \tag{A23} \\
&= \sum_{r=1}^n \overbrace{\sum_{f_k \in F_k} \cdots \sum_{f_{j+1} \in F_{j+1}}}^{k-j \text{ sums}} \overbrace{\left(\sum_{f_j \in F_j} \sum_{f_j \neq f_j^* \in F_j} \right)}^{1 \text{ special sum pair}} \overbrace{\left(\sum_{f_{j-1} \in F_{j-1}} \sum_{f_{j-1} \in F_{j-1}} \right) \cdots \left(\sum_{f_2 \in F_2} \sum_{f_2 \in F_2} \right)}^{j-2 \text{ sum pairs}} \\
&\quad \left(\mathbf{x}'_{r; \mathbf{f}^* (\mathbf{i}_{k:j})} - \bar{\mathbf{x}}'_{\mathbf{f}^* (\mathbf{i}_{k:j})} \right)' (\mathbf{x}_{r; \mathbf{f}} - \bar{\mathbf{x}}_{\mathbf{f}}),
\end{aligned}$$

where $\mathbf{f} = f_k, \dots, f_{j+1}, f_j, \dots, f_2$ and $\mathbf{f}^* (\mathbf{i}_{k:j}) = f_k, \dots, f_{j+1}, f_j^*, \dots, f_2^*$, and consequently, where the sums with subindex f_j or f_j^* with $j < 2$ do not appear in the above expression, is

$$tr \left(\Gamma_{\mathbf{x}}^{-1} \sum_{r=1}^n (\mathbf{x}_r - \bar{\mathbf{x}}) (\mathbf{x}_r - \bar{\mathbf{x}})' \right) = \sum_{j=1}^k tr \left[\left(\sum_{i=j}^k \mathbf{A}_i \right) \mathbf{B}_{k,j} \right].$$

Now, note that (A22) can be seen as

$$Q(\mathbf{x}_* : \bar{\mathbf{x}}_*, \Gamma_{\mathbf{x}_*}^{-1}) = \text{tr}(\Gamma_{\mathbf{x}_*}^{-1} \mathbf{C}), \quad (\text{A24})$$

where \mathbf{C} is a $np_{1,k} \times np_{1,k}$ block diagonal matrix where all the diagonal block are equal to \mathbf{blockC} , where

$$\mathbf{blockC} = \sum_{j=1}^k \left(\bigotimes_{h=1}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k:j,h}} \right) \otimes (\mathbf{C}_{k,j} - \mathbf{C}_{k,j+1}),$$

with, for $j = 1, \dots, k$,

$$\mathbf{C}_{k,j} = \frac{\mathbf{B}_{k,j}}{nq_{k,j}}, \quad (\text{A25})$$

where $\mathbf{B}_{k,j}$ is given by (A23) and

$$q_{k,j} = \begin{cases} \prod_{i=1}^{k-1} m_{k+1-i} = p_{2,k} & \text{if } j = 1 \\ \left(\prod_{i=1}^{k-j} m_{k+1-i} \right) m_j (m_j - 1) \left(\prod_{i=1}^{j-2} m_{j-i}^2 \right) & \text{if } j = 2, \dots, k \end{cases}, \quad (\text{A26})$$

where $\prod_{i=1}^0 m_{k+1-i} = \prod_{i=1}^0 m_{j-i} = 1$. Therefore, since (A19)

$$\begin{aligned} \log(L) &= -\frac{np_{1,k}}{2} \log(2\pi) - \frac{n}{2} \log |\Gamma_{\mathbf{x}}| - \frac{1}{2} \text{tr} \left(\begin{array}{cc} \Gamma_{\mathbf{x}}^{-1} & \mathbf{W} \\ p_{1,k} \times p_{1,k} & p_{1,k} \times p_{1,k} \end{array} \right) \\ &= -\frac{np_{1,k}}{2} \log(2\pi) - \frac{1}{2} \log |\Gamma_{\mathbf{x}_*}| - \frac{1}{2} \text{tr} \left(\begin{array}{cc} \Gamma_{\mathbf{x}_*}^{-1} & \mathbf{C} \\ np_{1,k} \times np_{1,k} & np_{1,k} \times np_{1,k} \end{array} \right), \end{aligned}$$

we can use lemma 3.2.2 of Anderson (2003) to find its maximum with respect to $\Gamma_{\mathbf{x}_*}$. This maximum is attained at $\Gamma_{\mathbf{x}_*} = \mathbf{C}$. From this, the maximum likelihood estimates of the k – *SSCS* covariance components are

$$\hat{\mathbf{U}}_{k,j} = \mathbf{C}_{k,j} = \frac{1}{nq_{k,j}} \quad (\text{A27})$$

$$\begin{aligned} & \cdot \sum_{r=1}^n \overbrace{\sum_{f_k \in F_k} \cdots \sum_{f_{j+1} \in F_{j+1}}}^{k-j \text{ sums}} \overbrace{\left(\sum_{f_j \in F_j} \sum_{f_j \neq f_j^* \in F_j} \right)}^{1 \text{ special sum pair}} \overbrace{\left(\sum_{f_{j-1} \in F_{j-1}} \sum_{f_{j-1}^* \in F_{j-1}} \right) \cdots \left(\sum_{f_2 \in F_2} \sum_{f_2^* \in F_2} \right)}^{j-2 \text{ sum pairs}} \\ & \left(x_{r; \mathbf{f}^*}(\mathbf{i}_{k:j}) - \bar{\mathbf{x}}_{\mathbf{f}^*}(\mathbf{i}_{k:j}) \right) \left(x'_{r; \mathbf{f}} - \bar{\mathbf{x}}'_{\mathbf{f}} \right), \end{aligned}$$

for $j = 1, \dots, k$, and the maximum likelihood estimate $\hat{\Gamma}_{\mathbf{x}}$ of $\Gamma_{\mathbf{x}}$ can be written as

$$\hat{\Gamma}_{\mathbf{x}} = \sum_{j=1}^k \left(\bigotimes_{h=1}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k:j,h}} \right) \otimes \left(\hat{\mathbf{U}}_{k,j} - \hat{\mathbf{U}}_{k,j+1} \right), \quad (\text{A28})$$

where $\hat{\mathbf{U}}_{k,h}$ is given in (A27).

A.4 Proof of Theorem 3

We use mathematical induction to prove that (19) with D_{i_k} is given by (20) is true for all natural numbers k . The proof of this result for $k = 2$ is given in Leiva (2007), and for $k = 3$ is given in ????. We assume is true for **any** $(k - 1)$ -SSCS matrix V_k (inductive hypothesis is given by (8), and we will prove that (19) is true for an arbitrary k -SSCS matrix V_{k+1} . Consider $\Gamma_{\mathbf{x}_r} = \mathbf{V}_{k+1}$ an arbitrary k -SSCS matrix with SSCS-component matrices $\mathbf{U}_{k,j}$, $j = 1, \dots, k$, it can be written as

$$\mathbf{V}_{k+1} = \mathbf{I}_{m_k} \otimes (\mathbf{V}_k - \mathbf{W}_k) + \mathbf{J}_{m_k} \otimes \mathbf{W}_k, \quad \begin{matrix} p_{1,k} \times p_{1,k} \\ p_{1,k-1} \times p_{1,k-1} \\ p_{1,k-1} \times p_{1,k-1} \end{matrix}$$

then

$$\begin{aligned} & (\mathbf{H}'_{m_k} \otimes \mathbf{I}_{p_{1,k-1}}) \mathbf{V}_{k+1} (\mathbf{H}_{m_k} \otimes \mathbf{I}_{p_{1,k-1}}) \\ &= \text{diag} \{ \mathbf{V}_k + (m_k - 1) \mathbf{W}_k; \mathbf{I}_{m_{k-1}} \otimes (\mathbf{V}_k - \mathbf{W}_k) \} \end{aligned} \quad (\text{A29})$$

where $\mathbf{V}_k - \mathbf{W}_k$ is the $(k - 1)$ -SSCS matrix given in (A3) and (A2), i.e.,

$$\begin{aligned} \mathbf{V}_k - \mathbf{W}_k &= \sum_{j=1}^{k-1} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:j,h}} \right) \otimes (\mathbf{U}_{k-1,j}^* - \mathbf{U}_{k-1,j+1}^*) \\ &= \sum_{j=1}^{k-2} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:j,h}} \right) \otimes (\mathbf{U}_{k,j} - \mathbf{U}_{k,j+1}) + \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:k-1,h}} \right) \otimes \mathbf{U}_{k,j}, \end{aligned}$$

with $\mathbf{U}_{k-1,k}^* = \mathbf{0}$, and where $\mathbf{V}_k + (m_k - 1) \mathbf{W}_k$ is the $k - 1$ -SSCS matrix given in (A7) and (A6), i.e,

$$\begin{aligned} \mathbf{V}_k + (m_k - 1) \mathbf{W}_k &= \sum_{j=1}^{k-1} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:j,h}} \right) \otimes (\mathbf{U}_{k-1,j}^{**} - \mathbf{U}_{k-1,j+1}^{**}) \\ &= \left[\sum_{j=1}^{k-2} \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}}^{i_{k-1:j,h}} \right) \otimes (\mathbf{U}_{k,j} - \mathbf{U}_{k,j+1}) \right] \\ &\quad + \left(\bigotimes_{h=1}^{k-2} \mathbf{J}_{m_{k-h}} \right) \otimes (\mathbf{U}_{k,k-1} + (m_k - 1) \mathbf{U}_{k,k}). \end{aligned}$$

By the inductive hypothesis, using $\mathbf{L}'_{k-1} = \mathbf{H}'_{m_{k-1}} \otimes \dots \otimes \mathbf{H}'_{m_2} \otimes \mathbf{I}_{m_1}$ we obtain

$$\begin{aligned} \mathbf{D}_{k-1}^* &= \mathbf{L}'_{k-1} (\mathbf{V}_k - \mathbf{W}_k) \mathbf{L}_{k-1} = \text{diag} \left\{ \mathbf{D}_{i_{k-1,k-1}^*}^* : i_{k-1,k-1}^* = 1, \dots, p_{2,k-1} \right\}, \quad \text{and} \\ \mathbf{D}_{k-1}^{**} &= \mathbf{L}'_{k-1} (\mathbf{V}_k + (m_k - 1) \mathbf{W}_k) \mathbf{L}_{k-1} = \text{diag} \left\{ \mathbf{D}_{i_{k-1,k-1}^{**}}^{**} : i_{k-1,k-1}^{**} = 1, \dots, p_{2,k-1} \right\} \end{aligned}$$

Therefore, pre and post multiplying (A29) = RICARDO, CAN YOU FINISH IT

$$\begin{aligned} \mathbf{D}_k &= (\mathbf{I}_{m_k} \otimes \mathbf{L}'_{k-1}) \text{diag} \{ \mathbf{V}_k + (m_k - 1) \mathbf{W}_k; \mathbf{I}_{m_{k-1}} \otimes (\mathbf{V}_k - \mathbf{W}_k) \} (\mathbf{I}_{m_k} \otimes \mathbf{L}_{k-1}) \\ &= \text{diag} \{ \mathbf{L}'_{k-1} [\mathbf{V}_k + (m_k - 1) \mathbf{W}_k] \mathbf{L}_{k-1}; \mathbf{I}_{m_{k-1}} \otimes \mathbf{L}'_{k-1} (\mathbf{V}_k - \mathbf{W}_k) \mathbf{L}_{k-1} \} \\ &= \text{diag} \{ \mathbf{D}_{k-1}^{**}; \mathbf{I}_{m_{k-1}} \otimes \mathbf{D}_{k-1}^* \}, \end{aligned}$$

where using (A10) and (A9) is

$$\begin{aligned}
& \mathbf{D}_{i_{k-1,k-1}^{**}} \\
= & \left\{ \begin{array}{ll} \begin{array}{l} \Delta_{k-1,k-1}^{**} = \Delta_{k,k} \text{ if } i_{k-1,k-1}^{**} = 1 \\ \Delta_{k-1,k-2}^{**} = \Delta_{k,k-2} \text{ if } i_{k-1,k-1}^{**} = 1 + i_{k-1,k-2}^{**} p_{2,k-1-1} \\ \Delta_{k-1,k-3}^{**} = \Delta_{k,k-3} \text{ if } i_{k-1,k-1}^{**} = 1 + \sum_{h=1}^2 i_{k-1,k-h}^{**} p_{2,k-1-h} \\ \vdots \\ \Delta_{k-1,2}^{**} = \Delta_{k,2} \text{ if } i_{k-1,k-1}^{**} = 1 + \sum_{h=1}^{k-2} i_{k-1,k-h}^{**} p_{2,k-1-h} \\ \Delta_{k-1,1}^{**} = \Delta_{k,1} \text{ if } i_{k-1,k-1}^{**} = 1 + \sum_{h=1}^{k-1} i_{k-h}^{**} p_{2,k-h} \end{array} & \text{for } \begin{cases} i_{k-1,k-2}^{**} = 1, \dots, m_{k-1} - 1 \\ i_{k-1,k-2}^{**} = 0, \dots, m_{k-1} - 1 \\ i_{k-1,k-3}^{**} = 1, \dots, m_{k-2} - 1 \\ \vdots \\ i_{k-1,k-2}^{**} = 0, \dots, m_{k-1} - 1 \\ \vdots \\ i_{k-1,3}^{**} = 0, \dots, m_4 - 1 \\ i_{k-1,2}^{**} = 1, \dots, m_3 - 1 \\ i_{k-1,k-2}^{**} = 0, \dots, m_{k-1} - 1 \\ \vdots \\ i_{k-1,2}^{**} = 0, \dots, m_3 - 1 \\ i_{k-1,1}^{**} = 1, \dots, m_2 - 1 \end{cases} \end{array} \right. \quad (\text{A30})
\end{aligned}$$

while \mathbf{D}_{k-1}^* appears repeated m_{k-1} times filling in the diagonal blocks the rows from $p_{1,k-1} + 1$ to $p_{1,k}$ (that is from the second diagonal $(m_1 \times m_1)$ - block to the $(p_{2,k})$ th diagonal $(m_1 \times m_1)$ - block repeating the following set of $p_{2,k}$ components $\mathbf{D}_{i_{k-1,k-1}^*}$.

$$\begin{aligned}
& \mathbf{D}_{i_{k-1,k-1}^*} \\
= & \left\{ \begin{array}{ll} \begin{array}{l} \Delta_{k-1,k-1}^* = \Delta_{k,k} \text{ if } i_{k-1,k-1}^* = 1 \\ \Delta_{k-1,k-2}^* = \Delta_{k,k-2} \text{ if } i_{k-1,k-1}^* = 1 + i_{k-1,k-2}^* p_{2,k-1-1} \\ \Delta_{k-1,k-3}^* = \Delta_{k,k-3} \text{ if } i_{k-1,k-1}^* = 1 + \sum_{h=1}^2 i_{k-1,k-h}^* p_{2,k-1-h} \\ \vdots \\ \Delta_{k-1,2}^* = \Delta_{k,2} \text{ if } i_{k-1,k-1}^* = 1 + \sum_{h=1}^{k-2} i_{k-1,k-h}^* p_{2,k-1-h} \\ \Delta_{k-1,1}^* = \Delta_{k,1} \text{ if } i_{k-1,k-1}^* = 1 + \sum_{h=1}^{k-1} i_{k-h}^* p_{2,k-h} \end{array} & \text{for } \begin{cases} i_{k-1,k-2}^* = 1, \dots, m_{k-1} - 1 \\ i_{k-1,k-2}^* = 0, \dots, m_{k-1} - 1 \\ i_{k-1,k-3}^* = 1, \dots, m_{k-1} - 1 \\ \vdots \\ i_{k-1,k-2}^* = 0, \dots, m_{k-1} - 1 \\ \vdots \\ i_{k-1,3}^* = 0, \dots, m_4 - 1 \\ i_{k-1,2}^* = 1, \dots, m_3 - 1 \\ i_{k-1,k-2}^* = 0, \dots, m_{k-1} - 1 \\ \vdots \\ i_{k-1,2}^* = 0, \dots, m_3 - 1 \\ i_{k-1,1}^* = 1, \dots, m_2 - 1 \end{cases} \end{array} \right. \quad (\text{A31})
\end{aligned}$$

$$\mathbf{L}'_{k-1} = \mathbf{H}'_{m_{k-1}} \otimes \cdots \otimes \mathbf{H}'_{m_2} \otimes \mathbf{I}_{m_1}$$

is

$$\mathbf{D}_k = (\mathbf{I}_{m_k} \otimes \mathbf{L}'_{k-1}) [\mathbf{I}_{m_k} \otimes (\mathbf{V}_k - \mathbf{W}_k) + \mathbf{J}_{m_k} \otimes \mathbf{W}_k] (\mathbf{I}_{m_k} \otimes \mathbf{L}_{k-1})$$

Alternatively, the result of Theorem 4 can be written as

$$\mathbf{L}'_k \boldsymbol{\Gamma}_x \mathbf{L}_k = \text{diag} \left\{ \mathbf{D}_f; \mathbf{f} = (f_2, f_3, \dots, f_k)' \in F = \prod_{j=2}^k F_j \right\}, \quad (\text{A32})$$

where the diagonal $(m_1 \times m_1)$ - matrices $\mathbf{D}_f = \mathbf{D}_{f_2, f_3, \dots, f_k}$ are given by

$$\mathbf{D}_{f_2, f_3, \dots, f_k} = \begin{cases} \Delta_{k,k} & \text{if } f_2 = 1, \dots, f_{k-1} = 1, f_k = 1 \\ \Delta_{k,k-1} & \text{if } f_2 = 1, \dots, f_{k-1} = 1, f_k \neq 1 \\ \Delta_{k,k-2} & \text{if } f_2 = 1, \dots, f_{k-2} = 1, f_{k-1} \neq 1 \\ \vdots & \vdots \\ \Delta_{k,2} & \text{if } f_2 = 1, f_3 \neq 1 \\ \Delta_{k,1} & \text{if } f_2 \neq 1 \end{cases} \quad (\text{A33})$$

A.5 Proof of Lemma 4

1. Using () and part 5 of Lemma 3, we know that

$$\begin{aligned} \Delta_{k,1} &= \mathbf{U}_{k,1} - \mathbf{U}_{k,2} \\ &= \frac{bTr_{p_{1,1}}(\boldsymbol{\Gamma}_x)}{p_{2,k}} - \frac{bSum_{p_{1,1}}(bTr_{p_{1,2}}(\boldsymbol{\Gamma}_x)) - bTr_{p_{1,1}}(\boldsymbol{\Gamma}_x)}{p_{2,k}(m_2 - 1)} \\ &= \frac{(m_2 - 1)bTr_{p_{1,1}}(\boldsymbol{\Gamma}_x) - bSum_{p_{1,1}}(bTr_{p_{1,2}}(\boldsymbol{\Gamma}_x)) + bTr_{p_{1,1}}(\boldsymbol{\Gamma}_x)}{p_{2,k}(m_2 - 1)} \\ &= \frac{m_2 \cdot bTr_{p_{1,1}}(\boldsymbol{\Gamma}_x) - bSum_{p_{1,1}}[bTr_{p_{1,2}}(\boldsymbol{\Gamma}_x)]}{p_{2,k}(m_2 - 1)}. \end{aligned}$$

Since

$$\begin{aligned} & p_{2,i}(\mathbf{U}_{k,i} - \mathbf{U}_{k,i+1}) \\ &= \frac{p_{2,i} \cdot bSum_{p_{1,1}} \{ bSum_{p_{1,i-1}}(bTr_{p_{1,i}}(\boldsymbol{\Gamma}_x)) - bTr_{p_{1,i-1}}(\boldsymbol{\Gamma}_x) \}}{p_{i+1,k} \cdot m_i (m_i - 1) \cdot p_{2,i-1}^2} \\ & \quad - \frac{p_{2,i} \cdot bSum_{p_{1,1}} \{ bSum_{p_{1,i}}(bTr_{p_{1,i+1}}(\boldsymbol{\Gamma}_x)) - bTr_{p_{1,i}}(\boldsymbol{\Gamma}_x) \}}{p_{i+2,k} \cdot m_{i+1} (m_{i+1} - 1) \cdot p_{2,i}^2} \\ &= \frac{m_i \cdot bSum_{p_{1,1}} \{ bSum_{p_{1,i-1}}(bTr_{p_{1,i}}(\boldsymbol{\Gamma}_x)) - bTr_{p_{1,i-1}}(\boldsymbol{\Gamma}_x) \}}{p_{i+1,k} \cdot m_i (m_i - 1) \cdot p_{2,i-1}} \\ & \quad - \frac{bSum_{p_{1,1}} \{ bSum_{p_{1,i}}(bTr_{p_{1,i+1}}(\boldsymbol{\Gamma}_x)) - bTr_{p_{1,i}}(\boldsymbol{\Gamma}_x) \}}{p_{i+2,k} \cdot m_{i+1} (m_{i+1} - 1) \cdot p_{2,i}}, \end{aligned}$$

then

$$\begin{aligned}
\Delta_{k,j} &= \sum_{i=1}^j p_{2,i} (\mathbf{U}_{k,i} - \mathbf{U}_{k,i+1}) \\
&= p_{2,1} \mathbf{U}_{k,1} + \left(\sum_{i=1}^{j-1} (p_{2,i+1} - p_{2,i}) \mathbf{U}_{k,i+1} \right) - p_{2,j} \mathbf{U}_{k,j+1} \\
&= \frac{bTr_{p_{1,1}}(\mathbf{\Gamma}_x)}{p_{2,k}} - p_{2,j} \mathbf{U}_{k,j+1} \\
&\quad + \left(\sum_{i=1}^{j-1} (m_{i+1} - 1) \cdot p_{2,i} \cdot \frac{bSum_{p_{1,1}} \{ bSum_{p_{1,i}} (bTr_{p_{1,i+1}}(\mathbf{\Gamma}_x)) - bTr_{p_{1,i}}(\mathbf{\Gamma}_x) \}}{p_{i+2,k} \cdot m_{i+1} (m_{i+1} - 1) \cdot p_{2,i}^2} \right) \\
&= \frac{bTr_{p_{1,1}}(\mathbf{\Gamma}_x)}{p_{2,k}} + \left(\sum_{i=1}^{j-1} \frac{bSum_{p_{1,1}} \{ bSum_{p_{1,i}} (bTr_{p_{1,i+1}}(\mathbf{\Gamma}_x)) - bTr_{p_{1,i}}(\mathbf{\Gamma}_x) \}}{p_{2,k}} \right) - p_{2,j} \mathbf{U}_{k,j+1} \\
&= \frac{bTr_{p_{1,1}}(\mathbf{\Gamma}_x)}{p_{2,k}} + \left(\sum_{i=1}^{j-1} \frac{bSum_{p_{1,1}} \{ bSum_{p_{1,i}} (bTr_{p_{1,i+1}}(\mathbf{\Gamma}_x)) - bTr_{p_{1,i}}(\mathbf{\Gamma}_x) \}}{p_{2,k}} \right) \\
&\quad - \frac{p_{2,j} \cdot bSum_{p_{1,1}} \{ bSum_{p_{1,j}} (bTr_{p_{1,j+1}}(\mathbf{\Gamma}_x)) - bTr_{p_{1,j}}(\mathbf{\Gamma}_x) \}}{p_{j+2,k} \cdot m_{j+1} (m_{j+1} - 1) \cdot p_{2,j}^2} \\
&= \frac{bTr_{p_{1,1}}(\mathbf{\Gamma}_x)}{p_{2,k}} + \left(\sum_{i=1}^{j-1} \frac{bSum_{p_{1,1}} \{ bSum_{p_{1,i}} (bTr_{p_{1,i+1}}(\mathbf{\Gamma}_x)) - bTr_{p_{1,i}}(\mathbf{\Gamma}_x) \}}{p_{2,k}} \right) \\
&\quad - \frac{bSum_{p_{1,1}} \{ bSum_{p_{1,j}} (bTr_{p_{1,j+1}}(\mathbf{\Gamma}_x)) - bTr_{p_{1,j}}(\mathbf{\Gamma}_x) \}}{p_{2,k} \cdot (m_{j+1} - 1)}.
\end{aligned}$$

Finally, the expression of $\Delta_{k,k}$ is obtained by replacing j with k in the above expression of $\Delta_{k,j}$ and noting that the last term is $p_{2,k} \mathbf{U}_{k,k+1} = \mathbf{0}$.

2. Since for $j = 1$ is $i_{k:1,h} = 0$ for each $h = 1, \dots, k-1$,

$$\begin{aligned}
&\mathbf{Q}_{k,1} \mathbf{\Gamma}_x \mathbf{Q}_{k,1} \\
&= \left[\left(\bigotimes_{h=1}^{k-1} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{I}_{m_1} \right] \left[\sum_{j=1}^k \left(\bigotimes_{h=1}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k:j,h}} \right) \otimes (\mathbf{U}_{k,j} - \mathbf{U}_{k,j+1}) \right] \\
&\quad \left[\left(\bigotimes_{h=1}^{k-1} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{I}_{m_1} \right] \\
&= \left[\sum_{j=1}^k \left(\bigotimes_{h=1}^{k-1} \mathbf{P}_{m_{k+1-h}} \mathbf{J}_{m_{k+1-h}}^{i_{k:j,h}} \mathbf{P}_{m_{k+1-h}} \right) \otimes (\mathbf{U}_{k,j} - \mathbf{U}_{k,j+1}) \right] \\
&= \left(\bigotimes_{h=1}^{k-1} \mathbf{P}_{m_{k+1-h}} \right) \otimes \sum_{j=1}^k \left(\prod_{h=1}^{k-1} m_{k+1-h}^{i_{k:j,h}} \right) (\mathbf{U}_{k,j} - \mathbf{U}_{k,j+1}),
\end{aligned}$$

and using (7) is

$$\begin{aligned}
\mathbf{Q}_{k,1} \Gamma_{\mathbf{x}} \mathbf{Q}_{k,1} &= \left(\bigotimes_{h=1}^{k-1} \mathbf{P}_{m_{k+1-h}} \right) \otimes \sum_{j=1}^k \mathbf{p}_{2,j} (\mathbf{U}_{k,j} - \mathbf{U}_{k,j+1}) \\
&= \left(\bigotimes_{h=1}^{k-1} \mathbf{P}_{m_{k+1-h}} \right) \otimes \Delta_{k,k}.
\end{aligned}$$

Similarly, using (25), for $j = 2, \dots, k$, is

$$\begin{aligned}
&\mathbf{Q}_{k,j} \Gamma_{\mathbf{x}} \mathbf{Q}_{k,j} \\
&= \left[\left(\bigotimes_{h=1}^{k-j} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{Q}_{m_j} \otimes \left(\bigotimes_{h=k-(j-2)}^{k-1} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{I}_{m_1} \right] \\
&\quad \left[\sum_{j^*=1}^k \left(\bigotimes_{h=1}^{k-1} \mathbf{J}_{m_{k+1-h}}^{i_{k:j^*,h}} \right) \otimes (\mathbf{U}_{k,j^*} - \mathbf{U}_{k,j^*+1}) \right] \\
&\quad \left[\left(\bigotimes_{h=1}^{k-j} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{Q}_{m_j} \otimes \left(\bigotimes_{h=k-(j-2)}^{k-1} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{I}_{m_1} \right] \\
&= \sum_{j^*=1}^k \left[\left(\bigotimes_{h=1}^{k-j} \mathbf{P}_{m_{k+1-h}} \mathbf{J}_{m_{k+1-h}}^{i_{k:j^*,h}} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{Q}_{m_j} \mathbf{J}_{m_{k+1-h}}^{i_{k:j^*,k-(j-1)}} \mathbf{Q}_{m_j} \right. \\
&\quad \left. \otimes \left(\bigotimes_{h=k-(j-2)}^{k-1} \mathbf{P}_{m_{k+1-h}} \mathbf{J}_{m_{k+1-h}}^{i_{k:j^*,h}} \mathbf{P}_{m_{k+1-h}} \right) \otimes (\mathbf{U}_{k,j^*} - \mathbf{U}_{k,j^*+1}) \right]
\end{aligned}$$

since $\mathbf{Q}_{m_j} \mathbf{J}_{m_{k+1-h}}^{i_{k:j^*,h}} \mathbf{Q}_{m_j} = 0$ for each $i_{k:j^*,h} = 1$, that is, for each $i_{k:j^*}$ with $j^* \geq j$, then

$$\begin{aligned}
& \mathbf{Q}_{k,j} \Gamma_x \mathbf{Q}_{k,j} \\
&= \sum_{j^*=1}^{j-1} \left[\left(\bigotimes_{h=1}^{k-j} \mathbf{P}_{m_{k+1-h}} \mathbf{J}_{m_{k+1-h}}^{i_{k:j^*,h}} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{Q}_{m_j} \mathbf{J}_{m_{k+1-h}}^{i_{k:j^*,k-(j-1)}} \mathbf{Q}_{m_j} \right. \\
&\quad \left. \otimes \left(\bigotimes_{h=k-(j-2)}^{k-1} \mathbf{P}_{m_{k+1-h}} \mathbf{J}_{m_{k+1-h}}^{i_{k:j^*,h}} \mathbf{P}_{m_{k+1-h}} \right) \otimes (\mathbf{U}_{k,j^*} - \mathbf{U}_{k,j^*+1}) \right] \\
&= \sum_{j^*=1}^{j-1} \left[\left(\bigotimes_{h=1}^{k-j} \mathbf{P}_{m_{k+1-h}} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{Q}_{m_j} \mathbf{J}_{m_{k+1-h}}^0 \mathbf{Q}_{m_j} \otimes \left(\bigotimes_{h=k-(j-2)}^{k-j^*} \mathbf{P}_{m_{k+1-h}} \mathbf{J}_{m_{k+1-h}}^0 \mathbf{P}_{m_{k+1-h}} \right) \right. \\
&\quad \left. \otimes \left(\bigotimes_{h=k-(j^*-1)}^{k-1} \mathbf{P}_{m_{k+1-h}} \mathbf{J}_{m_{k+1-h}}^1 \mathbf{P}_{m_{k+1-h}} \right) \otimes (\mathbf{U}_{k,j^*} - \mathbf{U}_{k,j^*+1}) \right] \\
&= \sum_{j^*=1}^{j-1} \left[\left(\bigotimes_{h=1}^{k-j} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{Q}_{m_j} \otimes \left(\bigotimes_{h=k-(j-2)}^{k-j^*} \mathbf{P}_{m_{k+1-h}} \right) \right. \\
&\quad \left. \otimes \left(\bigotimes_{h=k-(j^*-1)}^{k-1} m_{k+1-h} \mathbf{P}_{m_{k+1-h}} \right) \otimes (\mathbf{U}_{k,j^*} - \mathbf{U}_{k,j^*+1}) \right] \\
&= \left(\bigotimes_{h=1}^{k-j} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{Q}_{m_j} \left(\bigotimes_{h=k-(j-2)}^{k-1} \mathbf{P}_{m_{k+1-h}} \right) \\
&\quad \otimes \sum_{j^*=1}^{j-1} \left[\left(\prod_{h=k-(j^*-1)}^{k-1} m_{k+1-h} \right) (\mathbf{U}_{k,j^*} - \mathbf{U}_{k,j^*+1}) \right],
\end{aligned}$$

that is, using (6),

$$\begin{aligned}
& \mathbf{Q}_{k,j} \Gamma_x \mathbf{Q}_{k,j} \\
&= \left(\bigotimes_{h=1}^{k-j} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{Q}_{m_j} \otimes \left(\bigotimes_{h=k-(j-2)}^{k-1} \mathbf{P}_{m_{k+1-h}} \right) \\
&\quad \otimes \sum_{j^*=1}^{j-1} \left[\left(\prod_{h=k-(j^*-1)}^{k-1} m_{k+1-h} \right) (\mathbf{U}_{k,j^*} - \mathbf{U}_{k,j^*+1}) \right] \\
&= \left(\bigotimes_{h=1}^{k-j} \mathbf{P}_{m_{k+1-h}} \right) \otimes \mathbf{Q}_{m_j} \otimes \left(\bigotimes_{h=k-(j-2)}^{k-1} \mathbf{P}_{m_{k+1-h}} \right) \otimes \Delta_{k,j-1}.
\end{aligned}$$

3. Using the above part (2), the results to be proved are equivalent to

$$\begin{aligned}
\Delta_{k,k} &= bTr_{p_{1,1}} \left[\left(\bigotimes_{h=1}^{k-1} P_{m_{k+1-h}} \right) \otimes \Delta_{k,k} \right] \\
&= \frac{1}{p_{2,k}} bSum_{p_{1,1}} \left[\left(\bigotimes_{h=1}^{k-1} P_{m_{k+1-h}} \right) \otimes \Delta_{k,k} \right] \\
\Delta_{k,j-1} &= \frac{bTr_{p_{1,1}} \left[\left(\bigotimes_{h=1}^{k-j} P_{m_{k+1-h}} \right) \otimes Q_{m_j} \otimes \left(\bigotimes_{h=k-(j-2)}^{k-1} P_{m_{k+1-h}} \right) \otimes \Delta_{k,j-1} \right]}{m_j - 1}, \\
&\text{for } j = 2, \dots, k.
\end{aligned}$$

Noting that each $m_1 \times m_1$ - block of $\left(\bigotimes_{h=1}^{k-1} P_{m_{k+1-h}} \right) \otimes \Delta_{k,k} = \left(\bigotimes_{h=1}^{k-1} J_{m_{k+1-h}} \right) \otimes \frac{1}{p_{2,k}} \Delta_{k,k}$ is $\frac{1}{p_{2,k}} \Delta_{k,k}$, then

$$bTr_{p_{1,1}} \left[\left(\bigotimes_{h=1}^{k-1} P_{m_{k+1-h}} \right) \otimes \Delta_{k,k} \right] = p_{2,k} \cdot \frac{1}{p_{2,k}} \Delta_{k,k} = \Delta_{k,k},$$

and

$$bSum_{p_{1,1}} \left[\left(\bigotimes_{h=1}^{k-1} P_{m_{k+1-h}} \right) \otimes \Delta_{k,k} \right] = p_{2,k}^2 \cdot \frac{1}{p_{2,k}} \Delta_{k,k} = p_{2,k} \cdot \Delta_{k,k},$$

that is,

$$\begin{aligned}
\Delta_{k,k} &= bTr_{p_{1,1}} \left[\left(\bigotimes_{h=1}^{k-1} P_{m_{k+1-h}} \right) \otimes \Delta_{k,k} \right] \\
&= \frac{1}{p_{2,k}} bSum_{p_{1,1}} \left[\left(\bigotimes_{h=1}^{k-1} P_{m_{k+1-h}} \right) \otimes \Delta_{k,k} \right].
\end{aligned}$$

Similarly, the matrix $Q_{k,j} \otimes \Delta_{k,j-1}$ can be expressed as

$$\begin{aligned}
&Q_{k,j} \otimes \Delta_{k,j-1} \\
&= \left(\bigotimes_{h=1}^{k-j} \frac{1}{m_{k+1-h}} J_{m_{k+1-h}} \right) \otimes Q_{m_j} \otimes \left(\bigotimes_{h=k-(j-2)}^{k-1} \frac{1}{m_{k+1-h}} J_{m_{k+1-h}} \right) \otimes \Delta_{k,j-1} \\
&= \frac{1}{p_{j+1,k}} J_{p_{j+1,k}} \otimes \left(I_{m_j} - \frac{1}{m_j} J_{m_j} \right) \otimes \frac{1}{p_{2,j-1}} J_{p_{2,j-1}} \otimes \Delta_{k,j-1} \\
&= J_{p_{j+1,k}} \otimes \left((m_j - 1) I_{m_j} - (J_{m_j} - I_{m_j}) \right) \otimes J_{p_{2,j-1}} \otimes \frac{\Delta_{k,j-1}}{p_{2,k}} \\
&= J_{p_{j+1,k}} \otimes I_{m_j} \otimes J_{p_{2,j-1}} \otimes \frac{(m_j - 1) \Delta_{k,j-1}}{p_{2,k}} \\
&\quad - J_{p_{j+1,k}} \otimes (J_{m_j} - I_{m_j}) \otimes J_{p_{2,j-1}} \otimes \frac{\Delta_{k,j-1}}{p_{2,k}},
\end{aligned}$$

where all $m_1 \times m_1$ -block in the diagonal of $\mathbf{J}_{p_{j+1,k}} \otimes (\mathbf{J}_{m_j} - \mathbf{I}_{m_j}) \otimes \mathbf{J}_{p_{2,j-1}} \otimes \frac{\Delta_{k,j-1}}{p_{2,k}}$ are $\mathbf{0}$, and then

$$\begin{aligned} bTr_{p_{1,1}}(\mathbf{Q}_{k,j} \otimes \Delta_{k,j}) &= bTr_{p_{1,1}}\left(\mathbf{J}_{p_{j+1,k}} \otimes \mathbf{I}_{m_j} \otimes \mathbf{J}_{p_{2,j-1}} \otimes \frac{(m_j - 1) \Delta_{k,j-1}}{p_{2,k}}\right) \\ &= p_{j+1,k} \cdot m_j \cdot p_{2,j-1} \cdot \frac{(m_j - 1) \Delta_{k,j}}{p_{2,k}} = (m_j - 1) \Delta_{k,j}, \end{aligned}$$

that is,

$$\Delta_{k,j} = \frac{bTr_{p_{1,1}}(\mathbf{Q}_{k,j} \otimes \Delta_{k,j})}{m_j - 1}, \quad \text{for } j = 2, \dots, k.$$

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