Dimension-free Structured Covariance Estimation

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Abstract

Given a sample of i.i.d. high-dimensional centered random vectors, we consider a problem of estimation of their covariance matrix Σ with an additional assumption that Σ can be represented as a sum of a few Kronecker products of smaller matrices. Under mild conditions, we derive the first non-asymptotic dimension-free high-probability bound on the Frobenius distance between Σ and a widely used penalized permuted least squares estimate. Because of the hidden structure, the established rate of convergence is faster than in the standard covariance estimation problem. **Keywords:** Kronecker rank, effective rank, rearrangement operator, penalized permuted least squares estimate.

1. Introduction

Let $\mathbf{X}, \mathbf{X}_1, \dots, \mathbf{X}_n \in \mathbb{R}^d$ be i.i.d. centered random vectors. We are interested in estimation of the covariance matrix $\Sigma = \mathbb{E}\mathbf{X}\mathbf{X}^\top$ from observations $\mathbf{X}_1, \dots, \mathbf{X}_n$. This classical problem is of a great significance and it arises in various domains such as wireless communications (Werner and Jansson, 2007), economics and finance (Bai and Shi, 2011), biology and medicine (for example, functional MRI (Derado et al., 2010), genomics (Xie and Bentler, 2003), MEG/EEG (De Munck et al., 2004)). A standard approach to this problem is to consider the sample covariance

$$\widehat{\Sigma} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{X}_i \mathbf{X}_i^{\top}.$$

Unfortunately, if the number of available samples n is much less than the ambient dimension d (which is often the case in practical scenarios), the estimate $\hat{\Sigma}$ suffers from the curse of dimensionality. To overcome this issue, researchers have explored leveraging structural properties of covariance matrices to reduce their total number of degrees of freedom. This includes assumptions on the covariance matrix like sparsity (Banerjee et al., 2008; Ravikumar et al., 2011), low-rank (Fan et al., 2008), Toeplitz (Fuhrmann, 1991) and bandable model (Bickel and Levina, 2008ab). A reader is referred to the survey (Cai et al., 2016) for further examples. In situations when data can be represented as tensors, a popular modelling assumption is based on expansion of Σ into a Kronecker product of two smaller matrices (Wang et al., 2022):

$$\Sigma = \Phi \otimes \Psi$$
, where $\Phi \in \mathbb{R}^{p \times p}$, $\Psi \in \mathbb{R}^{q \times q}$, and $pq = d$. (1)

Each of the matrices Φ, Ψ corresponds to a certain index (mode) of the multivariate array and can be interpreted as a mode-wise covariance. For instance, when researchers deal with spatio-temporal

data, they use Kronecker product to separate spatial and temporal dimensions. Despite its simplicity, the Kronecker product model (1) appears to be useful in various applications (Werner and Jansson, 2007; Werner et al., 2008; Allen and Tibshirani, 2010; Guggenberger et al., 2023). In the present paper, we are concerned with a more expressive model that approximates the covariance matrix as a sum of Kronecker products:

$$\Sigma = \Phi_1 \otimes \Psi_1 + \dots + \Phi_K \otimes \Psi_K, \tag{2}$$

where $\Phi_1, \Psi_1, \ldots, \Phi_K, \Psi_K$ are symmetric positive semidefinite matrices, such that $\Phi_j \in \mathbb{R}^{p \times p}$, $\Psi_j \in \mathbb{R}^{q \times q}$ for all $j \in \{1, \ldots, K\}$ and pq = d. In this case, one says that Σ has a *Kronecker rank* equal to K. By summing multiple Kronecker products, the model can capture complex interactions and dependencies that may not be adequately represented by a single Kronecker product. We would like to note that any symmetric matrix of size $(pq \times pq)$ admits an expansion of the form (2) with $K = \min\{p^2, q^2\}$. However, even with a small number of Kronecker product terms, the model (2) has shown promising results in applications such as clutter covariance estimation for airborne STAP (Sun et al., 2018), MEG/EEG (De Munck et al., 2002, 2004; Bijma et al., 2005), video modelling (Greenewald et al., 2013), and SAR data analysis (Rucci et al., 2010). Notably, accurate approximations with a small number of Kronecker product terms have been demonstrated for the Matérn family of covariances (Litvinenko et al., 2019).

The rates of convergence in the covariance estimation problem with Σ of the form (1) or (2) were studied in numerous papers (see, for example, Werner et al. (2008); Tsiligkaridis and Hero (2013); Zhou (2014); Leng and Pan (2018); Masak et al. (2022)). However, the existing state-of-the-art results are either dimension-dependent or based on unsuitable for high-dimensional setting assumptions. At the same time, the recent advances in covariance estimation (Bunea and Xiao, 2015; Puchkin et al., 2023; Zhivotovskiy, 2024) allow to establish non-asymptotic high-probability bounds on the Frobenius and operator norm of $(\hat{\Sigma} - \Sigma)$ in terms of the effective rank $\mathbf{r}(\Sigma) = \text{Tr}(\Sigma)/||\Sigma||$ under mild assumptions, completely eliminating dependence on the ambient dimension *d*. For example, (Bunea and Xiao, 2015, Proposition A.3) prove that, for any $\delta \in (0, 1)$, with probability at least $1 - \delta$, we have

$$\left\|\widehat{\Sigma} - \Sigma\right\|_{\mathrm{F}} \lesssim \mathrm{Tr}(\Sigma) \left(\sqrt{\frac{\log(2/\delta)}{n}} \vee \frac{\log(2/\delta)}{n}\right). \tag{3}$$

Here and further in the paper, the sign \leq stands for an inequality up to an absolute multiplicative constant. This brings us to a question, whether it is possible to obtain sharper dimension-free bounds when Σ admits a Kronecker product expansion (2). The following motivating example gives a positive answer in the simple case K = 1.

Example 1.1 Let Σ have a Kronecker rank one, that is, it admits a representation (1) for some positive semidefinite matrices $\Phi \in \mathbb{R}^{p \times p}$ and $\Psi \in \mathbb{R}^{q \times q}$. Let $\mathbb{X}_1, \ldots, \mathbb{X}_n \in \mathbb{R}^{q \times p}$ be the matrices obtained by reshaping¹ of the vectors $\mathbf{X}_1, \ldots, \mathbf{X}_n$, respectively. Consider the estimates

$$\widehat{\Phi} = rac{1}{n} \sum_{i=1}^n \mathbb{X}_i^\top \mathbb{X}_i \quad and \quad \widehat{\Psi} = rac{1}{n} \sum_{i=1}^n \mathbb{X}_i \mathbb{X}_i^\top.$$

^{1.} More precisely, it holds that $\mathbf{vec}(\mathbb{X}_i) = \mathbf{X}_i$ for all $i \in \{1, ..., n\}$, where **vec** is the vectorization operator, stacking the matrix columns together (see the definition in Appendix A).

As shown by Leng and Pan (2018), $\widehat{\Phi}$ and $\widehat{\Psi}$ are unbiased estimates of $\operatorname{Tr}(\Psi)\Phi$ and $\operatorname{Tr}(\Phi)\Psi$, respectively. If, for any vectors $\mathbf{u} \in \mathbb{R}^p$, $\mathbf{v} \in \mathbb{R}^q$ and any $i \in \{1, \ldots, n\}$, it holds that

$$\frac{1}{\mathrm{Tr}(\Psi)} \left\| \mathbf{u}^\top \mathbb{X}_i^\top \mathbb{X}_i \mathbf{u} \right\|_{\psi_1} \lesssim \mathbf{u}^\top \Phi \mathbf{u} \quad and \quad \frac{1}{\mathrm{Tr}(\Phi)} \left\| \mathbf{v}^\top \mathbb{X}_i \mathbb{X}_i^\top \mathbf{v} \right\|_{\psi_1} \lesssim \mathbf{v}^\top \Psi \mathbf{v},$$

where $\|\cdot\|_{\psi_1}$ denotes the Orlicz norm (see the notation section below), then, similarly to the proof of Proposition A.3 from (Bunea and Xiao, 2015), we can show that

$$\left\|\widehat{\Phi}/\mathrm{Tr}(\Psi) - \Phi\right\|_{\mathrm{F}} \lesssim \mathrm{Tr}(\Phi) \left(\sqrt{\frac{\log(2/\delta)}{n}} \vee \frac{\log(2/\delta)}{n}\right)$$

and

$$\left\|\widehat{\Psi}/\mathrm{Tr}(\Phi) - \Psi\right\|_{\mathrm{F}} \lesssim \mathrm{Tr}(\Psi) \left(\sqrt{\frac{\log(2/\delta)}{n}} \vee \frac{\log(2/\delta)}{n}\right)$$

simultaneously on an event with probability at least $1 - \delta$. The trace product $\operatorname{Tr}(\Phi)\operatorname{Tr}(\Psi) = \operatorname{Tr}(\Sigma)$ can be easily estimated by $(\|\mathbf{X}_1\|^2 + \cdots + \|\mathbf{X}_n\|^2)/n$. Then the estimate

$$\breve{\Sigma} = \frac{\widehat{\Phi} \otimes \widehat{\Psi}}{\frac{1}{n} \sum_{i=1}^{n} \|\mathbf{X}_i\|^2},\tag{4}$$

suggested by Leng and Pan (2018), satisfies the following high probability bound:

$$\begin{split} \left\| \breve{\Sigma} - \Sigma \right\|_{\mathrm{F}} &\lesssim \left(\|\Psi\| \mathrm{Tr}(\Phi) + \|\Phi\| \mathrm{Tr}(\Psi) \right) \left(\sqrt{\frac{\log(2/\delta)}{n}} \vee \frac{\log(2/\delta)}{n} \right) \\ &= \|\Sigma\| \left(\mathbf{r}(\Phi) + \mathbf{r}(\Psi) \right) \left(\sqrt{\frac{\log(2/\delta)}{n}} \vee \frac{\log(2/\delta)}{n} \right), \end{split}$$

where $r(\Phi) = Tr(\Phi)/||\Phi||$ and $r(\Psi) = Tr(\Psi)/||\Psi||$, while (3) implies that

$$\begin{split} \left\| \widehat{\Sigma} - \Sigma \right\|_{\mathrm{F}} &\lesssim \mathrm{Tr}(\Sigma) \left(\sqrt{\frac{\log(2/\delta)}{n}} \vee \frac{\log(2/\delta)}{n} \right) \\ &= \| \Sigma \| \mathbf{r}(\Phi) \mathbf{r}(\Psi) \left(\sqrt{\frac{\log(2/\delta)}{n}} \vee \frac{\log(2/\delta)}{n} \right) \end{split}$$

Hence, the Kronecker structural assumption helped us to significantly improve the upper bound (3) *by replacing the product of effective ranks with their sum.*

Unfortunately, the estimate Σ from Example 1.1 significantly exploits the product structure (1) of Σ , which allows to estimate Φ and Ψ separately. This approach has no direct extension on the case of larger Kronecker rank. For this reason, the case, when Σ has a form (2) with K > 1, requires much more efforts.

Contribution. Our main contribution is a sharper upper bound on the performance of a regularized permuted least squares estimate $\tilde{\Sigma}$ (defined in (6)), which is widely used for covariance estimation in the presence of a Kronecker product structure. Under reasonable assumptions on the distribution of $\mathbf{X}, \mathbf{X}_1, \ldots, \mathbf{X}_n$, we show that, if Σ has a form (2), then

$$\left\|\widetilde{\Sigma} - \Sigma\right\|_{\mathrm{F}}^{2} \lesssim K\left(\sum_{j=1}^{K} \|\Phi_{j}\| \|\Psi_{j}\|\right)^{2} \cdot \left(\frac{1}{n} \max_{1 \leqslant j \leqslant K} \mathbf{r}(\Phi_{j})^{2} + \frac{1}{n} \max_{1 \leqslant j \leqslant K} \mathbf{r}(\Psi_{j})^{2} + \frac{\log(1/\delta)}{n}\right)$$

with probability at least $(1 - \delta)$. To our knowledge, this is the first dimension-free upper bound, capturing the Kronecker structure of the population covariance.

Notation. Throughout the paper, $\widehat{\Sigma}$ stands for the sample covariance. The identity matrix of size $(d \times d)$ and the zero matrix are denoted by I_d and O, respectively. For any matrix A, ||A||, $||A||_*$, and $||A||_F$ stand for the operator, nuclear, and Frobenius norms of A, respectively. Given arbitrary matrices $A \in \mathbb{R}^{p \times q}$ and $B \in \mathbb{R}^{r \times s}$, $A \otimes B$ denotes their Kronecker product:

$$A \otimes B = \begin{pmatrix} a_{11}B & \dots & a_{1q}B \\ \vdots & \ddots & \vdots \\ a_{p1}B & \dots & a_{pq}B \end{pmatrix} \in \mathbb{R}^{pr \times qs}.$$

For any matrix $U \in \mathbb{R}^{k \times \ell}$ with columns $\mathbf{u}_1, \ldots, \mathbf{u}_\ell$, $\mathbf{vec}(U) = (\mathbf{u}_1^\top, \ldots, \mathbf{u}_\ell^\top)^\top$ is a vector obtained by stacking the columns of U together. We also use the standard notation $\mathbf{r}(M) = \text{Tr}(M)/||M||$ for the effective rank of a symmetric positive semidefinite matrix M. Instead of $\min\{a, b\}$ and $\max\{a, b\}$, sometimes we will use $a \wedge b$ and $a \vee b$, respectively. The notation $f \leq g$ is equivalent to $f = \mathcal{O}(g)$. Finally, of any random variable ξ and any $s \geq 1$, the Orlicz norm $||\xi||_{\psi_s}$ is defined as

$$\|\xi\|_{\psi_s} = \inf\left\{t > 0 : \mathbb{E}e^{|\xi|^s/t^s} \leqslant 2\right\}.$$

The boldface font is reserved for vectors, while matrices and scalars are displayed in a regular font.

Paper structure. The rest of the paper is organized as follows. In Section 2, we present our main result, Theorem 2.5, discuss its novelty and compare with related work. Sections 3 and 4 are devoted to the proof of Theorem 2.5 and its main ingredient, Lemma 3.2. We also provide some useful information about Kronecker product and the vectorization operator vec in Appendix A. The proofs of some technical results are also deferred to Appendix.

2. Main results

This section contains the main result of this paper, but first, we have to introduce auxiliary definitions. One of the central objects when dealing with a covariance Σ of the form (2) is the rearrangement operator \mathcal{R} , defined below.

Definition 2.1 (rearrangement operator) Let M be a matrix of size $pq \times pq$ with a block structure

$$M = \begin{pmatrix} M(1,1) & \dots & M(1,p) \\ \vdots & \ddots & \vdots \\ M(p,1) & \dots & M(p,p) \end{pmatrix}, \text{ where } M(i,j) \in \mathbb{R}^{q \times q} \text{ for all } i, j \in \{1,\dots,p\}.$$

The rearrangement operator $\mathcal{R} : \mathbb{R}^{pq \times pq} \to \mathbb{R}^{p^2 \times q^2}$ is defined by the following identity: the ((j - 1)p + i)-th row of $\mathcal{R}(M)$ is $\mathbf{vec}(M(i, j))^{\top}$.

The importance of the rearrangement operator becomes clear from the properties formulated in the next proposition.

Proposition 2.2 The following holds.

- \mathcal{R} is a linear operator.
- \mathcal{R} defines an isometry between the Euclidean spaces $(\mathbb{R}^{pq \times pq}, \|\cdot\|_{\mathrm{F}})$ and $(\mathbb{R}^{p^2 \times q^2}, \|\cdot\|_{\mathrm{F}})$. As a consequence, there exists an inverse map \mathcal{R}^{-1} .
- If $M = A \otimes B$, where $A \in \mathbb{R}^{p \times p}$ and $B \in \mathbb{R}^{q \times q}$, then $\mathcal{R}(M) = \mathbf{vec}(A)\mathbf{vec}(B)^{\top}$.

The first and the second properties follow immediately from the definition of \mathcal{R} . The third one is well-known in the literature (see, for instance, the proof of Theorem 1 in (Van Loan and Pitsianis, 1993)). The rearrangement operator reduces our problem to low-rank matrix estimation. Indeed, if the covariance matrix Σ can be represented a sum of Kronecker products (2), then, due to Proposition 2.2,

$$\mathcal{R}(\Sigma) = \sum_{j=1}^{K} \mathcal{R}(\Phi_j \otimes \Psi_j) = \sum_{j=1}^{K} \mathbf{vec}(\Phi_j) \mathbf{vec}(\Psi_j)^{\top}.$$

In other words, if Σ has a Kronecker rank K, then $\mathcal{R}(\Sigma)$ has the same algebraic rank. This observation allows us to construct estimates based on the singular value decomposition of $\mathcal{R}(\hat{\Sigma})$, as in (Tsiligkaridis and Hero, 2013; Masak et al., 2022). For instance, Masak et al. (2022) considered an estimate based on K principal components of $\mathcal{R}(\hat{\Sigma})$:

$$\check{\Sigma} = \mathcal{R}^{-1}(\check{R}), \quad \text{where} \quad \check{R} = \sum_{j=1}^{K} \hat{\sigma}_j \hat{\mathbf{u}}_j \hat{\mathbf{v}}_j^{\top}, \tag{5}$$

where the values $\hat{\sigma}_1 \ge \ldots \ge \hat{\sigma}_K$ and the vectors $\hat{\mathbf{u}}_1, \hat{\mathbf{v}}_1, \ldots, \hat{\mathbf{u}}_K, \hat{\mathbf{v}}_K$ are defined from the singular value decomposition

$$\mathcal{R}(\widehat{\Sigma}) = \sum_{j=1}^{p^2 \wedge q^2} \widehat{\sigma}_j \widehat{\mathbf{u}}_j \widehat{\mathbf{v}}_j^{\top}$$

Let us note that the estimate (5) solves the optimization problem

$$\check{R} \in \operatorname*{argmin}_{R \in \mathbb{R}^{p^2 \times q^2}} \left\| R - \mathcal{R}(\hat{\Sigma}) \right\|_{\mathrm{F}}^2 + \lambda \operatorname{rank}(R), \quad \text{where } \hat{\sigma}_{K+1}^2 \leqslant \lambda \leqslant \hat{\sigma}_K^2.$$

In the present paper, we study the permuted least squares estimate suggested in (Tsiligkaridis and Hero, 2013), where the authors replaced rank(R) by nuclear norm penalization:

$$\widetilde{\Sigma} = \mathcal{R}^{-1}(\widetilde{R}), \quad \text{where} \quad \widetilde{R} \in \operatorname*{argmin}_{R \in \mathbb{R}^{p^2 \times q^2}} \left\{ \left\| R - \mathcal{R}(\widehat{\Sigma}) \right\|_{\mathrm{F}}^2 + \lambda \|R\|_* \right\}.$$
(6)

Similarly to \check{R} , the estimate \tilde{R} admits an explicit representation given by soft thresholding:

$$\widetilde{R} = \sum_{j=1}^{p^2 \wedge q^2} \left(\widehat{\sigma}_j - \lambda/2 \right)_+ \widehat{\mathbf{u}}_j \widehat{\mathbf{v}}_j^\top.$$

Our goal is to establish a dimension-free upper bound on the Frobenuis norm of $(\tilde{\Sigma} - \Sigma)$. Usually, results of such kind require some additional properties of the distribution of $\mathbf{X}, \mathbf{X}_1, \ldots, \mathbf{X}_n$. We impose the following assumption.

Assumption 2.3 There exists $\omega > 0$, such that the standardized random vector $\Sigma^{-1/2}\mathbf{X}$ satisfies the inequality

$$\log \mathbb{E} \exp\left\{ (\Sigma^{-1/2} \mathbf{X})^{\top} V (\Sigma^{-1/2} \mathbf{X}) - \operatorname{Tr}(V) \right\} \leqslant \omega^2 \|V\|_{\mathrm{F}}^2$$
(7)

for all $V \in \mathbb{R}^{d \times d}$, such that $\|V\|_{\mathrm{F}} \leq 1/\omega$.

An equivalent condition appeared in the paper (Puchkin et al., 2023), where the authors assumed that

$$\left\| (\Sigma^{-1/2} \mathbf{X})^{\top} V (\Sigma^{-1/2} \mathbf{X}) - \operatorname{Tr}(V) \right\|_{\psi_1} \lesssim \|V\|_{\mathrm{F}} \quad \text{for all } V \in \mathbb{R}^{d \times d}.$$
(8)

The fact that (8) yields (7) follows from, for instance, (Zhivotovskiy, 2024, Lemma 2). In (Puchkin et al., 2023), the authors argued that Assumption 2.3 holds for a large class of distributions. In particular, they discussed that it is fulfilled for all random vectors, satisfying the Hanson-Wright inequality. The examples include the Gaussian distribution $\mathcal{N}(\mathbf{0}, \Sigma)$ and, more generally, all distributions, such that $\Sigma^{-1/2}\mathbf{X}$ has independent components with finite ψ_2 -norms. Besides, random vectors satisfying log-Sobolev inequality or having the convex concentration property (Adamczak, 2015) also meet Assumption 2.3. Since a covariance matrix with a Kronecker product structure (2) often appears in the context of matrix models, we would like to give relevant examples from this field. For instance, if we have a matrix model

$$\mathbb{X} = B \mathbb{Y} A^\top,$$

where $B \in \mathbb{R}^{q \times q}$, $A \in \mathbb{R}^{p \times p}$, and $\mathbb{Y} \in \mathbb{R}^{q \times p}$ is a random matrix with i.i.d. standard Gaussian entries, then $\operatorname{vec}(\mathbb{X}) \sim \mathcal{N}(\mathbf{0}, (AA^{\top}) \otimes (BB^{\top}))$ and, consequently, it fulfils Assumption 2.3. In the proposition below, we provide another, more general example when the assumption is satisfied.

Proposition 2.4 Let

$$\mathbb{X} = \sum_{j=1}^{K} B_j \mathbb{Y}_j A_j^{\top},\tag{9}$$

where $\mathbb{Y}_1, \ldots, \mathbb{Y}_K \in \mathbb{R}^{q \times p}$ are independent centered random matrices. Assume that there exist positive numbers $\omega_1, \ldots, \omega_K$, such that for any $j \in \{1, \ldots, K\}$

$$\log \mathbb{E} \exp \left\{ \mathbf{vec}(\mathbb{Y}_j)^\top V \mathbf{vec}(\mathbb{Y}_j) - \mathrm{Tr}(V) \right\} \leq \omega_j^2 \|V\|_{\mathrm{F}}^2$$
(10)

for all $V \in \mathbb{R}^{d^2 \times d^2}$, satisfying the inequality $\|V\|_{\mathrm{F}} \leq 1/\omega_j$. Then $\operatorname{vec}(\mathbb{X})$ fulfils Assumption 2.3 with

$$\Sigma = \sum_{j=1}^{K} (A_j A_j^{\top}) \otimes (B_j B_j^{\top}) \quad and \quad \omega \leq \left(2\omega_{\max} \vee 16\sqrt{\frac{2+2\omega_{\max}}{\log 2}} \right),$$

where $\omega_{\max} = \max_{1 \leq j \leq K} \omega_j$.

The proof of Proposition 2.4 is quite technical. For this reason, we postpone it to Appendix B and move to the main result.

Theorem 2.5 Assume that the centered random vector **X** meets Assumption (2.3) and that its covariance Σ has a form (2). Let us fix any $\delta \in (0, 1)$, satisfying the constraint

$$\frac{1}{2n} \left(\max_{1 \le j \le K} \mathbf{r}(\Phi_j)^2 + \max_{1 \le j \le K} \mathbf{r}(\Psi_j)^2 \right) + \frac{\log(4/\delta)}{n} \le 1,$$

and take any $\lambda \in \mathbb{R}$, such that

$$\lambda \ge 2\omega \left(\sum_{j=1}^{K} \|\Phi_j\| \|\Psi_j\|\right) \sqrt{\frac{13}{2n} \left(\max_{1 \le j \le K} \mathbf{r}(\Phi_j)^2 + \max_{1 \le j \le K} \mathbf{r}(\Psi_j)^2\right) + \frac{13\log(4/\delta)}{n}}$$

Then, with probability at least $(1 - \delta)$, the permuted nuclear-norm penalized least squares estimate $\widetilde{\Sigma}$, defined in (6), fulfils the inequality

$$\left\|\widetilde{\Sigma} - \Sigma\right\|_{\mathrm{F}}^2 < \frac{3\lambda^2 K}{2}.$$

Remark 2.6 Theorem 2.5 requires a proper choice of $\lambda > 0$. To tune the parameter, we can fix a finite family $\Lambda = \{\lambda_0 \cdot 2^{-m} : 0 \le m \le M\}$, where $\lambda_0 > 0$ and $M \in \mathbb{N}$ are some constants, and perform model selection, using cross-validation or the random split procedure described in (Bickel and Levina, 2008b, Section 3). If the chosen λ meets the inequality

$$\lambda \leqslant C\omega \left(\sum_{j=1}^{K} \|\Phi_j\| \|\Psi_j\| \right) \sqrt{\frac{13}{2n} \left(\max_{1 \leqslant j \leqslant K} \mathbf{r}(\Phi_j)^2 + \max_{1 \leqslant j \leqslant K} \mathbf{r}(\Psi_j)^2 \right) + \frac{13 \log(4/\delta)}{n}}$$

with an absolute constant C > 2, then, under the conditions of Theorem 2.5, it holds that

$$\left\|\widetilde{\Sigma} - \Sigma\right\|_{\mathrm{F}}^{2} \lesssim \omega^{2} K \left(\sum_{j=1}^{K} \|\Phi_{j}\| \|\Psi_{j}\|\right)^{2} \left(\frac{1}{n} \max_{1 \leq j \leq K} \mathbf{r}(\Phi_{j})^{2} + \frac{1}{n} \max_{1 \leq j \leq K} \mathbf{r}(\Psi_{j})^{2} + \frac{\log(1/\delta)}{n}\right)$$

with probability at least $(1 - \delta)$.

To our knowledge, Theorem 2.5 provides the first dimension-free high-probability upper bound on the accuracy of covariance estimation with a Kronecker product structure. The most relevant papers to ours are (Masak et al., 2022) and (Tsiligkaridis and Hero, 2013), where the authors considered the estimates $\tilde{\Sigma}$ and $\tilde{\Sigma}$ (see (5), (6)), based on the hard and soft thresholding, respectively. In (Masak et al., 2022), the authors assumed only the existence of the fourth moment of $||\mathbf{X}||$ and proper decay of the singular values of $\mathcal{R}(\Sigma)$. Under these mild conditions, they proved the consistency of $\tilde{\Sigma}$. Unfortunately, the established rate of convergence includes the Frobenius norm of $(\hat{\Sigma} - \Sigma)$, which is of order $\mathbf{r}(\Sigma)/\sqrt{n}$ in the worst-case scenario and, in contrast to Theorem 2.5, shows no improvements compared to the unstructured case. In (Tsiligkaridis and Hero, 2013), the authors derived a non-asymptotic bound on the performance of the permuted least-squares estimate $\tilde{\Sigma}$. Assuming the observations $\mathbf{X}_1, \ldots, \mathbf{X}_n$ to have a Gaussian distribution $\mathcal{N}(\mathbf{0}, \Sigma)$, they showed that

$$\left\|\widetilde{\Sigma} - \Sigma\right\|_{\mathrm{F}}^2 \lesssim \frac{K(p^2 + q^2 + \log M)}{n} \vee \frac{K(p^2 + q^2 + \log M)^2}{n^2}$$

with probability at least $1 - M^{-c}$, where c > 0 is an absolute constant. In our paper, we derive a sharper dimension-free bound for a broader class of distributions, which remains valid in the extremely high-dimensional setup.

Let us elaborate on implications of Theorem 2.5 in the simpler case K = 1, which also got a considerable attention in the literature. In (Werner et al., 2008), the authors focused on the Gaussian case and showed the consistency of the maximum likelihood estimate and of non-iterative flip-flop algorithm. Later, Zhou (2014) suggested the Gemini method and obtained high-probability dimension-dependent bounds on the accuracy of covariance estimation, improving over the results of Werner, Jansson, and Stoica (2008). The Gemini estimator also exploits the fact that X_1, \ldots, X_n have the Gaussian distribution. In contrast, Leng and Pan (2018) considered a much broader class of distributions with finite 48-th moment. Under some technical assumptions, they derived a high-probability upper bound on the accuracy of covariance estimation in terms of both operator and Frobenius norms. Unfortunately, the analysis of Zhou (2014) and Leng and Pan (2018) imposes a severe restriction that the lowest eigenvalues of Φ and Ψ from the decomposition (1) should be bounded away from zero. This makes their theoretical guarantees vacuous in the high-dimensional setting. On the other hand, if the Kronecker rank of Σ is equal to one, then Theorem 2.5 yields that

$$\left\|\widetilde{\Sigma} - \Sigma\right\|_{\mathrm{F}}^2 \lesssim \omega^2 \|\Sigma\|^2 \cdot \frac{\mathbf{r}(\Phi)^2 + \mathbf{r}(\Psi)^2 + \log(1/\delta)}{n}$$

with probability at least $(1 - \delta)$. Note that this bound has a slightly better dependence on $\log(1/\delta)$, than the rate of convergence from Example 1.1.

3. Proof of Theorem 2.5

The first step in the proof of the rate of convergence of the permuted least squares estimate $\tilde{\Sigma}$ is identical to the one of Tsiligkaridis and Hero (2013). With a proper choice of λ , we have the following oracle inequality.

Theorem 3.1 (Tsiligkaridis and Hero (2013), Theorem 2) If $\lambda \ge 2 \|\mathcal{R}(\hat{\Sigma} - \Sigma)\|$, then

$$\left\|\widetilde{R} - \mathcal{R}(\Sigma)\right\|_{\mathrm{F}}^{2} \leq \inf_{R} \left\{ \|R - \mathcal{R}(\Sigma)\|_{\mathrm{F}}^{2} + \frac{(1+\sqrt{2})^{2}}{4}\lambda^{2} \mathrm{rank}(R) \right\}.$$
 (11)

Obviously, since Σ admits a representation (2), the rank of the matrix

$$\mathcal{R}(\Sigma) = \mathcal{R}\left(\sum_{j=1}^{K} \Phi_j \otimes \Psi_j\right) = \sum_{j=1}^{K} \mathcal{R}\left(\Phi_j \otimes \Psi_j\right) = \sum_{j=1}^{K} \mathbf{vec}(\Phi_j) \mathbf{vec}(\Psi_j)^{\top}$$
(12)

is equal to K. In view of (12), the oracle inequality (11) can be rewritten in the form

$$\left\|\widetilde{R} - \mathcal{R}(\Sigma)\right\|_{\mathrm{F}}^{2} \leq \frac{(1+\sqrt{2})^{2}\lambda^{2}K}{4}, \text{ provided that } \lambda \geq 2\|\mathcal{R}(\widehat{\Sigma} - \Sigma)\|.$$

Our main technical result, leading to superior guarantees on the performance of $\tilde{\Sigma}$ is the following dimension-free bound on the operator norm of $\mathcal{R}(\hat{\Sigma} - \Sigma)$.

Lemma 3.2 Let Assumption 2.3 hold and let us fix any $\delta \in (0, 1)$, satisfying the inequality

$$\frac{1}{2n} \left(\max_{1 \le j \le K} \mathbf{r}(\Phi_j)^2 + \max_{1 \le j \le K} \mathbf{r}(\Psi_j)^2 \right) + \frac{\log(4/\delta)}{n} \le 1.$$
(13)

Then, with probability at least $(1 - \delta)$, it holds that

$$\left\|\mathcal{R}(\widehat{\Sigma}-\Sigma)\right\| \leq \omega \left(\sum_{j=1}^{K} \|\Phi_j\| \|\Psi_j\|\right) \sqrt{\frac{13}{2n} \left(\max_{1 \leq j \leq K} \mathbf{r}(\Phi_j)^2 + \max_{1 \leq j \leq K} \mathbf{r}(\Psi_j)^2\right) + \frac{13\log(4/\delta)}{n}}$$

We present the proof of Lemma 3.2 in Section 4 below. With Lemma 3.2, we easily finish the proof of Theorem 2.5. Let λ be any number, satisfying the inequality

$$\lambda \ge 2\omega \left(\sum_{j=1}^{K} \|\Phi_j\| \|\Psi_j\| \right) \sqrt{\frac{13}{2n} \left(\max_{1 \le j \le K} \mathbf{r}(\Phi_j)^2 + \max_{1 \le j \le K} \mathbf{r}(\Psi_j)^2 \right) + \frac{13 \log(4/\delta)}{n}}$$

Then, according to Lemma 3.2, $\lambda \ge 2 \|\mathcal{R}(\hat{\Sigma} - \Sigma)\|$ on an event of probability at least $(1 - \delta)$. Hence, on this event, it holds that

$$\left\|\widetilde{\Sigma} - \Sigma\right\|_{\mathrm{F}}^{2} = \left\|\widetilde{R} - \mathcal{R}(\Sigma)\right\|_{\mathrm{F}}^{2} \leqslant \frac{(1+\sqrt{2})^{2}\lambda^{2}K}{4} = \frac{(3+2\sqrt{2})\lambda^{2}K}{4} < \frac{3\lambda^{2}K}{2}.$$

4. Proof of Lemma 3.2

The present section is devoted to the proof of our main technical result. For convenience, we split it into several steps, deferring auxiliary derivations to Appendix.

Step 1: reduction to an empirical process. We start with representing the operator norm of $\mathcal{R}(\hat{\Sigma} - \Sigma)$ in an appropriate form.

Lemma 4.1 Let $\mathbb{X}, \mathbb{X}_1, \ldots, \mathbb{X}_n$ be random matrices of size $(q \times p)$, such that $\mathbf{vec}(\mathbb{X}) = \mathbf{X}$ and $\mathbf{vec}(\mathbb{X}_i) = \mathbf{X}_i$ for all $i \in \{1, \ldots, n\}$. Then it holds that

$$\left\| \mathcal{R}(\widehat{\Sigma} - \Sigma) \right\| = \sup_{\substack{U \in \mathbb{R}^{p \times p}, V \in \mathbb{R}^{q \times q} \\ \|U\|_{F} = \|V\|_{F} = 1}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \operatorname{Tr} \left(\mathbb{X}_{i}^{\top} V^{\top} \mathbb{X}_{i} U \right) - \mathbb{E} \operatorname{Tr} \left(\mathbb{X}^{\top} V^{\top} \mathbb{X} U \right) \right\}.$$
(14)

The proof of Lemma 4.1 is postponed to Appendix C. Now we are in position to use powerful tools from the empirical process theory to derive a dimension-free bound on the supremum in the right-hand side of (14). The main ingredient of our proof is the following PAC-Bayesian variational inequality (see, for instance, (Catoni and Giulini, 2017, Proposition 2.1)).

Lemma 4.2 Let $\mathbf{X}, \mathbf{X}_1, \ldots, \mathbf{X}_n$ be i.i.d. random elements on a measurable space \mathcal{X} . Let Θ be a parameter space equipped with a measure μ (which is also referred to as prior). Let $f : \mathcal{X} \times \Theta \to \mathbb{R}$. Then, with probability at least $1 - \delta$, it holds that

$$\mathbb{E}_{\boldsymbol{\theta} \sim \rho} \frac{1}{n} \sum_{i=1}^{n} f(\mathbf{X}_{i}, \boldsymbol{\theta}) \leq \mathbb{E}_{\boldsymbol{\theta} \sim \rho} \log \mathbb{E}_{\mathbf{X}} e^{f(\mathbf{X}, \boldsymbol{\theta})} + \frac{\mathcal{KL}(\rho, \mu) + \log(1/\delta)}{n}$$

simultaneously for all $\rho \ll \mu$.

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Recently, Zhivotovskiy (2024) used a similar approach to prove that the operator norm of $(\hat{\Sigma} - \Sigma)$ is of order $\mathcal{O}(\sqrt{r(\Sigma)/n})$ with high probability. Unfortunately, the rate of convergence $\mathcal{O}(\sqrt{r(\Sigma)/n})$ is suboptimal in our case, because of the additional structure of the population covariance. In the rest of the proof, we deduce a sharper high-probability upper bound

$$\|\mathcal{R}(\widehat{\Sigma} - \Sigma)\| \lesssim \sqrt{\frac{1}{n}} \left(\max_{1 \le j \le K} \mathbf{r}(\Phi_j)^2 + \max_{1 \le j \le K} \mathbf{r}(\Psi_j)^2 \right),$$

leading to better guarantees on the accuracy of estimation of Σ .

Step 2: a variational inequality. On this step, we specify the prior and posterior distributions in order to apply Lemma 4.2 to our problem. In our case, both μ and ρ will be absolutely continuous with respect to the Lebesgue measure, so we identify them with the corresponding densities. Let μ be the density of a Gaussian measure on $\mathbb{R}^{p \times p} \times \mathbb{R}^{q \times q}$:

$$\mu(X,Y) = \frac{\alpha^{p^2/2} \beta^{q^2/2}}{(2\pi)^{p^2/2+q^2/2}} \exp\left\{-\frac{\alpha}{2} \|X\|_{\mathrm{F}}^2 - \frac{\beta}{2} \|Y\|_{\mathrm{F}}^2\right\}, \quad \text{where } X \in \mathbb{R}^{p \times p}, Y \in \mathbb{R}^{q \times q}, \quad (15)$$

and

$$\alpha = \max_{1 \le j \le K} \mathbf{r}(\Phi_j)^2, \quad \beta = \max_{1 \le j \le K} \mathbf{r}(\Psi_j)^2.$$
(16)

For any $U \in \mathbb{R}^{p \times p}$ and $V \in \mathbb{R}^{q \times q}$, define a set

$$\Upsilon(U,V) = \left\{ (X,Y) \in \mathbb{R}^{p \times p} \times \mathbb{R}^{q \times q} : \left\| \Sigma^{1/2} \left((X-U) \otimes (Y-V) \right) \Sigma^{1/2} \right\|_{\mathrm{F}}^{2} \leqslant \frac{4 \operatorname{Tr}(\Sigma)^{2}}{\alpha \beta}, \\ \left\| \left(\sum_{j=1}^{K} \|\Psi_{j}\| \Phi_{j} \right)^{1/2} (X-U) \left(\sum_{j=1}^{K} \|\Psi_{j}\| \Phi_{j} \right)^{1/2} \right\|_{\mathrm{F}}^{2} \leqslant \frac{4}{\alpha} \left(\sum_{j=1}^{K} \|\Psi_{j}\| \operatorname{Tr}(\Phi_{j}) \right)^{2},$$

$$\left\| \left(\sum_{j=1}^{K} \|\Phi_{j}\| \Psi_{j} \right)^{1/2} (Y-V) \left(\sum_{j=1}^{K} \|\Phi_{j}\| \Psi_{j} \right)^{1/2} \right\|_{\mathrm{F}}^{2} \leqslant \frac{4}{\beta} \left(\sum_{j=1}^{K} \|\Phi_{j}\| \operatorname{Tr}(\Psi_{j}) \right)^{2} \right\}$$

$$(17)$$

and a corresponding posterior density $\rho_{U,V}$, supported on $\Upsilon(U, V)$:

$$\rho_{U,V}(X,Y) = \begin{cases} \mu(X-U,Y-V)/\mathbf{Z}, & \text{if } (X,Y) \in \Upsilon(U,V), \\ 0, & \text{otherwise,} \end{cases}$$
(18)

where Z is a normalizing constant. It is not hard to show that Z is at least 1/4.

Lemma 4.3 With the notations introduced above, it holds that $Z \ge 1/4$.

The proof of Lemma 4.3 is deferred to Appendix D. Let $\nu > 0$ be a positive constant to be defined later. Considering a pair $(U, V) \in \mathbb{R}^{p \times p} \times \mathbb{R}^{q \times q}$ as an element of the parameter space

$$\Theta = \left\{ (U, V) \in \mathbb{R}^{p \times p} \times \mathbb{R}^{q \times q} \right\},\$$

we conclude that, according to Lemma 4.2,

$$\sup_{\substack{U \in \mathbb{R}^{p \times p}, V \in \mathbb{R}^{q \times q} \\ \|U\|_{\mathrm{F}} = \|V\|_{\mathrm{F}} = 1}} \left\{ \frac{\nu}{n} \sum_{i=1}^{n} \operatorname{Tr} \left(\mathbb{X}_{i}^{\top} V^{\top} \mathbb{X}_{i} U \right) - \nu \mathbb{E}_{\mathbb{X}} \operatorname{Tr} \left(\mathbb{X}^{\top} V^{\top} \mathbb{X} U \right) \right\}$$

$$= \sup_{\substack{U \in \mathbb{R}^{p \times p}, V \in \mathbb{R}^{q \times q} \\ \|U\|_{\mathrm{F}} = \|V\|_{\mathrm{F}} = 1}} \left\{ \frac{\nu}{n} \sum_{i=1}^{n} \mathbb{E}_{(P,Q) \sim \rho_{U,V}} \operatorname{Tr} \left(\mathbb{X}_{i}^{\top} Q^{\top} \mathbb{X}_{i} P \right) - \nu \mathbb{E}_{(P,Q) \sim \rho_{U,V}} \mathbb{E}_{\mathbb{X}} \operatorname{Tr} \left(\mathbb{X}^{\top} Q^{\top} \mathbb{X} P \right) \right\}$$

$$(19)$$

$$\leq \sup_{\substack{U \in \mathbb{R}^{p \times p}, V \in \mathbb{R}^{q \times q} \\ \|U\|_{\mathrm{F}} = \|V\|_{\mathrm{F}} = 1}} \left\{ \mathbb{E}_{(P,Q) \sim \rho_{U,V}} \log \left[\mathbb{E}_{\mathbb{X}} \exp \left\{ \nu \operatorname{Tr} \left(\mathbb{X}^{\top} Q^{\top} \mathbb{X} P \right) - \nu \mathbb{E}_{\mathbb{X}} \operatorname{Tr} \left(\mathbb{X}^{\top} Q^{\top} \mathbb{X} P \right) \right\} \right]$$

$$+ \frac{\mathcal{K} \mathcal{L}(\rho_{U,V}, \mu) + \log(1/\delta)}{n} \right\}.$$

with probability at least $(1 - \delta)$.

Step 3: a bound on the exponential moment. Our next goal is to bound the exponential moment

$$\mathbb{E}_{\mathbb{X}} \exp \left\{ \nu \operatorname{Tr} \left(\mathbb{X}^{\top} Q^{\top} \mathbb{X} P \right) - \nu \mathbb{E}_{\mathbb{X}} \operatorname{Tr} \left(\mathbb{X}^{\top} Q^{\top} \mathbb{X} P \right) \right\}.$$

We begin with the following auxiliary result.

Lemma 4.4 Let us fix any $U \in \mathbb{R}^{p \times p}$ and $V \in \mathbb{R}^{q \times q}$, such that $||U||_{\mathrm{F}} = ||V||_{\mathrm{F}} = 1$. Then

$$\left\|\Sigma^{1/2}(P\otimes Q)\Sigma^{1/2}\right\|_{\mathrm{F}}^{2} \leq 13\left(\sum_{j=1}^{K}\|\Phi_{j}\|\|\Psi_{j}\|\right)^{2} \quad \rho_{U,V}\text{-almost surely.}$$

The proof of Lemma 4.4 is moved to Appendix E. Applying this lemma and using the fact that $\mathbf{X} = \mathbf{vec}(\mathbb{X})$ satisfies Assumption 2.3, we obtain that

$$\log \mathbb{E}_{\mathbb{X}} \exp \left\{ \nu \operatorname{Tr} \left(\mathbb{X}^{\top} Q^{\top} \mathbb{X} P \right) - \nu \mathbb{E}_{\mathbb{X}} \operatorname{Tr} \left(\mathbb{X}^{\top} Q^{\top} \mathbb{X} P \right) \right\}$$

$$= \log \mathbb{E}_{\mathbb{X}} \exp \left\{ \nu \operatorname{vec}(\mathbb{X})^{\top} (P \otimes Q) \operatorname{vec}(\mathbb{X}) - \nu \mathbb{E}_{\mathbb{X}} \operatorname{vec}(\mathbb{X})^{\top} (P \otimes Q) \operatorname{vec}(\mathbb{X}) \right\}$$

$$= \log \mathbb{E}_{\mathbf{X}} \exp \left\{ \nu \mathbf{X}^{\top} (P \otimes Q) \mathbf{X} - \nu \mathbb{E}_{\mathbf{X}} \mathbf{X}^{\top} (P \otimes Q) \mathbf{X} \right\}$$

$$\leq \omega^{2} \nu^{2} \left\| \Sigma^{1/2} (P \otimes Q) \Sigma^{1/2} \right\|_{\mathrm{F}}^{2}$$

$$\leq 13 \omega^{2} \nu^{2} \left(\sum_{j=1}^{K} \|\Phi_{j}\| \|\Psi_{j}\| \right)^{2}$$
(20)

for all ν , such that

$$13\omega^{2}\nu^{2} \left(\sum_{j=1}^{K} \|\Phi_{j}\| \|\Psi_{j}\|\right)^{2} \leq 1,$$
(21)

and for all $U \in \mathbb{R}^{p \times p}$, $V \in \mathbb{R}^{q \times q}$ with unit Frobenius norms.

Step 4: a bound on the Kullback-Leibler divergence. We proceed with an upper bound on $\mathcal{KL}(\rho_{U,V}, \mu)$, where the densities μ and $\rho_{U,V}$ are defined in (15) and (18), respectively. It holds that

$$\mathcal{KL}(\rho_{U,V},\mu) = \int_{\Upsilon(U,V)} \log \frac{\rho_{U,V}(X,Y)}{\mu(X,Y)} \rho_{U,V}(X,Y) dX dY.$$

Substituting X and Y by X + U and Y + V, respectively, we immediately obtain that

$$\begin{split} \mathcal{KL}(\rho_{U,V},\mu) &= \int_{\Upsilon(O,O)} \log \frac{\rho_{U,V}(X+U,Y+V)}{\mu(X+U,Y+V)} \rho_{U,V}(X+U,Y+V) \mathrm{d}X \mathrm{d}Y \\ &= \int_{\Upsilon(O,O)} \log \frac{\rho_{O,O}(X,Y)}{\mu(X+U,Y+V)} \rho_{O,O}(X,Y) \mathrm{d}X \mathrm{d}Y \\ &= \log \frac{1}{Z} + \int_{\Upsilon(O,O)} \left(\alpha \mathrm{Tr}(U^{\top}X) + \beta \mathrm{Tr}(V^{\top}Y) \right) \rho_{O,O}(X,Y) \mathrm{d}X \mathrm{d}Y \\ &+ \frac{1}{2} \int_{\Upsilon(O,O)} \left(\alpha \|U\|_{\mathrm{F}}^{2} + \beta \|V\|_{\mathrm{F}}^{2} \right) \rho_{O,O}(X,Y) \mathrm{d}X \mathrm{d}Y \\ &= \log \frac{1}{Z} + \frac{\alpha \|U\|_{\mathrm{F}}^{2} + \beta \|V\|_{\mathrm{F}}^{2}}{2}. \end{split}$$

Here we took into account that $\Upsilon(O, O)$ and $\rho_{O,O}$ are symmetric around zero and, hence,

$$\int_{\Upsilon(O,O)} \operatorname{Tr}(U^{\top}X)\rho_{O,O}(X,Y) \mathrm{d}X \mathrm{d}Y = 0, \quad \int_{\Upsilon(O,O)} \operatorname{Tr}(V^{\top}Y)\rho_{O,O}(X,Y) \mathrm{d}X \mathrm{d}Y = 0.$$

Applying Lemma 4.3, we conclude that

$$\mathcal{KL}(\rho_{U,V},\mu) \leq 2\log 2 + \frac{\alpha+\beta}{2} = 2\log 2 + \frac{1}{2} \left(\max_{1 \leq j \leq K} \mathbf{r}(\Phi_j)^2 + \max_{1 \leq j \leq K} \mathbf{r}(\Psi_j)^2 \right)$$
(22)

for all $U \in \mathbb{R}^{p \times p}$, $V \in \mathbb{R}^{q \times q}$, such that $\|U\|_{\mathcal{F}} = \|V\|_{\mathcal{F}} = 1$.

Step 4: final bound. Summing up (14), (19), (20), and (22), we obtain that

$$\begin{split} \nu \left\| \mathcal{R}(\widehat{\Sigma} - \Sigma) \right\| &\leq 13\omega^2 \nu^2 \left(\sum_{j=1}^K \|\Phi_j\| \|\Psi_j\| \right)^2 \\ &+ \frac{1}{2n} \left(\max_{1 \leq j \leq K} \mathbf{r}(\Phi_j)^2 + \max_{1 \leq j \leq K} \mathbf{r}(\Psi_j)^2 \right) + \frac{\log(4/\delta)}{n} \end{split}$$

with probability at least $(1 - \delta)$. Let us take

$$\nu = \frac{1}{\omega\sqrt{13}} \left(\sum_{j=1}^{K} \|\Phi_j\| \|\Psi_j\| \right)^{-1} \sqrt{\frac{1}{2n} \left(\max_{1 \le j \le K} \mathbf{r}(\Phi_j)^2 + \max_{1 \le j \le K} \mathbf{r}(\Psi_j)^2 \right) + \frac{\log(4/\delta)}{n}}.$$

Note that the requirement (13) ensures that such choice of ν fulfils (21). Hence, with probability at least $(1 - \delta)$, it holds that

$$\left\| \mathcal{R}(\widehat{\Sigma} - \Sigma) \right\| \leq \omega \left(\sum_{j=1}^{K} \|\Phi_j\| \|\Psi_j\| \right) \sqrt{\frac{13}{2n} \left(\max_{1 \leq j \leq K} \mathbf{r}(\Phi_j)^2 + \max_{1 \leq j \leq K} \mathbf{r}(\Psi_j)^2 \right) + \frac{13 \log(4/\delta)}{n}}.$$

5. Conclusion and open problems

We showed that, if the covariance matrix Σ can be represented in the form (2), then it is possible to obtain a non-asymptotic dimension-free upper bound on the Frobenius distance between Σ and the penalized permuted least squares estimate $\tilde{\Sigma}$ under reasonable conditions. The rate of convergence is sharper compared to the standard unstructured case. There is an open question whether similar improvements are possible if we measure the estimation performance in terms of the operator norm. In particular, we are not aware of any (even dimension-dependent) bounds on $\|\tilde{\Sigma} - \Sigma\|$. We also leave open the question if the rate of convergence in Theorem 2.5 is optimal in the minimax sense. Another interesting question is how the result of Theorem 2.5 will change if we consider a misspecified model

$$\Sigma = \Phi_1 \otimes \Psi_1 + \ldots + \Phi_K \otimes \Psi_K + E,$$

where $E \in \mathbb{R}^{d \times d}$ is a (possibly unstructured) remainder. In (Greenewald and Hero, 2015), the authors studied the case when E is a sparse matrix and suggested a robust Kronecker PCA procedure for estimation of Σ in this situation. Finally, one can consider more complex models with higher-order Kronecker products (Pouryazdian et al., 2016; Hafner et al., 2020; McCormack and Hoff, 2023).

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Appendix A. Auxiliary results: Kronecker product and its properties

The goal of this section is to introduce key properties of Kronecker products that we utilize in this paper. For more details see, for instance, (Golub and Van Loan, 2013). We start with a basic fact also referred to as the mixed-product property:

$$(A \otimes B)(C \otimes D) = (AC) \otimes (BD), \tag{23}$$

The equality (23) has plenty of implications. In particular, if $A = U^{\top} \Lambda U$ and $B = V^{\top} M V$ are eigendecompositions of symmetric matrices $A \in \mathbb{R}^{p \times p}$ and $B \in \mathbb{R}^{q \times q}$, then

$$A \otimes B = (U^{\top} \Lambda U) \otimes (V^{\top} M V) = (U \otimes V)^{\top} (\Lambda \otimes M) (U \otimes V)$$

is the eigendecomposition of their Kronecker product. For this reason, we have

$$\operatorname{Tr}(A \otimes B) = \operatorname{Tr}(A)\operatorname{Tr}(B), \quad ||A \otimes B|| = ||A|| ||B||, \text{ and } ||A \otimes B||_{\mathrm{F}} = ||A||_{\mathrm{F}} ||B||_{\mathrm{F}}.$$
 (24)

Further properties of the Kronecker product, presented in this section, are related to the vectorization operator **vec** (see our notation in Section 1). Let us recall that, for any matrix U, **vec**(U) is a vector obtained by stacking the columns of U together. In our proofs, we will extensively use the following identities, which hold whenever the matrix products in the left- and the right-hand side are well defined:

$$(A \otimes B)\mathbf{vec}(U) = \mathbf{vec}(BUA^{\top}), \tag{25}$$

$$\operatorname{Tr}(V^{\top}BUA^{\top}) = \operatorname{vec}(V)^{\top}\operatorname{vec}(BUA^{\top}) = \operatorname{vec}(V)^{\top}(A \otimes B)\operatorname{vec}(U).$$
(26)

Appendix B. Proof of Proposition 2.4

Let us fix any $V \in \mathbb{R}^{d^2 \times d^2}$ and consider the exponential moment

$$\mathbb{E}\exp\left\{\operatorname{\mathbf{vec}}(\mathbb{X})^{\top}V\operatorname{\mathbf{vec}}(\mathbb{X})-\operatorname{Tr}(V\Sigma)\right\}.$$

According to (9), it holds that

$$\mathbb{E} \exp\left\{ \mathbf{vec}(\mathbb{X})^{\top} V \mathbf{vec}(\mathbb{X}) - \operatorname{Tr}(V\Sigma) \right\}$$

$$= \mathbb{E} \exp\left\{ \sum_{j,k=1}^{K} \mathbf{vec}(\mathbb{Y}_{j})^{\top} (A_{j}^{\top} \otimes B_{j}^{\top}) V (A_{k} \otimes B_{k}) \mathbf{vec}(\mathbb{Y}_{k}) - \operatorname{Tr}(V\Sigma) \right\}$$

$$= \mathbb{E} \exp\left\{ \sum_{j=1}^{K} \mathbf{vec}(\mathbb{Y}_{j})^{\top} (A_{j}^{\top} \otimes B_{j}^{\top}) V (A_{j} \otimes B_{j}) \mathbf{vec}(\mathbb{Y}_{j}) - \operatorname{Tr}(V\Sigma) + \sum_{j \neq k} \mathbf{vec}(\mathbb{Y}_{j})^{\top} (A_{j}^{\top} \otimes B_{j}^{\top}) V (A_{k} \otimes B_{k}) \mathbf{vec}(\mathbb{Y}_{k}) \right\}.$$
(27)

Applying the Cauchy-Schwarz inequality, we bound the expression in the right-hand side of (27) by a product of two terms:

$$\mathbb{E} \exp\left\{ \mathbf{vec}(\mathbb{X})^{\top} V \mathbf{vec}(\mathbb{X}) - \operatorname{Tr}(V\Sigma) \right\}$$

$$\leq \left[\mathbb{E} \exp\left\{ 2 \sum_{j=1}^{K} \mathbf{vec}(\mathbb{Y}_{j})^{\top} (A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{j} \otimes B_{j}) \mathbf{vec}(\mathbb{Y}_{j}) - 2 \operatorname{Tr}(V\Sigma) \right\} \right]^{1/2} \quad (28)$$

$$\cdot \left[\mathbb{E} \exp\left\{ 2 \sum_{j \neq k} \mathbf{vec}(\mathbb{Y}_{j})^{\top} (A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{k} \otimes B_{k}) \mathbf{vec}(\mathbb{Y}_{k}) \right\} \right]^{1/2} .$$

In the rest of the proof, we provide upper bounds on the exponential moments in the right-hand side of (28). For convenience, we split the proof into several steps.

Step 1: an upper bound on the first term in (28). An upper bound on the first term in the right-hand side of (28) simply follows from the conditions of the proposition. Since $\mathbb{Y}_1, \ldots, \mathbb{Y}_K$ are independent, we have

$$\mathbb{E} \exp\left\{2\sum_{j=1}^{K} \mathbf{vec}(\mathbb{Y}_{j})^{\top} (A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{j} \otimes B_{j}) \mathbf{vec}(\mathbb{Y}_{j}) - 2\mathrm{Tr}(V\Sigma)\right\}$$
$$= \prod_{j=1}^{K} \mathbb{E} \exp\left\{2\mathbf{vec}(\mathbb{Y}_{j})^{\top} (A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{j} \otimes B_{j}) \mathbf{vec}(\mathbb{Y}_{j}) - 2\mathrm{Tr}\left((A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{j} \otimes B_{j})\right)\right\}.$$

Then (10) yields that

$$\mathbb{E} \exp\left\{2\sum_{j=1}^{K} \mathbf{vec}(\mathbb{Y}_{j})^{\top} (A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{j} \otimes B_{j}) \mathbf{vec}(\mathbb{Y}_{j}) - 2\mathrm{Tr}(V\Sigma)\right\}$$

$$\leq \prod_{j=1}^{K} \mathbb{E} \exp\left\{4\omega_{j}^{2} \left\| (A_{j}A_{j}^{\top} \otimes B_{j}B_{j}^{\top})^{1/2} V(A_{j}A_{j}^{\top} \otimes B_{j}B_{j}^{\top})^{1/2} \right\|_{\mathrm{F}}^{2}\right\}$$

$$\leq \exp\left\{4\omega_{\max}^{2} \sum_{j=1}^{K} \left\| (A_{j}A_{j}^{\top} \otimes B_{j}B_{j}^{\top})^{1/2} V(A_{j}A_{j}^{\top} \otimes B_{j}B_{j}^{\top})^{1/2} \right\|_{\mathrm{F}}^{2}\right\}$$

$$(29)$$

for any V, such that

$$\left\| (A_j A_j^\top \otimes B_j B_j^\top)^{1/2} V (A_j A_j^\top \otimes B_j B_j^\top)^{1/2} \right\|_{\mathbf{F}} \leqslant \frac{1}{2\omega_{\max}}, \quad \text{where } \omega_{\max} = \max_{1 \leqslant j \leqslant r} \omega_j.$$

Step 2: decoupling. We move to the analysis of the second term in the right-hand side of (28). The proof of an upper bound on

$$\mathbb{E} \exp\left\{2\sum_{j\neq k} \mathbf{vec}(\mathbb{Y}_j)^\top (A_j^\top \otimes B_j^\top) V(A_k \otimes B_k) \mathbf{vec}(\mathbb{Y}_k)\right\}$$

extends the idea of decoupling (see (Vershynin, 2018, Theorem 6.1.1)) to the multivariate case. We proceed with the next auxiliary result.

Lemma B.1 Let ζ_1, \ldots, ζ_K be i.i.d. centered random vectors in \mathbb{R}^d and let $\{M_{jk} : 1 \leq j \leq K, 1 \leq k \leq K\}$ be a collection of deterministic matrices of size $(d \times d)$. Then, for any convex function $G : \mathbb{R} \to \mathbb{R}$ with the finite expectation

$$\mathbb{E}G\left(\sum_{j\neq k}\boldsymbol{\zeta}_{j}^{\top}M_{jk}\boldsymbol{\zeta}_{k}\right),$$

we have

$$\mathbb{E}G\left(\sum_{j\neq k}\boldsymbol{\zeta}_{j}^{\top}M_{jk}\boldsymbol{\zeta}_{k}\right) \leqslant \mathbb{E}G\left(4\sum_{j\neq k}\boldsymbol{\zeta}_{j}^{\top}M_{jk}\boldsymbol{\zeta}_{k}'\right),$$

where $\zeta'_1, \ldots, \zeta'_K$ are independent copies of ζ_1, \ldots, ζ_K .

The proof of Lemma B.1 is postponed to Appendix F. Applying this lemma to

$$\mathbb{E} \exp \left\{ 2 \sum_{j \neq k} \mathbf{vec}(\mathbb{Y}_j)^\top (A_j^\top \otimes B_j^\top) V(A_k \otimes B_k) \mathbf{vec}(\mathbb{Y}_k) \right\},\$$

we obtain that

$$\mathbb{E} \exp\left\{2\sum_{j\neq k} \mathbf{vec}(\mathbb{Y}_{j})^{\top} (A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{k} \otimes B_{k}) \mathbf{vec}(\mathbb{Y}_{k})\right\}$$
$$\leq \mathbb{E} \exp\left\{8\sum_{j\neq k} \mathbf{vec}(\mathbb{Y}_{j})^{\top} (A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{k} \otimes B_{k}) \mathbf{vec}(\mathbb{Y}_{k}')\right\},$$
(30)

where $\mathbb{Y}'_1, \ldots, \mathbb{Y}'_K$ are independent copies of $\mathbb{Y}_1, \ldots, \mathbb{Y}_K$.

Step 3: reduction to the Gaussian case. Let $\gamma_1, \ldots, \gamma_K \sim \mathcal{N}(\mathbf{0}, I_{d^2})$ be i.i.d Gaussian random vectors, which are independent of $\mathbb{Y}_1, \ldots, \mathbb{Y}_K$. We are going to show that the right-hand side of (30) does not exceed

$$\mathbb{E}\prod_{j=1}^{K} \exp\left\{\frac{128(1+\omega_{\max})}{\log 2} \left\|\sum_{k\neq j} (A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{k} \otimes B_{k}) \boldsymbol{\gamma}_{k}\right\|^{2}\right\}.$$

In other words, it is enough to consider the Gaussian case. To do so, we first make a small detour and consider the ψ_2 -norm of random variables of a form $\mathbf{u}^\top \mathbf{vec}(\mathbb{Y}_j)$, where $\mathbf{u} \in \mathbb{R}^{d^2}$ and $j \in \{1, \ldots, K\}$.

Lemma B.2 Assume that \mathbb{Y}_j satisfies (10), $j \in \{1, \ldots, K\}$. Then, for any $\mathbf{u} \in \mathbb{R}^{d^2}$, it holds that

$$\left\|\mathbf{u}^{\top}\mathbf{vec}(\mathbb{Y}_j)\right\|_{\psi_2}^2 \leqslant \frac{(1+\omega_j)\|\mathbf{u}\|^2}{\log 2}$$

The proof of Lemma B.2 is deferred to Appendix G. If a centered random variable has a finite ψ_2 -norm, we can bound its exponential moments, using the following lemma.

Lemma B.3 Let η be a centered random variable with a finite Orlicz norm $\|\eta\|_{\psi_2} \leq \sigma < +\infty$. Then, for any $\lambda \in \mathbb{R}$, it holds that

$$\mathbb{E}e^{\lambda\eta} \leqslant e^{\lambda^2\sigma^2}.$$

It is well-known that random variables with a finite ψ_2 -norm exhibit a sub-Gaussian behaviour (see, for instance, (Vershynin, 2018, Section 2.6)). However, the existing bounds in the literature include implicit absolute constants, while we are interested in tracking explicit ones. For this purpose, we carry out the proof of Lemma B.3 in Appendix H. Using this lemma and considering the expectation

$$\mathbb{E}\left[\exp\left\{8\sum_{j\neq k}\mathbf{vec}(\mathbb{Y}_j)^{\top}(A_j^{\top}\otimes B_j^{\top})V(A_k\otimes B_k)\mathbf{vec}(\mathbb{Y}_k')\right\} \middle| \mathbb{Y}_1,\ldots,\mathbb{Y}_K\right]$$

conditionally on $\mathbb{Y}_1, \ldots, \mathbb{Y}_K$, we obtain that

$$\mathbb{E} \exp\left\{8\sum_{j\neq k} \mathbf{vec}(\mathbb{Y}_{j})^{\top} (A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{k} \otimes B_{k}) \mathbf{vec}(\mathbb{Y}_{k}')\right\}$$

$$\leq \prod_{k=1}^{K} \mathbb{E} \exp\left\{\frac{64(1+\omega_{\max})}{\log 2} \left\|\sum_{j\neq k} (A_{k}^{\top} \otimes B_{k}^{\top}) V^{\top} (A_{j} \otimes B_{j}) \mathbf{vec}(\mathbb{Y}_{j})\right\|^{2}\right\}.$$
(31)

Now $\gamma_1, \ldots, \gamma_K$ come into the play. Using the fact that, for any $k \in \{1, \ldots, K\}$ and any $\mathbf{u} \in \mathbb{R}^{d^2}$, it holds that $\mathbb{E}e^{\mathbf{u}^\top \gamma_k} = e^{\|\mathbf{u}\|^2/2}$, we represent the right-hand side of (31) in the following form:

$$\begin{split} & \mathbb{E}_{\mathbb{Y}} \prod_{k=1}^{K} \exp\left\{ \frac{64(1+\omega_{\max})}{\log 2} \left\| \sum_{j \neq k} (A_{k}^{\top} \otimes B_{k}^{\top}) V^{\top} (A_{j} \otimes B_{j}) \mathbf{vec}(\mathbb{Y}_{j}) \right\|^{2} \right\} \\ &= \mathbb{E}_{\mathbb{Y}} \prod_{k=1}^{K} \mathbb{E}_{\boldsymbol{\gamma}_{k}} \exp\left\{ 8\sqrt{\frac{2+2\omega_{\max}}{\log 2}} \cdot \boldsymbol{\gamma}_{k}^{\top} \sum_{j \neq k} (A_{k}^{\top} \otimes B_{k}^{\top}) V^{\top} (A_{j} \otimes B_{j}) \mathbf{vec}(\mathbb{Y}_{j}) \right\} \\ &= \mathbb{E} \exp\left\{ 8\sqrt{\frac{2+2\omega_{\max}}{\log 2}} \cdot \sum_{j \neq k} \boldsymbol{\gamma}_{k}^{\top} (A_{k}^{\top} \otimes B_{k}^{\top}) V^{\top} (A_{j} \otimes B_{j}) \mathbf{vec}(\mathbb{Y}_{j}) \right\}. \end{split}$$

Applying Lemma B.2 and Lemma B.3 again, we obtain that

$$\mathbb{E} \exp\left\{8\sum_{j\neq k} \mathbf{vec}(\mathbb{Y}_{j})^{\top} (A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{k} \otimes B_{k}) \mathbf{vec}(\mathbb{Y}_{k}')\right\}$$

$$\leq \mathbb{E}_{\boldsymbol{\gamma}} \prod_{j=1}^{K} \mathbb{E}_{\mathbb{Y}_{j}} \exp\left\{8\sqrt{\frac{2+2\omega_{\max}}{\log 2}} \cdot \sum_{k\neq j} \boldsymbol{\gamma}_{k}^{\top} (A_{k}^{\top} \otimes B_{k}^{\top}) V^{\top} (A_{j} \otimes B_{j}) \mathbf{vec}(\mathbb{Y}_{j})\right\}$$

$$\leq \mathbb{E} \prod_{j=1}^{K} \exp\left\{\frac{128(1+\omega_{\max})}{\log 2} \left\|\sum_{k\neq j} (A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{k} \otimes B_{k}) \boldsymbol{\gamma}_{k}\right\|^{2}\right\}.$$
(32)

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Step 4: exponential moments of a Gaussian quadratic form. Let $\gamma = (\gamma_1^{\top}, \dots, \gamma_K^{\top})^{\top} \in \mathbb{R}^{d^2 K}$ denote a standard Gaussian random vector, obtained by stacking $\gamma_1, \dots, \gamma_K$ together and let $S = S^{\top} \in \mathbb{R}^{d^2 K \times d^2 K}$ be such that

$$\frac{128(1+\omega_{\max})}{\log 2} \sum_{j=1}^{K} \left\| \sum_{k\neq j} (A_j^{\top} \otimes B_j^{\top}) V(A_k \otimes B_k) \boldsymbol{\gamma}_k \right\|^2 = \boldsymbol{\gamma}^{\top} S \boldsymbol{\gamma}.$$
(33)

Obviously, $S \ge O$, because the corresponding quadratic form is always non-negative. Lemma B.2 from (Spokoiny, 2023) yields

$$\log \mathbb{E}e^{\boldsymbol{\gamma}^{\top}S\boldsymbol{\gamma}} \leq \operatorname{Tr}(S) + \frac{\operatorname{Tr}(S^2)}{1 - 2\|S\|} \leq \left(1 + \frac{\|S\|}{1 - 2\|S\|}\right) \operatorname{Tr}(S) \leq 2\operatorname{Tr}(S),$$

provided that $||S|| \leq \operatorname{Tr}(S) \leq 1/4$. Note that

$$\begin{aligned} \operatorname{Tr}(S) &= \mathbb{E} \boldsymbol{\gamma}^{\top} S \boldsymbol{\gamma} \\ &= \frac{128(1 + \omega_{\max})}{\log 2} \mathbb{E} \sum_{j=1}^{K} \left\| \sum_{k \neq j} (A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{k} \otimes B_{k}) \boldsymbol{\gamma}_{k} \right\|^{2} \\ &= \frac{128(1 + \omega_{\max})}{\log 2} \sum_{j=1}^{K} \left\| \sum_{k \neq j} (A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{k} \otimes B_{k}) \right\|_{\mathrm{F}}^{2} \end{aligned}$$
(34)
$$&= \frac{128(1 + \omega_{\max})}{\log 2} \left(\left\| \Sigma^{1/2} V \Sigma^{1/2} \right\|_{\mathrm{F}}^{2} - \sum_{j=1}^{K} \left\| (A_{j} A_{j}^{\top} \otimes B_{j} B_{j}^{\top})^{1/2} V(A_{j} A_{j}^{\top} \otimes B_{j} B_{j}^{\top})^{1/2} \right\|_{\mathrm{F}}^{2} \right). \end{aligned}$$

Thus, it holds that

$$\mathbb{E} \prod_{j=1}^{K} \exp\left\{ \frac{128(1+\omega_{\max})}{\log 2} \left\| \sum_{k\neq j} (A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{k} \otimes B_{k}) \boldsymbol{\gamma}_{k} \right\|^{2} \right\}$$

$$\leq \frac{256(1+\omega_{\max})}{\log 2} \left(\left\| \Sigma^{1/2} V \Sigma^{1/2} \right\|_{\mathrm{F}}^{2} - \sum_{j=1}^{K} \left\| (A_{j} A_{j}^{\top} \otimes B_{j} B_{j}^{\top})^{1/2} V(A_{j} A_{j}^{\top} \otimes B_{j} B_{j}^{\top})^{1/2} \right\|_{\mathrm{F}}^{2} \right)$$

$$(35)$$

for all $V \in \mathbb{R}^{d^2 \times d^2}$, such that

$$\frac{128(1+\omega_{\max})}{\log 2} \left\| \Sigma^{1/2} V \Sigma^{1/2} \right\|_{\rm F}^2 \le \frac{1}{4}.$$

Hence, due to the inequalities (30), (32), and (35), we have

$$\mathbb{E} \exp\left\{2\sum_{j\neq k} \mathbf{vec}(\mathbb{Y}_{j})^{\top} (A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{k} \otimes B_{k}) \mathbf{vec}(\mathbb{Y}_{k})\right\}$$

$$\leq \exp\left\{256(1+\omega_{\max}) \left(\left\|\Sigma^{1/2} V \Sigma^{1/2}\right\|_{\mathrm{F}}^{2} - \sum_{j=1}^{K} \left\|(A_{j} A_{j}^{\top} \otimes B_{j} B_{j}^{\top})^{1/2} V(A_{j} A_{j}^{\top} \otimes B_{j} B_{j}^{\top})^{1/2}\right\|_{\mathrm{F}}^{2}\right)\right\},$$

$$(36)$$

provided that

$$\frac{128(1+\omega_{\max})}{\log 2} \left\| \Sigma^{1/2} V \Sigma^{1/2} \right\|_{\mathrm{F}}^2 \leqslant \frac{1}{4}.$$

Step 5: final bound. Taking into account (29) and (36), we obtain that

$$\begin{split} &\mathbb{E} \exp\left\{ \mathbf{vec}(\mathbb{X})^{\top} V\mathbf{vec}(\mathbb{X}) - \mathrm{Tr}(V\Sigma) \right\} \\ &\leqslant \left[\mathbb{E} \exp\left\{ 2\sum_{j=1}^{K} \mathbf{vec}(\mathbb{Y}_{j})^{\top} (A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{j} \otimes B_{j}) \mathbf{vec}(\mathbb{Y}_{j}) - 2\mathrm{Tr}(V\Sigma) \right\} \right]^{1/2} \\ &\cdot \left[\mathbb{E} \exp\left\{ 2\sum_{j \neq k} \mathbf{vec}(\mathbb{Y}_{j})^{\top} (A_{j}^{\top} \otimes B_{j}^{\top}) V(A_{k} \otimes B_{k}) \mathbf{vec}(\mathbb{Y}_{k}) \right\} \right]^{1/2} \\ &\leqslant \exp\left\{ 2\omega_{\max}^{2} \sum_{j=1}^{K} \left\| (A_{j}A_{j}^{\top} \otimes B_{j}B_{j}^{\top})^{1/2} V(A_{j}A_{j}^{\top} \otimes B_{j}B_{j}^{\top})^{1/2} \right\|_{\mathrm{F}}^{2} \right\} \\ &\cdot \exp\left\{ \frac{128(1 + \omega_{\max})}{\log 2} \left(\left\| \Sigma^{1/2} V\Sigma^{1/2} \right\|_{\mathrm{F}}^{2} - \sum_{j=1}^{K} \left\| (A_{j}A_{j}^{\top} \otimes B_{j}B_{j}^{\top})^{1/2} V(A_{j}A_{j}^{\top} \otimes B_{j}B_{j}^{\top})^{1/2} \right\|_{\mathrm{F}}^{2} \right\} \\ &\leqslant \exp\left\{ \left(\frac{128(1 + \omega_{\max})}{\log 2} \vee 2\omega_{\max}^{2} \right) \left\| \Sigma^{1/2} V\Sigma^{1/2} \right\|_{\mathrm{F}}^{2} \right\}, \end{split}$$

provided that

$$\left\| (A_j A_j^\top \otimes B_j B_j^\top)^{1/2} V (A_j A_j^\top \otimes B_j B_j^\top)^{1/2} \right\|_{\mathcal{F}} \leqslant \frac{1}{2\omega_{\max}}$$
(37)

and

$$\frac{128(1+\omega_{\max})}{\log 2} \left\| \Sigma^{1/2} V \Sigma^{1/2} \right\|_{\mathcal{F}}^2 \leqslant \frac{1}{4}.$$

Note that, according to (34),

$$\left\|\Sigma^{1/2} V \Sigma^{1/2}\right\|_{\mathrm{F}}^{2} - \sum_{j=1}^{K} \left\| (A_{j} A_{j}^{\top} \otimes B_{j} B_{j}^{\top})^{1/2} V (A_{j} A_{j}^{\top} \otimes B_{j} B_{j}^{\top})^{1/2} \right\|_{\mathrm{F}}^{2} = \frac{\mathrm{Tr}(S) \log 2}{128(1 + \omega_{\max})} \ge 0,$$

where S is a positive semidefinite matrix, defined in (33). Thus, the condition

$$\left\| \Sigma^{1/2} V \Sigma^{1/2} \right\|_{\mathrm{F}} \leqslant \frac{1}{2 \omega_{\mathrm{max}}}$$

automatically yields (37). Hence, we proved that

$$\mathbb{E}\exp\left\{\mathbf{vec}(\mathbb{X})^{\top}V\mathbf{vec}(\mathbb{X}) - \mathrm{Tr}(V\Sigma)\right\} \leqslant \exp\left\{\left(\frac{128(1+\omega_{\max})}{\log 2} \vee 2\omega_{\max}^{2}\right) \left\|\Sigma^{1/2}V\Sigma^{1/2}\right\|_{\mathrm{F}}^{2}\right\}$$

for all $V \in \mathbb{R}^{d^2 \times d^2}$, such that

$$\left(4\omega_{\max}^2 \vee \frac{512(1+\omega_{\max})}{\log 2}\right) \left\|\Sigma^{1/2}V\Sigma^{1/2}\right\|_{\mathrm{F}}^2 \leqslant 1.$$

Appendix C. Proof of Lemma 4.1

We start with representing the operator norm of $\mathcal{R}(\hat{\Sigma} - \Sigma)$ in the following form:

$$\left\| \mathcal{R}(\widehat{\Sigma} - \Sigma) \right\| = \sup_{\substack{U \in \mathbb{R}^{p \times p}, V \in \mathbb{R}^{q \times q} \\ \|U\|_{F} = \|V\|_{F} = 1}} \operatorname{vec}(U)^{\top} \mathcal{R}(\widehat{\Sigma} - \Sigma) \operatorname{vec}(V).$$

Due to the linearity of the rearrangement operator \mathcal{R} , we have

$$\begin{aligned} \left\| \mathcal{R}(\hat{\Sigma} - \Sigma) \right\| &= \sup_{\substack{U \in \mathbb{R}^{p \times p}, V \in \mathbb{R}^{q \times q} \\ \|U\|_{\mathrm{F}} = \|V\|_{\mathrm{F}} = 1}} \operatorname{\mathbf{vec}}(U)^{\top} \mathcal{R}\left(\frac{1}{n} \sum_{i=1}^{n} \mathbf{X}_{i} \mathbf{X}_{i}^{\top} - \mathbb{E} \mathbf{X} \mathbf{X}^{\top}\right) \operatorname{\mathbf{vec}}(V) \end{aligned}$$
(38)
$$&= \sup_{\substack{U \in \mathbb{R}^{p \times p}, V \in \mathbb{R}^{q \times q} \\ \|U\|_{\mathrm{F}} = \|V\|_{\mathrm{F}} = 1}} \left\{\frac{1}{n} \sum_{i=1}^{n} \operatorname{\mathbf{vec}}(U)^{\top} \left[\mathcal{R}\left(\mathbf{X}_{i} \mathbf{X}_{i}^{\top}\right) - \mathbb{E}\mathcal{R}\left(\mathbf{X} \mathbf{X}^{\top}\right)\right] \operatorname{\mathbf{vec}}(V)\right\}. \end{aligned}$$

Let us show that, for any $U \in \mathbb{R}^{p \times p}$ and $V \in \mathbb{R}^{q \times q}$,

$$\operatorname{\mathbf{vec}}(U)^{\top} \mathcal{R}\left(\mathbf{X}\mathbf{X}^{\top}\right) \operatorname{\mathbf{vec}}(V) = \operatorname{Tr}\left(\mathbb{X}^{\top} V^{\top} \mathbb{X} U\right),$$

where \mathbb{X} is a matrix of size $(q \times p)$, such that $\mathbf{vec}(\mathbb{X}) = \mathbf{X}$. It holds that

$$\mathbf{vec}(U)^{\top} \mathcal{R}(\mathbf{X}\mathbf{X}^{\top}) \mathbf{vec}(V)$$

= $\sum_{i=1}^{p} \sum_{j=1}^{p} \sum_{k=1}^{q} \sum_{\ell=1}^{q} \mathbf{vec}(U)_{p(i-1)+j} \mathcal{R}(\mathbf{X}\mathbf{X}^{\top})_{p(i-1)+j,q(k-1)+\ell} \mathbf{vec}(V)_{q(k-1)+\ell}.$

The definition of the vectorization operator vec yields that

$$\mathbf{vec}(U)_{p(i-1)+j} = U_{ji}$$
 and $\mathbf{vec}(V)_{q(k-1)+\ell} = V_{\ell k}$.

At the same time, according to the definition of the rearrangement operator \mathcal{R} , we have

$$\mathcal{R}(\mathbf{X}\mathbf{X}^{\top})_{p(i-1)+j,q(k-1)+\ell} = \mathbf{vec} \left((\mathbf{X}\mathbf{X}^{\top})_{p(j-1):pj,p(i-1):pi} \right)_{q(k-1)+\ell}$$
$$= \left((\mathbf{X}\mathbf{X})_{(p-1)j:pj,(p-1)i:pi}^{\top} \right)_{\ell k}$$
$$= (\mathbf{X}\mathbf{X})_{(p-1)j+\ell,(p-1)i+k}^{\top}$$
$$= \mathbf{X}_{(p-1)j+\ell}\mathbf{X}_{(p-1)i+k} = \mathbb{X}_{\ell j}\mathbb{X}_{ki}.$$

Here $(\mathbf{X}\mathbf{X}^{\top})_{p(j-1):pj,p(i-1):pi}$ denotes a submatrix of $\mathbf{X}\mathbf{X}^{\top}$ on the intersection of the rows $p(j-1) + 1, \ldots, pj$ with the columns $p(i-1) + 1, \ldots, pi$. Hence, we obtain that

$$\mathbf{vec}(U)^{\top} \mathcal{R}(\mathbf{X}\mathbf{X}^{\top}) \mathbf{vec}(V) = \sum_{i=1}^{p} \sum_{j=1}^{p} \sum_{k=1}^{q} \sum_{\ell=1}^{q} U_{ji} \mathbb{X}_{\ell j} \mathbb{X}_{ki} V_{\ell k} = \mathrm{Tr}(V^{\top} \mathbb{X}U\mathbb{X}^{\top}).$$
(39)

Similarly, one can prove that

$$\mathbf{vec}(U)^{\top} \mathcal{R}\left(\mathbf{X}_{i} \mathbf{X}_{i}^{\top}\right) \mathbf{vec}(V) = \mathrm{Tr}\left(\mathbb{X}_{i}^{\top} V^{\top} \mathbb{X}_{i} U\right),$$
(40)

for any $U \in \mathbb{R}^{p \times p}$, $V \in \mathbb{R}^{q \times q}$, and any $i \in \{1, ..., n\}$, where $\mathbb{X}_1, ..., \mathbb{X}_n$ are the matrices of size $(q \times p)$, obtained by reshaping $\mathbf{X}_1, ..., \mathbf{X}_n$, respectively:

$$\mathbf{vec}(\mathbb{X}_i) = \mathbf{X}_i \quad \text{for all } i \in \{1, \dots, n\}.$$

Taking into account (38), (39), and (40), we deduce that

$$\begin{aligned} \left\| \mathcal{R}(\hat{\Sigma} - \Sigma) \right\| &= \sup_{\substack{U \in \mathbb{R}^{p \times p}, V \in \mathbb{R}^{q \times q} \\ \|U\|_{\mathrm{F}} = \|V\|_{\mathrm{F}} = 1}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \operatorname{\mathbf{vec}}(U)^{\top} \left[\mathcal{R} \left(\mathbf{X}_{i} \mathbf{X}_{i}^{\top} \right) - \mathbb{E} \mathcal{R} \left(\mathbf{X} \mathbf{X}^{\top} \right) \right] \operatorname{\mathbf{vec}}(V) \right\} \\ &= \sup_{\substack{U \in \mathbb{R}^{p \times p}, V \in \mathbb{R}^{q \times q} \\ \|U\|_{\mathrm{F}} = \|V\|_{\mathrm{F}} = 1}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \operatorname{Tr} \left(\mathbb{X}_{i}^{\top} V^{\top} \mathbb{X}_{i} U \right) - \mathbb{E} \operatorname{Tr} \left(\mathbb{X}^{\top} V^{\top} \mathbb{X} U \right) \right\}. \end{aligned}$$

Appendix D. Proof of Lemma 4.3

Let $X \in \mathbb{R}^{p \times p}$ and $Y \in \mathbb{R}^{q \times q}$ be random matrices with the joint distribution μ , defined in (15). That is, the entries of X and Y are independent centered Gaussian random variables, such that

$$\operatorname{Var}(\mathbb{X}_{ij}) = \frac{1}{\alpha}, \quad \operatorname{Var}(\mathbb{Y}_{k\ell}) = \frac{1}{\beta} \quad \text{for all } i, j \in \{1, \dots, p\} \text{ and } k, \ell \in \{1, \dots, q\}.$$

We are going to show that

$$\mathbb{P}\left(\left\|\Sigma^{1/2}(\mathbb{X}\otimes\mathbb{Y})\Sigma^{1/2}\right\|_{\mathrm{F}}^{2} \ge \frac{4\mathrm{Tr}(\Sigma)^{2}}{\alpha\beta}\right) \leqslant \frac{1}{4},\tag{41}$$

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$$\mathbb{P}\left(\left\|\left(\sum_{j=1}^{K}\|\Psi_{j}\|\Phi_{j}\right)^{1/2}\mathbb{X}\left(\sum_{j=1}^{K}\|\Psi_{j}\|\Phi_{j}\right)^{1/2}\right\|_{\mathrm{F}}^{2} \ge \frac{4}{\alpha}\left(\sum_{j=1}^{K}\|\Psi_{j}\|\mathrm{Tr}(\Phi_{j})\right)^{2}\right) \le \frac{1}{4},\qquad(42)$$

and

$$\mathbb{P}\left(\left\|\left(\sum_{j=1}^{K}\|\Phi_{j}\|\Psi_{j}\right)^{1/2}\mathbb{Y}\left(\sum_{j=1}^{K}\|\Phi_{j}\|\Psi_{j}\right)^{1/2}\right\|_{\mathrm{F}}^{2} \leqslant \frac{4}{\beta}\left(\sum_{j=1}^{K}\|\Phi_{j}\|\operatorname{Tr}(\Psi_{j})\right)^{2}\right) \leqslant \frac{1}{4}.$$
 (43)

Then the union bound implies that

$$\mathbf{Z} = \mathbb{P}\left((\mathbb{X}, \mathbb{Y}) \in \Upsilon(O, O)\right) = 1 - \mathbb{P}\left((\mathbb{X}, \mathbb{Y}) \notin \Upsilon(O, O)\right) \ge 1 - \frac{3}{4} = \frac{1}{4}$$

For convenience, the rest of the proof is divided into three parts.

Step 1: proof of (41). Since the covariance matrix Σ has a Kronecker product structure

$$\Sigma = \sum_{j=1}^{K} \Phi_j \otimes \Psi_j,$$

it holds that

$$\begin{split} \left\| \Sigma^{1/2} (\mathbb{X} \otimes \mathbb{Y}) \Sigma^{1/2} \right\|_{\mathrm{F}}^{2} &= \mathrm{Tr} \left(\Sigma (\mathbb{X} \otimes \mathbb{Y})^{\top} \Sigma (\mathbb{X} \otimes \mathbb{Y}) \right) \\ &= \sum_{j=1}^{K} \sum_{k=1}^{K} \mathrm{Tr} \left((\Phi_{j} \otimes \Psi_{j}) (\mathbb{X}^{\top} \otimes \mathbb{Y}^{\top}) (\Phi_{k} \otimes \Psi_{k}) (\mathbb{X} \otimes \mathbb{Y}) \right) \\ &= \sum_{j=1}^{K} \sum_{k=1}^{K} \mathrm{Tr} \left((\Phi_{j} \mathbb{X}^{\top} \Phi_{k} \mathbb{X}) \otimes (\Psi_{j} \mathbb{Y}^{\top} \Psi_{k} \mathbb{Y}) \right). \end{split}$$

Using the property (24) about the trace of Kronecker product, we obtain that

$$\begin{split} \left\| \Sigma^{1/2} (\mathbb{X} \otimes \mathbb{Y}) \Sigma^{1/2} \right\|_{\mathrm{F}}^{2} &= \sum_{j=1}^{K} \sum_{k=1}^{K} \operatorname{Tr} \left((\Phi_{j} \mathbb{X}^{\top} \Phi_{k} \mathbb{X}) \otimes (\Psi_{j} \mathbb{Y}^{\top} \Psi_{k} \mathbb{Y}) \right) \\ &= \sum_{j=1}^{K} \sum_{k=1}^{K} \operatorname{Tr} (\Phi_{j} \mathbb{X}^{\top} \Phi_{k} \mathbb{X}) \operatorname{Tr} (\Psi_{j} \mathbb{Y}^{\top} \Psi_{k} \mathbb{Y}). \end{split}$$

For any j and k from $\{1, \ldots, K\}$, we have

$$\mathbb{E}\mathrm{Tr}(\Phi_j \mathbb{X}^\top \Phi_k \mathbb{X}) = \mathbb{E}\mathbf{vec}(\mathbb{X})^\top (\Phi_j \otimes \Phi_k) \mathbf{vec}(\mathbb{X}) = \frac{1}{\alpha} \mathrm{Tr}(\Phi_j \otimes \Phi_k) = \frac{1}{\alpha} \mathrm{Tr}(\Phi_j) \mathrm{Tr}(\Phi_k)$$

and, similarly,

$$\mathbb{E}\mathrm{Tr}(\Psi_{j}\mathbb{Y}^{\top}\Psi_{k}\mathbb{Y}) = \mathbb{E}\mathbf{vec}(\mathbb{Y})^{\top}(\Psi_{j}\otimes\Psi_{k})\mathbf{vec}(\mathbb{Y}) = \frac{1}{\beta}\mathrm{Tr}(\Psi_{j}\otimes\Psi_{k}) = \frac{1}{\beta}\mathrm{Tr}(\Psi_{j})\mathrm{Tr}(\Psi_{k}).$$

This yields that

$$\mathbb{E} \left\| \Sigma^{1/2} (\mathbb{X} \otimes \mathbb{Y}) \Sigma^{1/2} \right\|_{\mathrm{F}}^{2} = \frac{1}{\alpha \beta} \sum_{j=1}^{K} \sum_{k=1}^{K} \mathrm{Tr}(\Phi_{j}) \mathrm{Tr}(\Phi_{k}) \mathrm{Tr}(\Psi_{j}) \mathrm{Tr}(\Psi_{k})$$
$$= \frac{1}{\alpha \beta} \left(\sum_{j=1}^{K} \mathrm{Tr}(\Phi_{j}) \mathrm{Tr}(\Psi_{j}) \right)^{2} = \frac{\mathrm{Tr}(\Sigma)^{2}}{\alpha \beta},$$

and, applying Markov's inequality, we obtain (41).

Step 2: proof of (42) **and** (43). Similarly to the first step, the proof of (42) and (43) relies on Markov's inequality and computation of the expectations

$$\mathbb{E} \left\| \left(\sum_{j=1}^{K} \|\Psi_j\| \Phi_j \right)^{1/2} \mathbb{X} \left(\sum_{j=1}^{K} \|\Psi_j\| \Phi_j \right)^{1/2} \right\|_{\mathrm{F}}^2$$
$$\mathbb{E} \left\| \left(\sum_{j=1}^{K} \|\Phi_j\| \Psi_j \right)^{1/2} \mathbb{Y} \left(\sum_{j=1}^{K} \|\Phi_j\| \Psi_j \right)^{1/2} \right\|_{\mathrm{F}}^2.$$

First, let us show that

and

$$\mathbb{E} \left\| \left(\sum_{j=1}^{K} \| \Psi_j \| \Phi_j \right)^{1/2} \mathbb{X} \left(\sum_{j=1}^{K} \| \Psi_j \| \Phi_j \right)^{1/2} \right\|_{\mathrm{F}}^2 = \frac{1}{\alpha} \left(\sum_{j=1}^{K} \| \Psi_j \| \operatorname{Tr}(\Phi_j) \right)^2.$$

Indeed, it holds that

$$\mathbb{E} \left\| \left(\sum_{j=1}^{K} \|\Psi_{j}\| \Phi_{j} \right)^{1/2} \mathbb{X} \left(\sum_{j=1}^{K} \|\Psi_{j}\| \Phi_{j} \right)^{1/2} \right\|_{\mathrm{F}}^{2}$$
$$= \mathbb{E} \mathrm{Tr} \left[\left(\sum_{j=1}^{K} \|\Psi_{j}\| \Phi_{j} \right) \mathbb{X}^{\top} \left(\sum_{k=1}^{K} \|\Psi_{k}\| \Phi_{k} \right) \mathbb{X} \right]$$
$$= \sum_{j=1}^{K} \sum_{k=1}^{K} \|\Psi_{j}\| \|\Psi_{k}\| \mathbb{E} \mathrm{Tr} \left(\Phi_{j} \mathbb{X}^{\top} \Phi_{k} \mathbb{X} \right).$$

Since for any j and k from $\{1, \ldots, K\}$ the expectation of $\operatorname{Tr}(\Phi_j \mathbb{X}^\top \Phi_k \mathbb{X})$ is equal to

$$\mathbb{E}\mathrm{Tr}\left(\Phi_{j}\mathbb{X}^{\top}\Phi_{k}\mathbb{X}\right) = \mathbb{E}\mathbf{vec}(\mathbb{X})^{\top}(\Phi_{j}\otimes\Phi_{k})\mathbf{vec}(\mathbb{X}) = \frac{1}{\alpha}\mathrm{Tr}(\Phi_{j}\otimes\Phi_{k}) = \frac{1}{\alpha}\mathrm{Tr}(\Phi_{j})\mathrm{Tr}(\Phi_{k}),$$

we obtain that

$$\mathbb{E} \left\| \left(\sum_{j=1}^{K} \|\Psi_{j}\|\Phi_{j} \right)^{1/2} \mathbb{X} \left(\sum_{j=1}^{K} \|\Psi_{j}\|\Phi_{j} \right)^{1/2} \right\|_{\mathrm{F}}^{2} = \frac{1}{\alpha} \sum_{j=1}^{K} \sum_{k=1}^{K} \|\Psi_{j}\| \|\Psi_{k}\| \operatorname{Tr}(\Phi_{j}) \operatorname{Tr}(\Phi_{k})$$
$$= \frac{1}{\alpha} \left(\sum_{j=1}^{K} \|\Psi_{j}\| \operatorname{Tr}(\Phi_{j}) \right)^{2},$$

and (42) follows from Markov's inequality. The proof of (43) is absolutely similar.

Appendix E. Proof of Lemma 4.4

Note that

$$\begin{split} \left\| \Sigma^{1/2} (P \otimes Q) \Sigma^{1/2} \right\|_{\mathcal{F}}^{2} &\leq 4 \left\| \Sigma^{1/2} \left((P - U) \otimes (Q - V) \right) \Sigma^{1/2} \right\|_{\mathcal{F}}^{2} \\ &+ 4 \left\| \Sigma^{1/2} \left(U \otimes (Q - V) \right) \Sigma^{1/2} \right\|_{\mathcal{F}}^{2} \\ &+ 4 \left\| \Sigma^{1/2} \left((P - U) \otimes V \right) \Sigma^{1/2} \right\|_{\mathcal{F}}^{2} \\ &+ 4 \left\| \Sigma^{1/2} (U \otimes V) \Sigma^{1/2} \right\|_{\mathcal{F}}^{2}. \end{split}$$

The definition of the support $\Upsilon(U, V)$ (see (17)) implies that

$$\|\Sigma^{1/2} \left((P-U) \otimes (Q-V) \right) \Sigma^{1/2} \|_{\mathbf{F}}^2 \leqslant \frac{4 \operatorname{Tr}(\Sigma)^2}{\alpha \beta} \quad \rho_{U,V} \text{-almost surely.}$$
(44)

Moreover, on $\Upsilon(U, V)$ it holds that

$$\begin{split} & \left\| \Sigma^{1/2} \big((P-U) \otimes V \big) \Sigma^{1/2} \right\|_{\mathrm{F}}^{2} = \mathrm{Tr} \left(\Sigma \big((P-U) \otimes V \big)^{\mathsf{T}} \Sigma \big((P-U) \otimes V \big) \big) \\ &= \sum_{j=1}^{K} \sum_{k=1}^{K} \mathrm{Tr} \left((\Phi_{j} \otimes \Psi_{j}) \big((P-U) \otimes V \big)^{\mathsf{T}} (\Phi_{k} \otimes \Psi_{k}) \big((P-U) \otimes V \big) \big) \\ &= \sum_{j=1}^{K} \sum_{k=1}^{K} \mathrm{Tr} \big(\Phi_{j} (P-U)^{\mathsf{T}} \Phi_{k} (P-U) \big) \mathrm{Tr} \big(\Psi_{j} V^{\mathsf{T}} \Psi_{k} V \big) \big) \\ &= \sum_{j=1}^{K} \sum_{k=1}^{K} \mathrm{Tr} \big(\Phi_{j} (P-U)^{\mathsf{T}} \Phi_{k} (P-U) \big) \left\| \Psi_{j}^{1/2} V \Psi_{k}^{1/2} \right\|_{\mathrm{F}}^{2}. \end{split}$$

Since $||V||_{\mathbf{F}} = 1$, we have

$$\left\|\Psi_{j}^{1/2}V\Psi_{k}^{1/2}\right\|_{\mathcal{F}}^{2} \leq \left\|\Psi_{j}^{1/2}\right\|^{2} \cdot \left\|V\right\|_{\mathcal{F}}^{2} \cdot \left\|\Psi_{k}^{1/2}\right\|^{2} \leq \left\|\Psi_{j}\right\|\left\|\Psi_{k}\right\| \quad \text{for all } j,k \in \{1,\ldots,K\},$$

and thus,

$$\begin{split} \left\| \Sigma^{1/2} \big((P-U) \otimes V \big) \Sigma^{1/2} \right\|_{\mathrm{F}}^{2} &\leq \sum_{j=1}^{K} \sum_{k=1}^{K} \|\Psi_{j}\| \|\Psi_{k}\| \mathrm{Tr} \big(\Phi_{j} (P-U)^{\top} \Phi_{k} (P-U) \big) \\ &= \left\| \left(\sum_{j=1}^{K} \|\Psi_{j}\| \Phi_{j} \right)^{1/2} (P-U) \left(\sum_{k=1}^{K} \|\Psi_{k}\| \Phi_{k} \right)^{1/2} \right\|_{\mathrm{F}}^{2} \qquad (45) \\ &\leq \frac{4}{\alpha} \left(\sum_{j=1}^{K} \|\Psi_{j}\| \mathrm{Tr} (\Phi_{j}) \right)^{2} \quad \rho_{U,V} \text{-almost surely,} \end{split}$$

where the last inequality is due to (17). Similarly, one can show that

$$\left\|\Sigma^{1/2} \left(U \otimes (Q - V)\right) \Sigma^{1/2}\right\|_{\mathcal{F}}^2 \leqslant \frac{4}{\beta} \left(\sum_{j=1}^K \|\Phi_j\| \operatorname{Tr}(\Psi_j)\right)^2 \quad \rho_{U,V}\text{-almost surely.}$$
(46)

Finally,

$$\left\| \Sigma^{1/2} (U \otimes V) \Sigma^{1/2} \right\|_{\mathbf{F}}^{2} \leq \left\| \Sigma^{1/2} \right\|^{2} \cdot \left\| U \otimes V \right\|_{\mathbf{F}}^{2} \cdot \left\| \Sigma^{1/2} \right\|^{2} = \left\| \Sigma \right\|^{2}.$$

This inequality and the bounds (44), (45), (46) yield that

$$\begin{split} \left\| \Sigma^{1/2} (P \otimes Q) \Sigma^{1/2} \right\|_{\mathcal{F}}^2 &\leq \| \Sigma \|^2 + \frac{4}{\alpha} \left(\sum_{j=1}^K \| \Psi_j \| \operatorname{Tr}(\Phi_j) \right)^2 \\ &+ \frac{4}{\beta} \left(\sum_{j=1}^K \| \Phi_j \| \operatorname{Tr}(\Psi_j) \right)^2 + \frac{4 \operatorname{Tr}(\Sigma)^2}{\alpha \beta} \quad \rho_{U,V} \text{-almost surely.} \end{split}$$

It only remains to recall the definition of α and β (see (16)) to conclude the proof:

$$\begin{split} \left\| \Sigma^{1/2} (P \otimes Q) \Sigma^{1/2} \right\|_{\mathrm{F}}^{2} \\ &\leqslant \left\| \sum_{j=1}^{K} \Phi_{j} \otimes \Psi_{j} \right\|^{2} + \frac{4}{\underset{1 \leqslant j \leqslant K}{\max} \mathbf{r}(\Phi_{j})^{2}} \left(\sum_{j=1}^{K} \|\Psi_{j}\| \mathrm{Tr}(\Phi_{j}) \right)^{2} \\ &+ \frac{4}{\underset{1 \leqslant j \leqslant K}{\max} \mathbf{r}(\Psi_{j})^{2}} \left(\sum_{j=1}^{K} \|\Phi_{j}\| \mathrm{Tr}(\Psi_{j}) \right)^{2} + \frac{4}{\underset{1 \leqslant j \leqslant K}{\max} \mathbf{r}(\Phi_{j})^{2} \mathbf{r}(\Psi_{j})^{2}} \left(\sum_{j=1}^{K} \mathrm{Tr}(\Phi_{j}) \mathrm{Tr}(\Psi_{j}) \right)^{2} \\ &\leqslant \sum_{j=1}^{K} \|\Phi_{j} \otimes \Psi_{j}\|^{2} + 12 \left(\sum_{j=1}^{K} \|\Phi_{j}\| \|\Psi_{j}\| \right)^{2} \\ &= 13 \left(\sum_{j=1}^{K} \|\Phi_{j}\| \|\Psi_{j}\| \right)^{2} \quad \rho_{U,V} \text{-almost surely.} \end{split}$$

Appendix F. Proof of Lemma B.1

Let $\varepsilon_1, \ldots, \varepsilon_K \sim \text{Be}(1/2)$ be i.i.d. Bernoulli random variables. Then

$$\sum_{j \neq k} \boldsymbol{\zeta}_j^\top M_{jk} \boldsymbol{\zeta}_k = 4 \mathbb{E}_{\varepsilon} \sum_{j \neq k} \varepsilon_j (1 - \varepsilon_k) \boldsymbol{\zeta}_j^\top M_{jk} \boldsymbol{\zeta}_k \quad \text{almost surely,}$$

where \mathbb{E}_{ε} stands for the expectation with respect to $\varepsilon_1, \ldots, \varepsilon_K$ conditionally on ζ_1, \ldots, ζ_K . Let us define a random set $\mathcal{I} \subseteq \{1, \ldots, K\}$ as follows:

$$\mathcal{I} = \{j \in \{1, \dots, K\} : \varepsilon_j = 1\}.$$

Then we can rewrite the sum

$$\sum_{j\neq k} \varepsilon_j (1-\varepsilon_k) \boldsymbol{\zeta}_j^\top M_{jk} \boldsymbol{\zeta}_k$$

in the form

$$\sum_{j \neq k} \varepsilon_j (1 - \varepsilon_k) \boldsymbol{\zeta}_j^\top M_{jk} \boldsymbol{\zeta}_k = \sum_{j \in \mathcal{I}} \sum_{k \in \mathcal{I}^c} \boldsymbol{\zeta}_j^\top M_{jk} \boldsymbol{\zeta}_k,$$

where $\mathcal{I}^c = \{1, \ldots, K\} \setminus \mathcal{I}$ denotes the complement of \mathcal{I} . With the notation introduced above, we obtain that

$$\mathbb{E}G\left(\sum_{j\neq k}\boldsymbol{\zeta}_{j}^{\top}M_{jk}\boldsymbol{\zeta}_{k}\right) = \mathbb{E}_{\boldsymbol{\zeta}}G\left(4\mathbb{E}_{\varepsilon}\sum_{j\in\mathcal{I}}\sum_{k\in\mathcal{I}^{c}}\boldsymbol{\zeta}_{j}^{\top}M_{jk}\boldsymbol{\zeta}_{k}\right).$$

Here \mathbb{E}_{ζ} stands for the expectation with respect to ζ_1, \ldots, ζ_K . Applying Jensen's inequality and taking into account that, for any realization of $\varepsilon_1, \ldots, \varepsilon_K$, the collection $\{\zeta_j : j \in \mathcal{I}\}$ is independent of $\{\zeta_k : k \in \mathcal{I}\}$, we deduce that

$$\mathbb{E}G\left(\sum_{j\neq k}\boldsymbol{\zeta}_{j}^{\top}M_{jk}\boldsymbol{\zeta}_{k}\right) \leqslant \mathbb{E}_{\varepsilon}\mathbb{E}_{\boldsymbol{\zeta}}G\left(4\sum_{j\in\mathcal{I}}\sum_{k\in\mathcal{I}^{c}}\boldsymbol{\zeta}_{j}^{\top}M_{jk}\boldsymbol{\zeta}_{k}\right) \leqslant \mathbb{E}_{\varepsilon}\mathbb{E}_{\boldsymbol{\zeta},\boldsymbol{\zeta}'}G\left(4\sum_{j\in\mathcal{I}}\sum_{k\in\mathcal{I}^{c}}\boldsymbol{\zeta}_{j}^{\top}M_{jk}\boldsymbol{\zeta}_{k}'\right)$$

Note that, for any realization of $\varepsilon_1, \ldots, \varepsilon_r$, the sum

$$\sum_{j \in \mathcal{I}^c} \sum_{k \in \mathcal{I}} \boldsymbol{\zeta}_j^\top M_{jk} \boldsymbol{\zeta}_k' \quad \text{is independent of} \quad \sum_{j \in \mathcal{I}} \sum_{k \in \mathcal{I}^c} \boldsymbol{\zeta}_j^\top M_{jk} \boldsymbol{\zeta}_k'$$

and

$$\mathbb{E}\sum_{j\in\mathcal{I}^c}\sum_{k\in\mathcal{I}}\boldsymbol{\zeta}_j^\top M_{jk}\boldsymbol{\zeta}_k'=0.$$

Then Lemma 6.1.2 from the book (Vershynin, 2018) implies that

$$\mathbb{E}_{\boldsymbol{\zeta},\boldsymbol{\zeta}'}G\left(4\sum_{j\in\mathcal{I}}\sum_{k\in\mathcal{I}^c}\boldsymbol{\zeta}_j^{\top}M_{jk}\boldsymbol{\zeta}_k'\right) \leqslant \mathbb{E}_{\boldsymbol{\zeta},\boldsymbol{\zeta}'}G\left(4\sum_{j\in\mathcal{I}}\sum_{k\in\mathcal{I}^c}\boldsymbol{\zeta}_j^{\top}M_{jk}\boldsymbol{\zeta}_k' + 4\sum_{j\in\mathcal{I}^c}\sum_{k\in\mathcal{I}}\boldsymbol{\zeta}_j^{\top}M_{jk}\boldsymbol{\zeta}_k'\right)$$
$$= \mathbb{E}_{\boldsymbol{\zeta},\boldsymbol{\zeta}'}G\left(4\sum_{j\neq k}\boldsymbol{\zeta}_j^{\top}M_{jk}\boldsymbol{\zeta}_k'\right).$$

Hence, we obtain that

$$\mathbb{E}G\left(\sum_{j\neq k}\boldsymbol{\zeta}_{j}^{\top}M_{jk}\boldsymbol{\zeta}_{k}\right) \leqslant \mathbb{E}_{\varepsilon}\mathbb{E}_{\boldsymbol{\zeta},\boldsymbol{\zeta}'}G\left(4\sum_{j\in\mathcal{I}}\sum_{k\in\mathcal{I}^{c}}\boldsymbol{\zeta}_{j}^{\top}M_{jk}\boldsymbol{\zeta}_{k}'\right)$$
$$\leqslant \mathbb{E}_{\varepsilon}\mathbb{E}_{\boldsymbol{\zeta},\boldsymbol{\zeta}'}G\left(4\sum_{j\neq k}\boldsymbol{\zeta}_{j}^{\top}M_{jk}\boldsymbol{\zeta}_{k}'\right)$$
$$= \mathbb{E}_{\boldsymbol{\zeta},\boldsymbol{\zeta}'}G\left(4\sum_{j\neq k}\boldsymbol{\zeta}_{j}^{\top}M_{jk}\boldsymbol{\zeta}_{k}'\right).$$

Appendix G. Proof of Lemma B.2

Let us denote

$$t = \|\mathbf{u}\| \sqrt{\frac{1+\omega_j}{\log 2}} \ge \|\mathbf{u}\| \sqrt{\omega_j}$$

and show that

$$\mathbb{E} \exp\left\{\frac{\left(\mathbf{u}^{\top}\mathbf{vec}(\mathbb{Y}_j)\right)^2}{t^2}\right\} \leqslant 2.$$

Since $\mathbf{vec}(\mathbb{Y}_j)$ satisfies (10), we have

$$\log \mathbb{E} \exp\left\{\frac{\left(\mathbf{u}^{\top} \mathbf{vec}(\mathbb{Y}_{j})\right)^{2}}{t^{2}}\right\} \leqslant \frac{\operatorname{Tr}(\mathbf{u}\mathbf{u}^{\top})}{t^{2}} + \frac{\omega_{j}^{2} \|\mathbf{u}\mathbf{u}^{\top}\|_{\mathrm{F}}^{2}}{t^{4}}$$
$$= \frac{\|\mathbf{u}\|^{2}}{t^{2}} + \frac{\omega_{j}^{2} \|\mathbf{u}\|^{4}}{t^{4}} = \frac{\|\mathbf{u}\|^{2}}{t^{2}} \left(1 + \omega_{j} \cdot \frac{\omega_{j} \|\mathbf{u}\|^{2}}{t^{2}}\right) \qquad (47)$$
$$\leqslant \frac{(1 + \omega_{j}) \|\mathbf{u}\|^{2}}{t^{2}} \leqslant \log 2.$$

Here we took into account that $\omega_j \|\mathbf{u}\|^2 < t^2$. The inequality (47) yields that

$$\|\mathbf{u}^{\top}\mathbf{vec}(\mathbb{Y}_j)\|_{\psi_2}^2 \leqslant \frac{(1+\omega_j)\|\mathbf{u}\|^2}{\log 2}.$$

Step 1: a bound on $\mathbb{E}\eta^{2k}$. The goal of this step is to prove that

$$\mathbb{E}\eta^{2k} \leqslant 2 \cdot k! \cdot \sigma^{2k}$$

Note that Markov's inequality and the definition of the Orlicz norm yield that

$$\mathbb{P}\left(|\eta| \ge t\right) \leqslant e^{-t^2/\sigma^2} \mathbb{E}e^{\eta^2/\sigma^2} \leqslant 2e^{-t^2/\sigma^2} \quad \text{for all } t > 0.$$

Then it holds that

$$\mathbb{E}\eta^{2k} = \int_{0}^{+\infty} \mathbb{P}\left(\eta^{2k} \ge t\right) \mathrm{d}t = \int_{0}^{+\infty} \mathbb{P}\left(|\eta| \ge t^{1/(2k)}\right) \mathrm{d}t \le 2 \int_{0}^{+\infty} \exp\left\{-\frac{t^{1/k}}{\sigma^2}\right\} \mathrm{d}t.$$

Substituting t with $\sigma^{2k}u^k$, we obtain that

$$\mathbb{E}\eta^{2k} \leqslant 2k\,\sigma^{2k}\,\int_{0}^{+\infty} u^{k-1}e^{-u}\mathrm{d}u = 2k\,\sigma^{2k}\,\Gamma(k) = 2\cdot k!\cdot\sigma^{2k}.\tag{48}$$

Step 2: a bound on $\mathbb{E}\eta^2$. For the second moment, it is possible to prove a bit better bound, than (48). It holds that

$$\mathbb{E}\eta^2 = \int_0^{+\infty} \mathbb{P}\left(\eta^2 \ge t\right) \mathrm{d}t \leqslant \int_0^{\sigma^2 \log 2} \mathrm{d}t + \int_0^{\sigma^2 \log 2} \mathbb{P}\left(\eta^2 \ge t\right) \mathrm{d}t \leqslant \sigma^2 \log 2 + 2 \int_{\sigma^2 \log 2}^{+\infty} e^{-t/\sigma^2} \mathrm{d}t.$$

Let us replace t with $\sigma^2(u + \log 2)$, where $u \in (0, +\infty)$. Then

$$\mathbb{E}\eta^2 \leqslant \sigma^2 \log 2 + \sigma^2 \int_0^{+\infty} e^{-u} \mathrm{d}u = \sigma^2 (1 + \log 2).$$
(49)

Step 3: a bound on exponential moments. Let us fix any $\lambda > 0$ and consider $\mathbb{E}e^{\lambda\eta}$. Using Taylor's expansion and taking into account that $\mathbb{E}\eta = 0$, we obtain that

$$\mathbb{E}e^{\lambda\eta} = 1 + \sum_{k=2}^{\infty} \frac{\lambda^k \mathbb{E}\eta^k}{k!} = 1 + \sum_{k=1}^{\infty} \frac{\lambda^{2k} \mathbb{E}\eta^{2k}}{(2k)!} + \sum_{k=1}^{\infty} \frac{\lambda^{2k+1} \mathbb{E}\eta^{2k+1}}{(2k+1)!}.$$

According to the Cauchy-Schwarz inequality, we have

$$\lambda^{2k+1} \mathbb{E} \eta^{2k+1} \leqslant \frac{\lambda^{2k} \mathbb{E} \eta^{2k}}{2} + \frac{\lambda^{2k+2} \mathbb{E} \eta^{2k+2}}{2},$$

and thus,

$$\begin{split} \mathbb{E}e^{\lambda\eta} &= 1 + \sum_{k=1}^{\infty} \frac{\lambda^{2k} \mathbb{E}\eta^{2k}}{(2k)!} + \sum_{k=1}^{\infty} \frac{\lambda^{2k+1} \mathbb{E}\eta^{2k+1}}{(2k+1)!} \\ &\leqslant 1 + \frac{7\lambda^2 \mathbb{E}\eta^2}{12} + \sum_{k=2}^{\infty} \left(\frac{1}{(2k)!} + \frac{1}{2(2k-1)!} + \frac{1}{2(2k+1)!}\right) \lambda^{2k} \mathbb{E}\eta^{2k}. \end{split}$$

Due to (48), it holds that

$$\begin{split} \mathbb{E}e^{\lambda\eta} &\leqslant 1 + \frac{7\lambda^2 \mathbb{E}\eta^2}{12} + \sum_{k=2}^{\infty} \left(\frac{1}{(2k)!} + \frac{1}{2(2k-1)!} + \frac{1}{2(2k+1)!}\right) \lambda^{2k} \cdot \left(2 \cdot k! \cdot \sigma^{2k}\right) \\ &\leqslant 1 + \frac{7\lambda^2 \mathbb{E}\eta^2}{12} + \sum_{k=2}^{\infty} \frac{2(k!)^2}{(2k)!} \left(1 + k + \frac{1}{2(2k+1)}\right) \cdot \frac{\lambda^{2k} \sigma^{2k}}{k!}. \end{split}$$

Note that, for any integer $k \ge 2$, we have

$$\begin{aligned} \frac{2(k!)^2}{(2k)!} \left(1+k+\frac{1}{2(2k+1)}\right) &= \left(2+2k+\frac{1}{2k+1}\right) \prod_{j=1}^k \frac{j \cdot j}{(2j-1) \cdot 2j} \\ &= \frac{1}{2^k} \left(2+2k+\frac{1}{2k+1}\right) \prod_{j=1}^k \frac{j}{(2j-1)} \\ &\leqslant \frac{2k+3}{2^k} \prod_{j=1}^k \frac{j}{(2j-1)} \leqslant \frac{2k+3}{2^k} \cdot \frac{1}{3} < 1. \end{aligned}$$

Hence, it holds that

$$\begin{split} \mathbb{E}e^{\lambda\eta} &\leqslant 1 + \frac{7\lambda^2 \mathbb{E}\eta^2}{12} + \sum_{k=2}^{\infty} \left(\frac{1}{(2k)!} + \frac{1}{2(2k-1)!} + \frac{1}{2(2k+1)!} \right) \lambda^{2k} \cdot \left(2 \cdot k! \cdot \sigma^{2k} \right) \\ &\leqslant 1 + \frac{7\lambda^2 \mathbb{E}\eta^2}{12} + \sum_{k=2}^{\infty} \frac{\lambda^{2k} \sigma^{2k}}{k!}. \end{split}$$

The sharper bound (49) on $\mathbb{E}\eta^2$ implies that

$$\frac{7\lambda^2 \mathbb{E}\eta^2}{12} \leqslant \frac{7\lambda^2 \sigma^2 (1+\log 2)}{12} \leqslant \lambda^2 \sigma^2.$$

Thus, we finally obtain that

$$\mathbb{E}e^{\lambda\eta} \leq 1 + \lambda^2 \sigma^2 + \sum_{k=2}^{\infty} \frac{\lambda^{2k} \sigma^{2k}}{k!} \leq e^{\lambda^2 \sigma^2} \quad \text{for any } \lambda \ge 0.$$

The proof for negative λ is absolutely similar.