Asymptotic properties of the first principal component and equality tests of covariance matrices in high-dimension, low-sample-size context

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Abstract

A common feature of high-dimensional data is that the data dimension is high, however, the sample size is relatively low. We call such data HDLSS data. In this paper, we study asymptotic properties of the first principal component in the HDLSS context and apply them to equality tests of covariance matrices for high-dimensional data sets. We consider HDLSS asymptotic theories as the dimension grows for both the cases when the sample size is fixed and the sample size goes to infinity. We introduce an eigenvalue estimator by the noise-reduction methodology and provide asymptotic distributions of the largest eigenvalue in the HDLSS context. We construct a confidence interval of the first contribution ratio and give a one-sample test. We give asymptotic properties both for the first PC direction and PC score as well. We apply the findings to equality tests of two covariance matrices in the HDLSS context. We provide numerical results and discussions about the performances both on the estimates of the first PC and the equality tests of two covariance matrices.

Keywords: Contribution ratio, Equality test of covariance matrices, HDLSS, Noise-reduction methodology, PCA
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1. Introduction

One of the features of modern data is the data dimension d is high and the sample size n is relatively low. We call such data HDLSS data. In HDLSS situations such as $d/n \to \infty$, new theories and methodologies are required to develop for statistical inference. One of the approaches is to study geometric representations of HDLSS data and investigate the possibilities to make use of them in HDLSS statistical inference. Hall et al. (2005), Ahn et al. (2007), and Yata and Aoshima (2012) found several conspicuous geometric descriptions of HDLSS data when $d \to \infty$ while n is fixed. The HDLSS asymptotic studies usually assume either the normality as the population distribution or a ρ-mixing condition as the dependency of random variables in a sphered data matrix. See Jung and Marron (2009) and Jung et al. (2012). However, Yata and Aoshima (2009) developed an HDLSS asymptotic theory without assuming those assumptions and showed that the conventional principal component analysis (PCA) cannot give consistent estimation in the HDLSS context. In order to overcome this inconvenience, Yata and Aoshima (2012) provided the *noise-reduction (NR) methodology* that can successfully give consistent estimators of both the eigenvalues and eigenvectors together with the principal component (PC) scores. Furthermore, Yata and Aoshima (2010, 2013) created the *cross-data-matrix (CDM) methodology* that is a nonparametric method to ensure consistent estimation of those quantities. Given this background, Aoshima and Yata (2011, 2015) developed a variety of inference for HDLSS data such as given-bandwidth confidence regions, two-sample tests, tests of equality of two covariance matrices, classification, variable selection, regression, pathway analysis and so on along with the sample size determination to ensure prespecified accuracy for each inference.

In this paper, suppose we have a $d \times n$ data matrix, $\boldsymbol{X}_{(d)} = [\boldsymbol{x}_{1(d)}, ..., \boldsymbol{x}_{n(d)}]$, where $\boldsymbol{x}_{j(d)} = (x_{1j(d)}, ..., x_{dj(d)})^T,\ j = 1, ..., n$, are independent and identically distributed (i.i.d.) as a d-dimensional distribution with a mean vector $\boldsymbol{\mu}_d$ and covariance matrix $\boldsymbol{\Sigma}_d$ $(\geq \boldsymbol{O})$. We assume $n \geq 3$. The eigen-decomposition of $\boldsymbol{\Sigma}_d$ is given by $\boldsymbol{\Sigma}_d = \boldsymbol{H}_d \boldsymbol{\Lambda}_d \boldsymbol{H}_d^T$, where $\boldsymbol{\Lambda}_d$ =diag$(\lambda_{1(d)}, ..., \lambda_{d(d)})$ is a diagonal matrix of eigenvalues, $\lambda_{1(d)} \geq \cdots \geq \lambda_{d(d)} (\geq 0)$, and $\boldsymbol{H}_d = [\boldsymbol{h}_{1(d)}, ..., \boldsymbol{h}_{d(d)}]$ is an orthogonal matrix of the corresponding eigenvectors. Let $\boldsymbol{X}_{(d)} - [\boldsymbol{\mu}_d, ..., \boldsymbol{\mu}_d] = \boldsymbol{H}_d \boldsymbol{\Lambda}_d^{1/2} \boldsymbol{Z}_{(d)}$. Then, $\boldsymbol{Z}_{(d)}$ is a $d \times n$ sphered data matrix from a distribution with the zero mean and the identity covariance matrix. Let $\boldsymbol{Z}_{(d)} = [\boldsymbol{z}_{1(d)}, ..., \boldsymbol{z}_{d(d)}]^T$ and $\boldsymbol{z}_{i(d)} = (z_{i1(d)}, ..., z_{in(d)})^T,\ i = 1, ..., d$. Note that $E(z_{ij(d)} z_{i'j(d)}) = 0\ (i \neq i')$ and Var$(\boldsymbol{z}_{i(d)}) = \boldsymbol{I}_n$, where $\boldsymbol{I}_n$ is the n-dimensional identity matrix. The i-th true PC score of $\boldsymbol{x}_{j(d)}$ is given by $\boldsymbol{h}_{i(d)}^T (\boldsymbol{x}_{j(d)} - \boldsymbol{\mu}_d) = \lambda_{i(d)}^{1/2} z_{ij(d)}$ (hereafter called

$s_{ij(d)}$). Note that $\text{Var}(s_{ij(d)}) = \lambda_{i(d)}$ for all i, j. Hereafter, the subscript d will be omitted for the sake of simplicity when it does not cause any confusion. Let $\boldsymbol{z}_{oi} = \boldsymbol{z}_i - (\bar{z}_i, ..., \bar{z}_i)^T,\ i = 1, ..., d$, where $\bar{z}_i = n^{-1}\sum_{k=1}^n z_{ik}$. We assume that λ_1 has multiplicity one in the sense that $\liminf_{d\to\infty} \lambda_1/\lambda_2 > 1$. Also, we assume that $\limsup_{d\to\infty} E(z_{ij}^4) < \infty$ for all i, j and $P(\lim_{d\to\infty} ||\boldsymbol{z}_{o1}|| \neq 0) = 1$. Note that if $\boldsymbol{X}$ is Gaussian, z_{ij}s are i.i.d. as the standard normal distribution, $N(0, 1)$. As necessary, we consider the following assumption for the normalized first PC scores, z_{1j} $(= s_{1j}/\lambda_1^{1/2})$, $j = 1, ..., n$:

(A-i) $\quad z_{1j},\ j = 1, ..., n,$ are i.i.d. as $N(0, 1)$.

Note that $P(\lim_{d\to\infty} ||\boldsymbol{z}_{o1}|| \neq 0) = 1$ under (A-i) from the fact that $||\boldsymbol{z}_{o1}||^2$ is distributed as χ^2_{n-1}, where χ^2_ν denotes a random variable distributed as χ^2 distribution with ν degrees of freedom. Let us write the sample covariance matrix as $\boldsymbol{S} = (n-1)^{-1}(\boldsymbol{X} - \overline{\boldsymbol{X}})(\boldsymbol{X} - \overline{\boldsymbol{X}})^T = (n-1)^{-1}\sum_{j=1}^n(\boldsymbol{x}_j - \bar{\boldsymbol{x}})(\boldsymbol{x}_j - \bar{\boldsymbol{x}})^T$, where $\overline{\boldsymbol{X}} = [\bar{\boldsymbol{x}}, ..., \bar{\boldsymbol{x}}]$ and $\bar{\boldsymbol{x}} = \sum_{j=1}^n \boldsymbol{x}_j/n$. Then, we define the $n \times n$ dual sample covariance matrix by $\boldsymbol{S}_D = (n-1)^{-1}(\boldsymbol{X} - \overline{\boldsymbol{X}})^T(\boldsymbol{X} - \overline{\boldsymbol{X}})$. Let $\hat{\lambda}_1 \geq \cdots \geq \hat{\lambda}_{n-1} \geq 0$ be the eigenvalues of $\boldsymbol{S}_D$. Let us write the eigen-decomposition of $\boldsymbol{S}_D$ as $\boldsymbol{S}_D = \sum_{j=1}^{n-1}\hat{\lambda}_j\hat{\boldsymbol{u}}_j\hat{\boldsymbol{u}}_j^T$, where $\hat{\boldsymbol{u}}_j = (\hat{u}_{j1}, ..., \hat{u}_{jn})^T$ denotes a unit eigenvector corresponding to $\hat{\lambda}_j$. Note that $\boldsymbol{S}$ and $\boldsymbol{S}_D$ share non-zero eigenvalues. Also, note that $\text{tr}(\boldsymbol{S}) = \text{tr}(\boldsymbol{S}_D)$.

Here, we emphasize that the first principal component is quite important for high-dimensional data because λ_1 often becomes much larger than the other eigenvalues as d increases in the sense that $\lambda_j/\lambda_1 \to 0$ as $d \to \infty$ for all $j \geq 2$. See Figure 1 in Yata and Aoshima (2013) or Table 1 in Section 2 for example. In other words, the first principal component contains much useful information about high-dimensional data sets. In addition, λ_1 and $\boldsymbol{h}_1$ can be accurately estimated for high-dimensional data by using the NR methodology even when n is fixed. It is likely that the first principal component is applicable to high-dimensional statistical inferences such as tests of mean vectors and covariance matrices. That is the reason why we focus on the first principal component in this paper.

In this paper, we study asymptotic properties of the first principal component in the HDLSS context. We apply them to a one-sample test and equality tests of covariance matrices for high-dimensional data sets. We consider HDLSS asymptotic theories as $d \to \infty$ for both the cases when n is fixed and $n \to \infty$. In Section 2, we introduce an eigenvalue estimator by the NR methodology and provide asymptotic distributions of the largest eigenvalue in the HDLSS context. We construct a confidence interval of the first contribution ratio and give a one-sample test. In Section 3, we give asymptotic properties both for the first PC direction and PC score as well. In Section 4, we apply the findings to equality tests of two covariance matrices in the HDLSS context. Finally, in Section 5, we provide numerical results and discussions about the performances both on the estimates of the first PC and the equality tests of two covariance matrices.

2. Largest eigenvalue estimation and its applications

In this section, we give asymptotic properties of the largest eigenvalue. We construct a confidence interval of the first contribution ratio and give a one-sample test.

2.1. Asymptotic distributions of the largest eigenvalue

Let $\delta_i = \text{tr}(\boldsymbol{\Sigma}^2) - \sum_{s=1}^{i} \lambda_s^2 = \sum_{s=i+1}^{d} \lambda_s^2$ for $i = 1, ..., d-1$. We consider the following assumptions for the largest eigenvalue:

(A-ii) $\dfrac{\delta_1}{\lambda_1^2} = o(1)$ as $d \to \infty$ when n is fixed; $\dfrac{\delta_{i_*}}{\lambda_1^2} = o(1)$ as $d \to \infty$ for some fixed i_* $(< d)$ when $n \to \infty$.

(A-iii) $\dfrac{\sum_{r,s\geq 2}^{d} \lambda_r \lambda_s E\{(z_{rk}^2 - 1)(z_{sk}^2 - 1)\}}{n\lambda_1^2} = o(1)$ as $d \to \infty$ either when n is fixed or $n \to \infty$.

Note that (A-ii) implies the conditions that $\lambda_2/\lambda_1 \to 0$ as $d \to \infty$ when n is fixed and $\lambda_{i_*+1}/\lambda_1 \to 0$ as $d \to \infty$ for some fixed i_* when $n \to \infty$. Also, note that (A-iii) holds when $\boldsymbol{X}$ is Gaussian and (A-ii) is met. See Remark 2.2.

Remark 2.1. For a spiked model such as

$$\lambda_j = a_j d^{\alpha_j} \ (j = 1, ..., m) \quad \text{and} \quad \lambda_j = c_j \ (j = m+1, ..., d)$$

with positive (fixed) constants, a_js, c_js and α_js, and a positive (fixed) integer m, (A-ii) holds under the condition that $\alpha_1 > 1/2$ and $\alpha_1 > \alpha_2$ when n is fixed. When $n \to \infty$, (A-ii) holds under $\alpha_1 > 1/2$ even if $\alpha_1 = \alpha_m$. See Yata and Aoshima (2012) for the details.

Remark 2.2. For several statistical inferences of high-dimensional data, Bai and Saranadasa (1996), Chen and Qin (2010) and Aoshima and Yata (2015) assumed a general factor model as follows:

$$\boldsymbol{x}_j = \boldsymbol{\Gamma} \boldsymbol{w}_j + \boldsymbol{\mu}$$

for $j = 1, ..., n$, where $\mathbf{\Gamma}$ is a $d \times r$ matrix for some $r > 0$ such that $\mathbf{\Gamma}\mathbf{\Gamma}^T = \mathbf{\Sigma}$, and $\boldsymbol{w}_j,\ j = 1, ..., n$, are i.i.d. random vectors having $E(\boldsymbol{w}_j) = \mathbf{0}$ and Var$(\boldsymbol{w}_j) = \boldsymbol{I}_r$. As for $\boldsymbol{w}_j = (w_{1j}, ..., w_{rj})^T$, assume that $E(w_{qj}^2 w_{sj}^2) = 1$ and $E(w_{qj}w_{sj}w_{tj}w_{uj}) = 0$ for all $q \neq s, t, u$. From Lemma 1 in Yata and Aoshima (2013), one can claim that (A-iii) holds under (A-ii) in the factor model. Also, we note that the factor model naturally holds when $\boldsymbol{X}$ is Gaussian.

Let $\kappa = \mathrm{tr}(\mathbf{\Sigma}) - \lambda_1 = \sum_{s=2}^{d} \lambda_s$. Then, we have the following result.

Proposition 2.1. *Under (A-ii) and (A-iii), it holds that*

$$\frac{\hat{\lambda}_1}{\lambda_1} - ||\boldsymbol{z}_{o1}/\sqrt{n-1}||^2 - \frac{\kappa}{\lambda_1(n-1)} = o_p(1)$$

as $d \to \infty$ either when n is fixed or $n \to \infty$.

Remark 2.3. (A-ii) and (A-iii) are milder when $n \to \infty$ compared to when fixed. Jung et al. (2012) gave a result similar to Proposition 2.1 when $\boldsymbol{X}$ is Gaussian, $\boldsymbol{\mu} = \mathbf{0}$ and n is fixed.

It holds that $E(||\boldsymbol{z}_{o1}/\sqrt{n-1}||^2) = 1$ and $||\boldsymbol{z}_{o1}/\sqrt{n-1}||^2 = 1 + o_p(1)$ as $n \to \infty$. If $\kappa/(n\lambda_1) = o(1)$ as $d \to \infty$ and $n \to \infty$, $\hat{\lambda}_1$ is a consistent estimator of λ_1. When n is fixed, the condition '$\kappa/\lambda_1 = o(1)$' is equivalent to '$\lambda_1/\mathrm{tr}(\mathbf{\Sigma}) = 1 + o(1)$' in which the contribution ratio of the first principal component is asymptotically 1. In that sense, '$\kappa/\lambda_1 = o(1)$' is quite strict condition in real high-dimensional data analyses. *Hereafter, we assume* $\liminf_{d\to\infty} \kappa/\lambda_1 > 0$.

Yata and Aoshima (2012) proposed a method for eigenvalue estimation called the *noise-reduction (NR) methodology* that was brought by a geometric representation of $\boldsymbol{S}_D$. If one applies the NR method to the present case, λ_is are estimated by

$$\tilde{\lambda}_i = \hat{\lambda}_i - \frac{\mathrm{tr}(\boldsymbol{S}_D) - \sum_{j=1}^{i} \hat{\lambda}_j}{n-1-i} \quad (i = 1, ..., n-2). \tag{2.1}$$

Note that $\tilde{\lambda}_i \geq 0$ w.p.1 for $i = 1, ..., n-2$. Also, note that the second term in (2.1) with $i = 1$ is an estimator of $\kappa/(n-1)$. See Lemma 2.1 in Section 2.2 for the details. Yata and Aoshima (2012, 2013) showed that $\tilde{\lambda}_i$ has several consistency properties when $d \to \infty$ and $n \to \infty$. On the other hand, Ishii et al. (2014) gave asymptotic properties of $\tilde{\lambda}_1$ when $d \to \infty$ while n is fixed. The following theorem summarizes their findings:

Theorem 2.1 (Yata and Aoshima (2013), Ishii et al. (2014))**.** *Under (A-ii) and (A-iii), it holds that as* $d \to \infty$

$$\frac{\tilde{\lambda}_1}{\lambda_1} = \begin{cases} ||\boldsymbol{z}_{o1}/\sqrt{n-1}||^2 + o_p(1) & \textit{when } n \textit{ is fixed}, \\ 1 + o_p(1) & \textit{when } n \to \infty. \end{cases}$$

Under (A-i) to (A-iii), it holds that as $d \to \infty$

$$(n-1)\frac{\tilde{\lambda}_1}{\lambda_1} \Rightarrow \chi^2_{n-1} \qquad \textit{when } n \textit{ is fixed},$$
$$\sqrt{\frac{n-1}{2}}\Big(\frac{\tilde{\lambda}_1}{\lambda_1} - 1\Big) \Rightarrow N(0,1) \quad \textit{when } n \to \infty.$$

Here, " $\Rightarrow$ *" denotes the convergence in distribution.*

2.2. Confidence interval of the first contribution ratio

We consider a confidence interval for the contribution ratio of the first principal component. Let a and b be constants satisfying $P(a \le \chi^2_{n-1} \le b) = 1 - \alpha$, where $\alpha \in (0,1)$. Then, from Theorem 2.1, under (A-i) to (A-iii), it holds that

$$\begin{aligned} &P\Big(\frac{\lambda_1}{\text{tr}(\boldsymbol{\Sigma})} \in \Big[\frac{(n-1)\tilde{\lambda}_1}{b\kappa + (n-1)\tilde{\lambda}_1}, \frac{(n-1)\tilde{\lambda}_1}{a\kappa + (n-1)\tilde{\lambda}_1}\Big]\Big) \\ &= P\Big(a \le (n-1)\frac{\tilde{\lambda}_1}{\lambda_1} \le b\Big) = 1 - \alpha + o(1) \end{aligned} \tag{2.2}$$

as $d \to \infty$ when n is fixed. We need to estimate κ in (2.2). Here, we give a consistent estimator of κ by $\tilde{\kappa} = (n-1)(\text{tr}(\boldsymbol{S}_D) - \hat{\lambda}_1)/(n-2) = \text{tr}(\boldsymbol{S}_D) - \tilde{\lambda}_1$. Then, we have the following results.

Lemma 2.1. *Under (A-ii) and (A-iii), it holds that*

$$\frac{\tilde{\kappa}}{\kappa} = 1 + o_p(1) \quad \textit{and} \quad \frac{\tilde{\kappa}}{\lambda_1} = \frac{\kappa}{\lambda_1} + o_p(1)$$

as $d \to \infty$ *either when* n *is fixed or* $n \to \infty$*.*

Theorem 2.2. *Under (A-i) to (A-iii), it holds that*

$$P\Big(\frac{\lambda_1}{\textit{tr}(\boldsymbol{\Sigma})} \in \Big[\frac{(n-1)\tilde{\lambda}_1}{b\tilde{\kappa} + (n-1)\tilde{\lambda}_1}, \frac{(n-1)\tilde{\lambda}_1}{a\tilde{\kappa} + (n-1)\tilde{\lambda}_1}\Big]\Big) = 1 - \alpha + o(1) \tag{2.3}$$

as $d \to \infty$ *when* n *is fixed.*

Remark 2.4. From Theorem 2.1 and Lemma 2.1, under (A-ii) and (A-iii), it holds that tr$(\boldsymbol{S}_D)/$tr$(\boldsymbol{\Sigma}) = (\tilde{\kappa} + \tilde{\lambda}_1)/tr(\boldsymbol{\Sigma}) = 1 + o_p(1)$ as $d \to \infty$ and $n \to \infty$. We have that

$$\frac{\tilde{\lambda}_1}{\mathrm{tr}(\boldsymbol{S}_D)} = \frac{\lambda_1}{\mathrm{tr}(\boldsymbol{\Sigma})}\{1 + o_p(1)\}.$$

Remark 2.5. The constants $(a,\ b)$ should be chosen for (2.3) to have the minimum length. If $\lambda_1/\kappa = o(1)$, the length of the confidence interval becomes close to $\{(n-1)\tilde{\lambda}_1/\tilde{\kappa}\}(1/a - 1/b)$ under (A-ii) and (A-iii) when $d \to \infty$ and n is fixed. Thus, we recommend to choose constants $(a,\ b)$ such that

$$\underset{a,b}{\mathrm{argmin}}(1/a - 1/b) \quad \text{subject to } \ G_{n-1}(b) - G_{n-1}(a) = 1 - \alpha,$$

where $G_{n-1}(\cdot)$ denotes the c.d.f. of χ^2_{n-1}.

We used gene expression data sets and constructed a confidence interval for the contribution ratio of the first principal component. The microarray data sets were as follows: Lymphoma data with 7129 $(= d)$ genes consisting of diffuse large B-cell (DLBC) lymphoma (58 samples) and follicular lymphoma (19 samples) given by Shipp et al. (2002); and prostate cancer data with 12625 $(= d)$ genes consisting of normal prostate (50 samples) and prostate tumor (52 samples) given by Singh et al. (2002). The data sets are given in Jeffery et al. (2006). We standardized each sample so as to have the unit variance. Then, it holds that tr$(\boldsymbol{S})$ $(=$ tr$(\boldsymbol{S}_D)) = d$, so that $\tilde{\lambda}_1 + \tilde{\kappa} = d$. We gave estimates of the first five eigenvalues by $\hat{\lambda}_j$s and $\tilde{\lambda}_j$s in Table 1. We observed that the first eigenvalues are much larger than the others especially for prostate cancer data. We also observed that $\hat{\lambda}_j$ was larger than $\tilde{\lambda}_j$ for $j = 1, ..., 5$, as expected theoretically from the fact that $\hat{\lambda}_j/\tilde{\lambda}_j \geq 0$ w.p.1 for all j. We considered an estimator of δ_1 by $\tilde{\delta}_1 = W_n - \tilde{\lambda}_1^2$ having W_n by (4) in Aoshima and Yata (2015), where W_n is an unbiased and consistent estimator of tr$(\boldsymbol{\Sigma}^2)$. We calculated that $\tilde{\delta}_1/\tilde{\lambda}_1^2 = 0.163$ for DLBC lymphoma, $\tilde{\delta}_1/\tilde{\lambda}_1^2 = -0.082$ for follicular lymphoma, $\tilde{\delta}_1/\tilde{\lambda}_1^2 = -0.245$ for normal prostate and $\tilde{\delta}_1/\tilde{\lambda}_1^2 = -0.235$ for prostate tumor. From these observations, we concluded that these data sets satisfy (A-ii). In addition, from Remark 3.1 given in Section 3, by using Jarque-Bera test, we could confirm that these data sets satisfy (A-i) with the level of significance 0.05. On the other hand, it is difficult to check whether (A-iii) holds or not. However, from Remark 2.2, (A-iii) must be a natural condition under (A-ii), so that we assume (A-iii) for these data sets. Hence, from Theorem 2.2, we constructed a 95% confidence interval of the first contribution rate for each data set by choosing $(a,\ b)$ as in Remark 2.5. The results are summarized in Table 2.

Table 1. Estimates of the first five eigenvalues by $\hat{\lambda}_j$s and $\tilde{\lambda}_j$s, for the microarray data sets.

	n	$\hat{\lambda}_1,\ \hat{\lambda}_2,\ \hat{\lambda}_3,\ \hat{\lambda}_4,\ \hat{\lambda}_5$	$\tilde{\lambda}_1,\ \tilde{\lambda}_2,\ \tilde{\lambda}_3,\ \tilde{\lambda}_4,\ \tilde{\lambda}_5$
Lymphoma data with 7129 $(= d)$ genes given by Shipp et al. (2002)			
DLBC	58	1862, 564, 490, 398, 324	1768, 479, 412, 326, 257
Follicular	19	2476, 704, 614, 533, 369	2203, 457, 392, 333, 182
Prostate cancer data with 12625 $(= d)$ genes given by Singh et al (2002)			
Normal	50	6760, 562, 426, 371, 304	6637, 450, 320, 271, 209
Prostate	52	6106, 687, 512, 462, 298	5976, 568, 401, 359, 199

Table 2. The 95% confidence interval (CI) of the first contribution ratio, together with $\tilde{\lambda}_1$ and $\tilde{\kappa}$, for the microarray data sets.

	(n, d)	CI	$\tilde{\lambda}_1$	$\tilde{\kappa}$
DLBC lymphoma	$(58, 7129)$	$[0.183, 0.322]$	1768	5361
Follicular lymphoma	$(19, 7129)$	$[0.178, 0.467]$	2203	4926
Normal prostate	$(50, 12625)$	$[0.422, 0.622]$	6637	5988
Prostate tumor	$(52, 12625)$	$[0.374, 0.569]$	5976	6649

2.3. Test of mean vector

We consider the following one-sample test for the mean vector:

$$H_0:\ \boldsymbol{\mu} = \boldsymbol{\mu}_0 \quad \text{vs.} \quad H_1:\ \boldsymbol{\mu} \neq \boldsymbol{\mu}_0, \tag{2.4}$$

where $\boldsymbol{\mu}_0$ is a candidate mean vector such as $\boldsymbol{\mu}_0 = \mathbf{0}$. Here, we have the following result.

Lemma 2.2. *Under (A-ii), it holds that*

$$\frac{||\bar{\boldsymbol{x}} - \boldsymbol{\mu}||^2 - tr(\boldsymbol{S}_D)/n}{\lambda_1} = \bar{z}_1^2 - \frac{||\boldsymbol{z}_{o1}/\sqrt{n-1}||^2}{n} + o_p(1)$$

as $d \to \infty$ when n is fixed.

Let

$$F_0 = \frac{n||\bar{\boldsymbol{x}} - \boldsymbol{\mu}_0||^2 - \text{tr}(\boldsymbol{S}_D)}{\tilde{\lambda}_1} + 1.$$

Note that $E(\tilde{\lambda}_1(F_0-1)/n)=||\boldsymbol{\mu}-\boldsymbol{\mu}_0||^2$. Then, by combining Theorem 2.1 and Lemma 2.2, we have the following result.

Theorem 2.3. *Under (A-i) to (A-iii), it holds that*

$$F_0 \Rightarrow F_{1,n-1} \text{ under } H_0 \text{ in (2.4)}$$

as $d\to\infty$ when n is fixed, where F_{ν_1,ν_2} denotes a random variable distributed as F distribution with degrees of freedom, ν_1 and ν_2.

For a given $\alpha\in(0,1/2)$ we test (2.4) by

$$\text{accepting } H_1 \Longleftrightarrow F_0 > F_{1,n-1}(\alpha),$$

where $F_{\nu_1,\nu_2}(\alpha)$ denotes the upper $\alpha\%$ point of F distribution with degrees of freedom, ν_1 and ν_2. Then, under (A-i) to (A-iii), it holds that

$$\text{size} = \alpha + o(1)$$

as $d\to\infty$ when n is fixed.

For the same gene expression data as in Section 2.2, we tested (2.4) with $\boldsymbol{\mu}_0=\mathbf{0}$ and $\alpha=0.05$. We observed that H_1 was accepted for all four data sets.

3. First PC direction and PC score

In this section, we give asymptotic properties of the first PC direction and PC score in the HDLSS context.

3.1. Asymptotic properties of the first PC direction

Let $\hat{\boldsymbol{H}}=[\hat{\boldsymbol{h}}_1,...,\hat{\boldsymbol{h}}_d]$, where $\hat{\boldsymbol{H}}$ is a $d\times d$ orthogonal matrix of the sample eigenvectors such that $\hat{\boldsymbol{H}}^T\boldsymbol{S}\hat{\boldsymbol{H}}=\hat{\boldsymbol{\Lambda}}$ having $\hat{\boldsymbol{\Lambda}}=\text{diag}(\hat{\lambda}_1,...,\hat{\lambda}_d)$. We assume $\boldsymbol{h}_i^T\hat{\boldsymbol{h}}_i\ge 0$ w.p.1 for all i without loss of generality. Note that $\hat{\boldsymbol{h}}_i$ can be calculated by $\hat{\boldsymbol{h}}_i=\{(n-1)\hat{\lambda}_i\}^{-1/2}(\boldsymbol{X}-\overline{\boldsymbol{X}})\hat{\boldsymbol{u}}_i$. First, we have the following result.

Lemma 3.1. *Under (A-ii) and (A-iii), it holds that*

$$\hat{\boldsymbol{h}}_1^T\boldsymbol{h}_1-\Big(1+\frac{\kappa}{\lambda_1||\boldsymbol{z}_{o1}||^2}\Big)^{-1/2}=o_p(1)$$

as $d\to\infty$ either when n is fixed or $n\to\infty$.

If $\kappa/(n\lambda_1) = o(1)$ as $d \to \infty$ and $n \to \infty$, $\hat{\boldsymbol{h}}_1$ is a consistent estimator of $\boldsymbol{h}_1$ in the sense that $\hat{\boldsymbol{h}}_1^T \boldsymbol{h}_1 = 1 + o_p(1)$. When n is fixed, $\hat{\boldsymbol{h}}_1$ is not a consistent estimator because $\liminf_{d\to\infty} \kappa/\lambda_1 > 0$. In order to overcome this inconvenience, we consider applying the NR methodology to the PC direction vector. Let $\tilde{\boldsymbol{h}}_i = \{(n-1)\tilde{\lambda}_i\}^{-1/2}(\boldsymbol{X} - \overline{\boldsymbol{X}})\hat{\boldsymbol{u}}_i$. From Lemma 3.1, we have the following result.

Theorem 3.1. *Under (A-ii) and (A-iii), it holds that*

$$\tilde{\boldsymbol{h}}_1^T \boldsymbol{h}_1 = 1 + o_p(1)$$

as $d \to \infty$ either when n is fixed or $n \to \infty$.

Note that $||\tilde{\boldsymbol{h}}_1||^2 = \hat{\lambda}_1/\tilde{\lambda}_1 \geq 1$ w.p.1. We emphasize that $\tilde{\boldsymbol{h}}_1$ is a consistent estimator of $\boldsymbol{h}_1$ in the sense of the inner product even when n is fixed though $\tilde{\boldsymbol{h}}_1$ is not a unit vector. We give an application of $\tilde{\boldsymbol{h}}_1$ in Section 4.

3.2. Asymptotic properties of the first PC score

Let $z_{oij} = z_{ij} - \bar{z}_i$ for all i, j. Note that $\boldsymbol{z}_{oi} = (z_{oi1}, ..., z_{oin})^T$ for all i. First, we have the following result.

Lemma 3.2. *Under (A-ii) and (A-iii), it holds that*

$$\hat{u}_{1j} = z_{o1j}/||\boldsymbol{z}_{o1}|| + o_p(1) \quad \textit{for } j = 1, ..., n$$

as $d \to \infty$ when n is fixed.

Remark 3.1. From Lemma 3.2, by using $\hat{u}_{1j}$s and the test of normality such as Jarque-Bera test, one can check whether (A-i) holds or not.

By applying the NR methodology to the first PC score, we obtain an estimate by $\tilde{s}_{1j} = \sqrt{(n-1)\tilde{\lambda}_1}\hat{u}_{1j},\ j = 1, ..., n$. A sample mean squared error of the first PC score is given by $\text{MSE}(\tilde{s}_1) = n^{-1}\sum_{j=1}^n (\tilde{s}_{1j} - s_{1j})^2$. Then, from Theorem 2.1 and Lemma 3.2, we have the following result.

Theorem 3.2. *Under (A-ii) and (A-iii), it holds that*

$$\frac{1}{\sqrt{\lambda_1}}(\tilde{s}_{1j} - s_{1j}) = -\bar{z}_1 + o_p(1) \quad \textit{for } j = 1, ..., n$$

as $d \to \infty$ when n is fixed. Under (A-i) to (A-iii), it holds that

$$\sqrt{\frac{n}{\lambda_1}}(\tilde{s}_{1j} - s_{1j}) \Rightarrow N(0,1) \quad \textit{for } j = 1, ..., n; \quad \textit{and} \quad n\frac{\textit{MSE}(\tilde{s}_1)}{\lambda_1} \Rightarrow \chi_1^2$$

as $d \to \infty$ when n is fixed.

Remark 3.2. The conventional estimator of the first PC score is given by $\hat{s}_{1j} = \sqrt{(n-1)\hat{\lambda}_1}\hat{u}_{1j},\ j = 1, ..., n$. From Theorems 8.1 and 8.2 in Yata and Aoshima (2013), under (A-ii) and (A-iii), it holds that as $d \to \infty$ and $n \to \infty$

$$\frac{\text{MSE}(\hat{s}_1)}{\lambda_1} = o_p(1) \text{ if } \kappa/(n\lambda_1) = o(1), \quad \text{and} \quad \frac{\text{MSE}(\tilde{s}_1)}{\lambda_1} = o_p(1).$$

4. Equality tests of two covariance matrices

In this section, we consider the test of equality of two covariance matrices in the HDLSS context. Even though there are a variety of tests to deal with covariance matrices when $d \to \infty$ and $n \to \infty$, there seem to be no tests available in the HDLSS context such as $d \to \infty$ while n is fixed. Suppose we have two independent $d \times n_i$ data matrices, $\boldsymbol{X}_i = [\boldsymbol{x}_{1(i)}, ..., \boldsymbol{x}_{n_i(i)}],\ i = 1, 2$, where $\boldsymbol{x}_{j(i)},\ j = 1, ..., n_i$, are i.i.d. as a d-dimensional distribution, π_i, having a mean vector $\boldsymbol{\mu}_i$ and covariance matrix $\boldsymbol{\Sigma}_i\ (\geq \boldsymbol{O})$. We assume $n_i \geq 3,\ i = 1, 2$. The eigen-decomposition of $\boldsymbol{\Sigma}_i$ is given by $\boldsymbol{\Sigma}_i = \boldsymbol{H}_i \boldsymbol{\Lambda}_i \boldsymbol{H}_i^T$, where $\boldsymbol{\Lambda}_i = \text{diag}(\lambda_{1(i)}, ..., \lambda_{d(i)})$ having $\lambda_{1(i)} \geq \cdots \geq \lambda_{d(i)} (\geq 0)$ and $\boldsymbol{H}_i = [\boldsymbol{h}_{1(i)}, ..., \boldsymbol{h}_{d(i)}]$ is an orthogonal matrix of the corresponding eigenvectors. We assume that $\liminf_{d\to\infty} \lambda_{1(i)}/\lambda_{2(i)} > 0$ for $i = 1, 2$. Also, we assume that $\limsup_{d\to\infty} E(z_{sj}^4) < \infty$ for all s, j and $P(\lim_{d\to\infty} ||\boldsymbol{z}_{o1}|| \neq 0) = 1$, for each π_i.

4.1. Equality test using the largest eigenvalues

We consider the following test for the largest eigenvalues:

$$H_0 : \lambda_{1(1)} = \lambda_{1(2)} \quad \text{vs.} \quad H_a : \lambda_{1(1)} \neq \lambda_{1(2)} \ \ (\text{or } \ H_b : \lambda_{1(1)} < \lambda_{1(2)}). \tag{4.1}$$

Let $\tilde{\lambda}_{1(i)}$ be the estimate of $\lambda_{1(i)}$ by the NR methodology as in (2.1) for π_i. Let $\nu_1 = n_1 - 1$ and $\nu_2 = n_2 - 1$. From Theorem 2.1, we have the following result.

Corollary 4.1. *Under (A-i) to (A-iii) for each π_i, it holds that*

$$\frac{\tilde{\lambda}_{1(1)}/\lambda_{1(1)}}{\tilde{\lambda}_{1(2)}/\lambda_{1(2)}} \Rightarrow F_{\nu_1,\nu_2}$$

as $d \to \infty$ when n_is are fixed.

Let $F_1 = \tilde{\lambda}_{1(1)}/\tilde{\lambda}_{1(2)}$. For a given $\alpha \in (0, 1/2)$ we test (4.1) by

$$\text{accepting } H_a \Longleftrightarrow F_1 \notin [\{F_{\nu_2,\nu_1}(\alpha/2)\}^{-1}, F_{\nu_1,\nu_2}(\alpha/2)] \tag{4.2}$$
$$\text{or} \quad \text{accepting } H_b \Longleftrightarrow F_1 < \{F_{\nu_2,\nu_1}(\alpha)\}^{-1}. \tag{4.3}$$

Then, under (A-i) to (A-iii) for each π_i, it holds that

$$\text{size} = \alpha + o(1)$$

as $d \to \infty$ when n_is are fixed.

Now, we consider a test by the conventional estimator, $\hat{\lambda}_{1(i)}$. Let $\kappa_i = \text{tr}(\boldsymbol{\Sigma}_i) - \lambda_{1(i)} = \sum_{s=2}^{d} \lambda_{s(i)}$ for $i = 1, 2$. From Proposition 2.1, if $\kappa_i/\lambda_{1(i)} = o(1)$, $i = 1, 2$, under (A-i) for each π_i it holds that

$$\frac{\hat{\lambda}_{1(1)}/\lambda_{1(1)}}{\hat{\lambda}_{1(2)}/\lambda_{1(2)}} \Rightarrow F_{\nu_1,\nu_2}$$

as $d \to \infty$ when n_is are fixed. As mentioned in Section 2, the condition '$\kappa_i/\lambda_{1(i)} = o(1)$ for $i = 1, 2$' is quite strict in real high-dimensional data analyses. See Table 2 for example. *Hereafter, we assume* $\liminf_{d\to\infty} \kappa_i/\lambda_{1(i)} > 0$ *for* $i = 1, 2$.

4.2. Equality test using the largest eigenvalues and their PC directions

We consider the following test using the largest eigenvalues and their PC directions:

$$H_0 : (\lambda_{1(1)}, \boldsymbol{h}_{1(1)}) = (\lambda_{1(2)}, \boldsymbol{h}_{1(2)}) \quad \text{vs.} \quad H_a : (\lambda_{1(1)}, \boldsymbol{h}_{1(1)}) \neq (\lambda_{1(2)}, \boldsymbol{h}_{1(2)}). \tag{4.4}$$

Let $\tilde{\boldsymbol{h}}_{1(i)}$ be the estimator of the first PC direction for π_i by the NR methodology given in Section 3.1. We assume $\boldsymbol{h}_{1(i)}^T \tilde{\boldsymbol{h}}_{1(i)} \geq 0$ w.p.1 for $i = 1, 2$, without loss of generality. Here, we have the following result.

Lemma 4.1. *Under (A-ii) and (A-iii) for each π_i, it holds that*

$$\tilde{\boldsymbol{h}}_{1(1)}^T \tilde{\boldsymbol{h}}_{1(2)} = \boldsymbol{h}_{1(1)}^T \boldsymbol{h}_{1(2)} + o_p(1)$$

as $d \to \infty$ either when n_i is fixed or $n_i \to \infty$ for $i = 1, 2$.

We note that under H_0 in (4.4)

$$(\lambda_{1(i)} \boldsymbol{h}_{1(i)})^T (\lambda_{1(j)}^{-1} \boldsymbol{h}_{1(j)}) = 1 \quad \text{for } i = 1, 2;\ j \neq i.$$

Hence, one may consider a test statistic such as $F_1 |\tilde{\boldsymbol{h}}_{1(1)}^T \tilde{\boldsymbol{h}}_{1(2)}|$ or $F_1 |\tilde{\boldsymbol{h}}_{1(1)}^T \tilde{\boldsymbol{h}}_{1(2)}|^{-1}$. From Corollary 4.1 and Lemma 4.1, $F_1 |\tilde{\boldsymbol{h}}_{1(1)}^T \tilde{\boldsymbol{h}}_{1(2)}|$ and $F_1 |\tilde{\boldsymbol{h}}_{1(1)}^T \tilde{\boldsymbol{h}}_{1(2)}|^{-1}$ are asymptotically distributed as F_{ν_1,ν_2}. Let $\tilde{h} = \max\{|\tilde{\boldsymbol{h}}_{1(1)}^T \tilde{\boldsymbol{h}}_{1(2)}|, |\tilde{\boldsymbol{h}}_{1(1)}^T \tilde{\boldsymbol{h}}_{1(2)}|^{-1}\}$. Note that $\tilde{h} \geq 1$ w.p.1. Then, in view of the power, we give a test statistic for (4.4) as follows:

$$F_2 = \frac{\tilde{\lambda}_{1(1)}}{\tilde{\lambda}_{1(2)}}\tilde{h}_* \ \ (= F_1\tilde{h}_*),$$

where

$$\tilde{h}_* = \begin{cases} \tilde{h} & \text{if } \tilde{\lambda}_{1(1)} \geq \tilde{\lambda}_{1(2)}, \\ \tilde{h}^{-1} & \text{otherwise}. \end{cases}$$

From Lemma 4.1, we have the following result.

Theorem 4.1. *Under (A-i) to (A-iii) for each π_i, it holds that*

$$F_2 \Rightarrow F_{\nu_1,\nu_2} \text{ under } H_0 \text{ in (4.4)}$$

as $d \to \infty$ when n_is are fixed.

From Theorem 4.1, we consider testing (4.4) by (4.2) with F_2 instead of F_1. Then, the size becomes close to α as d increases.

4.3. Equality test of the covariance matrices

We consider the following test for the covariance matrices:

$$H_0 : \boldsymbol{\Sigma}_1 = \boldsymbol{\Sigma}_2 \quad \text{vs.} \quad H_a : \boldsymbol{\Sigma}_1 \neq \boldsymbol{\Sigma}_2. \tag{4.5}$$

When $d \to \infty$ and n_is are fixed, one can estimate $\lambda_{1(i)}$s and $\boldsymbol{h}_{1(i)}$s by the NR methodology, however, one cannot estimate $\lambda_{j(i)}$s and $\boldsymbol{h}_{j(i)}$s for $j = 2, ..., d$. Instead, we consider estimating κ_is. Let $\boldsymbol{S}_{D(i)}$ be the dual sample covariance matrix for π_i. We estimate κ_i by $\tilde{\kappa}_i = \text{tr}(\boldsymbol{S}_{D(i)}) - \tilde{\lambda}_{1(i)}$ for $i = 1, 2$. From Lemma 2.1, under (A-ii) and (A-iii) for each π_i, $\tilde{\kappa}_i$s are consistent estimators of κ_is in the sense that $\tilde{\kappa}_i/\kappa_i = 1+o_p(1)$ as $d \to \infty$ when n_is are fixed. Let $\tilde{\gamma} = \max\{\tilde{\kappa}_1/\tilde{\kappa}_2, \tilde{\kappa}_2/\tilde{\kappa}_1\}$. Similar to F_2, we give a test statistic for (4.5) as follows:

$$F_3 = \frac{\tilde{\lambda}_{1(1)}}{\tilde{\lambda}_{1(2)}}\tilde{h}_*\tilde{\gamma}_* \ \ (= F_2\tilde{\gamma}_*),$$

where

$$\tilde{\gamma}_* = \begin{cases} \tilde{\gamma} & \text{if } \tilde{\lambda}_{1(1)} \geq \tilde{\lambda}_{1(2)}, \\ \tilde{\gamma}^{-1} & \text{otherwise}. \end{cases}$$

Then, we have the following result.

Theorem 4.2. *Under (A-i) to (A-iii) for each π_i, it holds that*

$$F_3 \Rightarrow F_{\nu_1,\nu_2} \text{ under } H_0 \text{ in (4.5)}$$

as $d \to \infty$ when n_is are fixed.

From Theorem 4.2, we consider testing (4.5) by (4.2) with F_3 instead of F_1. Then, the size becomes close to α as d increases.

We analyzed lymphoma data given by Shipp et al. (2002) and prostate cancer data given by Singh et al. (2002) which are the same gene expression data as in Section 2.2. When each sample is standardized, we note that $\tilde{\kappa}_1 \approx \tilde{\kappa}_2$ if $\lambda_{1(i)}/\kappa_i = o(1),\ i = 1, 2$, since $\text{tr}(\boldsymbol{S}_{D(1)}) = \text{tr}(\boldsymbol{S}_{D(2)}) = d$, so that one loses information about the difference between κ_1 and κ_2. Hence, we did not standardize each sample. We set $\alpha = 0.05$. We considered two cases: (I) π_1 : DLBC lymphoma ($n_1 = 58$) and π_2 : follicular lymphoma ($n_2 = 19$) and (II) π_1 : normal prostate ($n_1 = 50$) and π_2 : prostate tumor ($n_2 = 52$). We compared the performance of F_3 with two other test statistics, Q_2^2 and T_2^2, by Srivastava and Yanagihara (2010). The results are summarized in Table 3. We observed that F_3 accepted H_a for (I) and H_0 for (II), namely, F_3 rejected H_0 in (4.5) for (I). On the other hand, Q_2^2 and T_2^2 did not work for these data sets because Q_2^2 and T_2^2 are established under the severe conditions that $0 < \lim_{d\to\infty} \text{tr}(\boldsymbol{\Sigma}^i)/d < \infty\ (i = 1, ..., 4)$ and $d^{1/2}/n = o(1)$. As observed in Table 1, the conditions seem not to hold for these data sets. Hence, there is no theoretical guarantee for the results by Q_2^2 and T_2^2.

Table 3. Tests of $H_0 : \boldsymbol{\Sigma}_1 = \boldsymbol{\Sigma}_2$ vs. $H_a : \boldsymbol{\Sigma}_1 \neq \boldsymbol{\Sigma}_2$ with size 0.05 for two data sets: (I) lymphoma data with $d = 7129$ given by Shipp et al. (2002) and (II) prostate cancer data with $d = 12625$ given by Singh et al. (2002).

	H_a by F_3	H_a by Q_2^2	H_a by T_2^2
(I) π_1: DLBC, π_2: Follicular	Accept	Accept	Reject
(II) π_1: Normal, π_2: Tumor	Reject	Reject	Reject

5. Numerical results and discussions

5.1. Comparisons of the estimates on the first PC

In this section, we compared the performance of $\tilde{\lambda}_1$, $\tilde{\boldsymbol{h}}_1$ and $\tilde{s}_{1j}$ with their conventional counterparts by Monte Carlo simulations. We set $d = 2^k,\ k = 3, ..., 11$

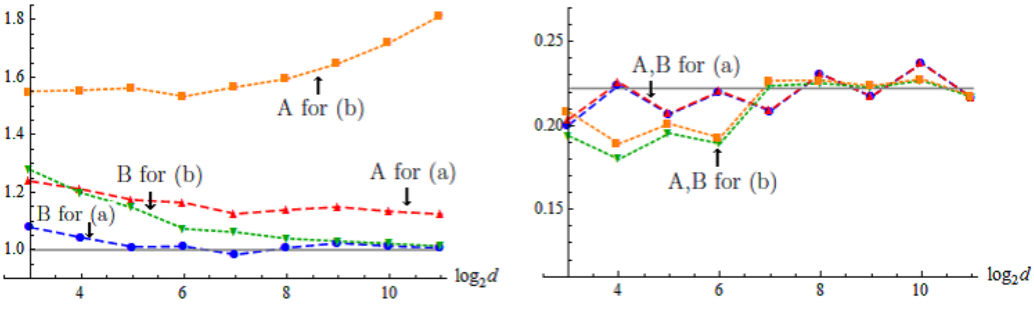
and $n = 10$. We considered two cases for λ_is: (a) $\lambda_i = d^{1/i}$, $i = 1, ..., d$ and (b) $\lambda_i = d^{3/(2+2i)}$, $i = 1, ..., d$. Note that $\lambda_1 = d$ for (a) and $\lambda_1 = d^{3/4}$ for (b). Also, note that (A-ii) holds both for (a) and (b). Let $d_* = \lceil d^{1/2} \rceil$, where $\lceil x \rceil$ denotes the smallest integer $\geq x$. We considered a non-Gaussian distribution as follows: $(z_{1j}, ..., z_{d-d_*j})^T,\ j = 1, ..., n$, are i.i.d. as $N_{d-d_*}(\mathbf{0}, \boldsymbol{I}_{d-d_*})$ and $(z_{d-d_*+1j}, ..., z_{dj})^T,\ j = 1, ..., n$, are i.i.d. as the d_*-variate t-distribution, $t_{d_*}(\mathbf{0}, \boldsymbol{I}_{d_*}, 10)$ with mean zero, covariance matrix $\boldsymbol{I}_{d_*}$ and degrees of freedom 10, where $(z_{1j}, ..., z_{d-d_*j})^T$ and $(z_{d-d_*+1j}, ..., z_{dj})^T$ are independent for each j. Note that (A-i) and (A-iii) hold both for (a) and (b) from the fact that $\sum_{r,s\geq 2}^{d} \lambda_r \lambda_s E\{(z_{rk}^2 - 1)(z_{sk}^2 - 1)\} = 2\sum_{s=2}^{d-d_*} \lambda_s^2 + O(\sum_{r,s\geq d-d_*+1}^{d} \lambda_r\lambda_s) = o(\lambda_1^2)$.

The findings were obtained by averaging the outcomes from 2000 ($= R$, say) replications. Under a fixed scenario, suppose that the r-th replication ends with estimates, ($\hat{\lambda}_{1r}$, $\hat{\boldsymbol{h}}_{1r}$, MSE$(\hat{s}_1)_r$) and ($\tilde{\lambda}_{1r}$, $\tilde{\boldsymbol{h}}_{1r}$, MSE$(\tilde{s}_1)_r$) $(r = 1, ..., R)$. Let us simply write $\hat{\lambda}_1 = R^{-1}\sum_{r=1}^{R} \hat{\lambda}_{1r}$ and $\tilde{\lambda}_1 = R^{-1}\sum_{r=1}^{R} \tilde{\lambda}_{1r}$. We also considered the Monte Carlo variability by var$(\hat{\lambda}_1/\lambda_1) = (R-1)^{-1}\sum_{r=1}^{R}(\hat{\lambda}_{1r} - \hat{\lambda}_1)^2/\lambda_1^2$ and var$(\tilde{\lambda}_1/\lambda_1) = (R-1)^{-1}\sum_{r=1}^{R}(\tilde{\lambda}_{1r} - \tilde{\lambda}_1)^2/\lambda_1^2$. Figure 1 shows the behaviors of ($\hat{\lambda}_1/\lambda_1$, $\tilde{\lambda}_1/\lambda_1$) in the left panel and (var$(\hat{\lambda}_1/\lambda_1)$, var$(\tilde{\lambda}_1/\lambda_1)$) in the right panel for (a) and (b). We gave the asymptotic variance of $\tilde{\lambda}_1/\lambda_1$ by Var$\{\chi_{n-1}^2/(n-1)\} = 0.222$ from Theorem 2.1 and showed it by the solid line in the right panel. We observed that the sample mean and variance of $\tilde{\lambda}_1/\lambda_1$ become close to those asymptotic values as d increases.

Similarly, we plotted ($\hat{\boldsymbol{h}}_1^T\boldsymbol{h}_1$, $\tilde{\boldsymbol{h}}_1^T\boldsymbol{h}_1$) and (var$(\hat{\boldsymbol{h}}_1^T\boldsymbol{h}_1)$, var$(\tilde{\boldsymbol{h}}_1^T\boldsymbol{h}_1)$) in Figure 2 and (MSE$(\hat{s}_1)/\lambda_1$, MSE$(\tilde{s}_1)/\lambda_1$) and (var(MSE$(\hat{s}_1)/\lambda_1$), var(MSE$(\tilde{s}_1)/\lambda_1$)) in Figure 3. From Theorem 3.2, we gave the asymptotic mean of MSE$(\tilde{s}_1)/\lambda_1$ by $E(\chi_1^2/n) = 0.1$ and showed it by the solid line in the left panel of Figure 3. We also gave the asymptotic variance of MSE$(\tilde{s}_1)/\lambda_1$ by Var$(\chi_1^2/n) = 0.02$ in the right panel of Figure 3. Throughout, the estimators by the NR method gave good performances both for (a) and (b) when d is large. However, the conventional estimators gave poor performances especially for (b). This is probably because the bias of the conventional estimators, $\kappa/\{(n-1)\lambda_1\}$, is large for (b) compared to (a). See Proposition 2.1 for the details.

5.2. Equality tests of two covariance matrices

We used computer simulations to study the performance of the test procedures by (4.2) with F_1 for (4.1), F_2 for (4.4) and F_3 for (4.5). We set $\alpha = 0.05$. Independent pseudo-random normal observations were generated from $\pi_i : N_d(\mathbf{0}, \boldsymbol{\Sigma}_i)$, $i = 1, 2$. We set $(n_1, n_2) = (15, 25)$. We considered the cases: $d = 2^k,\ k = 4, ..., 12$,



A: $\hat{\lambda}_1/\lambda_1$ and B: $\tilde{\lambda}_1/\lambda_1$ A: $\text{var}(\hat{\lambda}_1/\lambda_1)$ and B: $\text{var}(\tilde{\lambda}_1/\lambda_1)$

Figure 1. The values of A: $\hat{\lambda}_1/\lambda_1$ and B: $\tilde{\lambda}_1/\lambda_1$ are denoted by the dashed lines for (a) and by the dotted lines for (b) in the left panel. The values of A: $\text{var}(\hat{\lambda}_1/\lambda_1)$ and B: $\text{var}(\tilde{\lambda}_1/\lambda_1)$ are denoted by the dashed lines for (a) and by the dotted lines for (b) in the left panel. The asymptotic variance of $\tilde{\lambda}_1/\lambda_1$ was given by $\text{Var}\{\chi^2_{n-1}/(n-1)\} = 0.222$ and denoted by the solid line in the left panel.

and

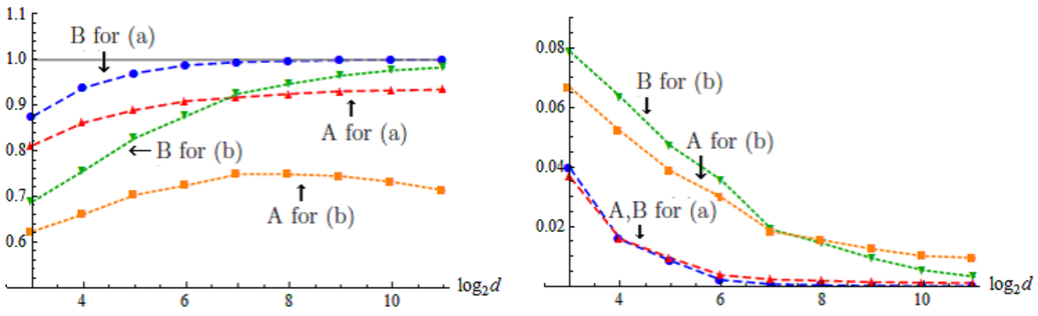
$$\boldsymbol{\Sigma}_i = \begin{pmatrix} \boldsymbol{\Sigma}_{i(1)} & \boldsymbol{O}_{2,d-2} \\ \boldsymbol{O}_{d-2,2} & \boldsymbol{\Sigma}_{i(2)} \end{pmatrix},\ i = 1, 2, \tag{5.1}$$

where $\boldsymbol{O}_{k,l}$ is the $k \times l$ zero matrix, $\boldsymbol{\Sigma}_{1(1)} = \text{diag}(d^{3/4}, d^{1/2})$ and $\boldsymbol{\Sigma}_{1(2)} = (0.3^{|s-t|})$. When considered the alternative hypotheses, we set

$$\boldsymbol{\Sigma}_{2(1)} = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \text{diag}(3d^{3/4}, 1.5d^{1/2}) \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \tag{5.2}$$

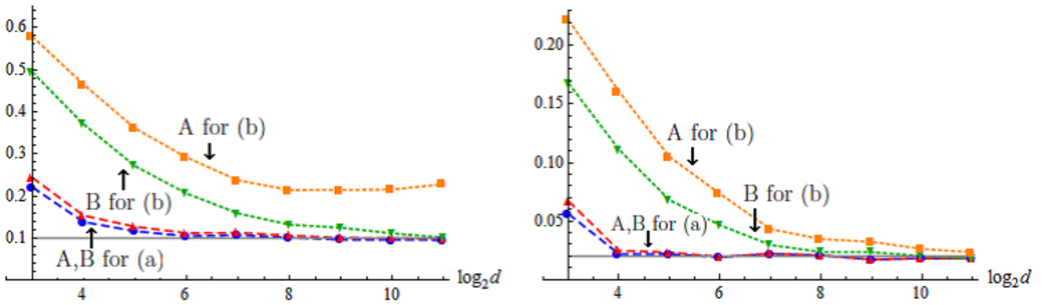
and $\boldsymbol{\Sigma}_{2(2)} = 1.5(0.3^{|s-t|})$. Note that $\lambda_{1(2)}/\lambda_{1(1)} = 3$, $\kappa_2/\kappa_1 = 1.5$ and $\boldsymbol{h}_{1(1)}^T\boldsymbol{h}_{1(2)} = 1/\sqrt{2}$. Also, note that (A-i) to (A-iii) hold for each π_i. Let $h = \max\{|\boldsymbol{h}_{1(1)}^T\boldsymbol{h}_{1(2)}|, |\boldsymbol{h}_{1(1)}^T\boldsymbol{h}_{1(2)}|^{-1}\}$ and $\gamma = \max\{\kappa_1/\kappa_2, \kappa_2/\kappa_1\}$. From Lemmas 2.1 and 4.1, it holds that $\tilde{h} = h + o_p(1)$ and $\tilde{\gamma} = \gamma + o_p(1)$. Thus, from Corollary 4.1, Theorems 4.1 and 4.2, we obtained the asymptotic powers of F_1, F_2 and F_3 with $(\tilde{h}_*, \tilde{\gamma}_*) = (h^{-1}, \gamma^{-1})$ as follows:

$$\begin{aligned} &\text{Power}(F_1) = P\big\{(\lambda_{1(1)}/\lambda_{1(2)})f \notin [\{F_{\nu_2,\nu_1}(\alpha/2)\}^{-1}, F_{\nu_1,\nu_2}(\alpha/2)]\big\} = 0.577, \\ &\text{Power}(F_2) = P\big\{h^{-1}(\lambda_{1(1)}/\lambda_{1(2)})f \notin [\{F_{\nu_2,\nu_1}(\alpha/2)\}^{-1}, F_{\nu_1,\nu_2}(\alpha/2)]\big\} = 0.823 \\ &\text{and}\ \ \text{Power}(F_3) = P\big\{\gamma^{-1}h^{-1}(\lambda_{1(1)}/\lambda_{1(2)})f \notin [\{F_{\nu_2,\nu_1}(\alpha/2)\}^{-1}, F_{\nu_1,\nu_2}(\alpha/2)]\big\} \\ &\qquad\qquad\qquad = 0.963, \end{aligned}$$



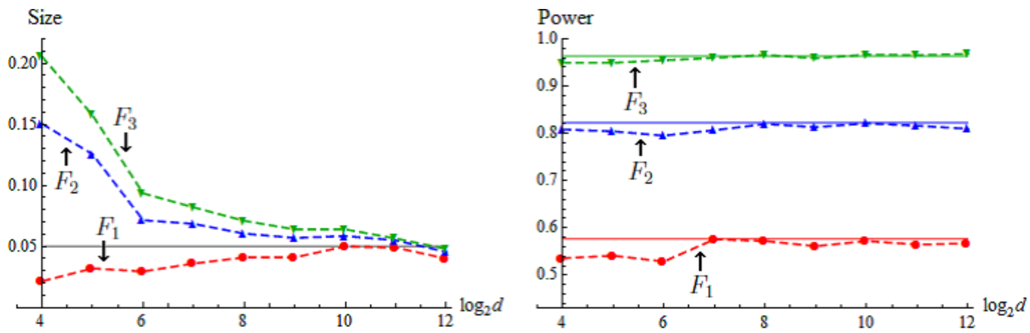
A: $\hat{\boldsymbol{h}}_1^T \boldsymbol{h}_1$ and B: $\tilde{\boldsymbol{h}}_1^T \boldsymbol{h}_1$ A: var$(\hat{\boldsymbol{h}}_1^T \boldsymbol{h}_1)$ and B: var$(\tilde{\boldsymbol{h}}_1^T \boldsymbol{h}_1)$

Figure 2. The values of A: $\hat{\boldsymbol{h}}_1^T \boldsymbol{h}_1$ and B: $\tilde{\boldsymbol{h}}_1^T \boldsymbol{h}_1$ are denoted by the dashed lines for (a) and by the dotted lines for (b) in the left panel. The values of A: var$(\hat{\boldsymbol{h}}_1^T \boldsymbol{h}_1)$ and B: var$(\tilde{\boldsymbol{h}}_1^T \boldsymbol{h}_1)$ are denoted by the dashed lines for (a) and by the dotted lines for (b) in the right panel.



A: MSE$(\hat{s}_1)/\lambda_1$ and B: MSE$(\tilde{s}_1)/\lambda_1$ A: var(MSE$(\hat{s}_1)/\lambda_1$) and B: var(MSE$(\tilde{s}_1)/\lambda_1$)

Figure 3. The values of A: MSE$(\hat{s}_1)/\lambda_1$ and B: MSE$(\tilde{s}_1)/\lambda_1$ are denoted by the dashed lines for (a) and by the dotted lines for (b) in the left panel. The values of A: var(MSE$(\hat{s}_1)/\lambda_1$) and B: var(MSE$(\tilde{s}_1)/\lambda_1$) are denoted by the dashed lines for (a) and by the dotted lines for (b) in the right panel. The asymptotic mean and variance of MSE$(\tilde{s}_1)/\lambda_1$ were given by $E(\chi_1^2/n) = 0.1$ and Var$(\chi_1^2/n) = 0.02$ and denoted by the solid lines in both panels.



Sizes of F_1, F_2 and F_3 Powers of F_1, F_2 and F_3

Figure 4. The values of $\overline{\alpha}$ are denoted by the dashed lines in the left panel and the values of $1-\overline{\beta}$ are denoted by the dashed lines in the right panel for F_1, F_2 and F_3. The asymptotic powers were given by Power$(F_1) = 0.577$, Power$(F_2) = 0.823$ and Power$(F_3) = 0.963$ which were denoted by the solid lines in the right panel.

where f denotes a random variable distributed as F distribution with degrees of freedom, ν_1 and ν_2. Note that Power(F_2) and Power(F_3) give lower bounds of the asymptotic powers when $\tilde{h}_* = h^{-1}$ and $\tilde{\gamma}_* = \gamma^{-1}$.

In Figure 4, we summarized the findings obtained by averaging the outcomes from 4000 $(= R$, say) replications. Here, the first 2000 replications were generated by setting $\boldsymbol{\Sigma}_2 = \boldsymbol{\Sigma}_1$ as in (5.1) and the last 2000 replications were generated by setting $\boldsymbol{\Sigma}_2$ as in (5.2). Let F_{ir} $(i = 1, 2, 3)$ be the rth observation of F_i for $r = 1, ..., 4000$. We defined $P_r = 1$ (or 0) when H_0 was falsely rejected (or not) for $r = 1, ..., 2000$, and H_a was falsely rejected (or not) for $r = 2001, ..., 4000$. We defined $\overline{\alpha} = (R/2)^{-1}\sum_{r=1}^{R/2} P_r$ to estimate the size and $1 - \overline{\beta} = 1 - (R/2)^{-1}\sum_{r=R/2+1}^{R} P_r$ to estimate the power. Their standard deviations are less than 0.011. When d is not sufficiently large, we observed that the sizes of F_2 and F_3 are quite higher than α. This is probably because $\tilde{h}_*$ (≥ 1) and $\tilde{\gamma}_*$ (≥ 1) are much larger than 1. Actually, the sizes became close to α as d increases. When d is large, F_3 gave excellent performances both for the size and power.

Appendix A.

Throughout, let $\boldsymbol{P}_n = \boldsymbol{I}_n - \boldsymbol{1}_n\boldsymbol{1}_n^T/n$, where $\boldsymbol{1}_n = (1, ..., 1)^T$. Let $\boldsymbol{e}_n = (e_1, ..., e_n)^T$ be an arbitrary (random) n-vector such that $||\boldsymbol{e}_n|| = 1$ and $\boldsymbol{e}_n^T\boldsymbol{1}_n = 0$.

Proof of Proposition 2.1. We assume $\boldsymbol{\mu} = \mathbf{0}$ without loss of generality. We write that $\boldsymbol{X}^T\boldsymbol{X} = \sum_{s=1}^{i_*}\lambda_s\boldsymbol{z}_s\boldsymbol{z}_s^T + \sum_{s=i_*+1}^{d}\lambda_s\boldsymbol{z}_s\boldsymbol{z}_s^T$ for $i_* = 1$ when n is fixed, and for some fixed $i_*(\geq 1)$ when $n \to \infty$. Here, by using Markov's inequality, for any $\tau > 0$, under (A-ii) and (A-iii), we have that

$$P\Big\{\sum_{j=1}^{n}\Big(\sum_{s=i_*+1}^{d}\frac{\lambda_s(z_{sj}^2-1)}{n\lambda_1}\Big)^2 > \tau\Big\} \leq \frac{\sum_{r,s\geq 2}^{d}\lambda_r\lambda_s E\{(z_{rk}^2-1)(z_{sk}^2-1)\}}{\tau n\lambda_1^2} \to 0$$

$$\text{and } P\Big\{\sum_{j\neq j'}^{n}\Big(\sum_{s=i_*+1}^{d}\frac{\lambda_s z_{sj}z_{sj'}}{n\lambda_1}\Big)^2 > \tau\Big\} \leq \frac{\delta_{i_*}}{\tau\lambda_1^2} \to 0 \tag{A.1}$$

as $d \to \infty$ either when n is fixed or $n \to \infty$. Note that $\sum_{j=1}^{n} e_j^4 \leq 1$ and $\sum_{j\neq j'}^{n} e_j^2 e_{j'}^2 \leq 1$. Then, under (A-ii) and (A-iii), we have that

$$\begin{aligned}\Big|\sum_{j=1}^{n}e_j^2\sum_{s=i_*+1}^{d}\frac{\lambda_s(z_{sj}^2-1)}{n\lambda_1}\Big| &\leq \Big\{\sum_{j=1}^{n}e_j^4\Big\}^{1/2}\Big\{\sum_{j=1}^{n}\Big(\sum_{s=i_*+1}^{d}\frac{\lambda_s(z_{sj}^2-1)}{n\lambda_1}\Big)^2\Big\}^{1/2}\\ &= o_p(1) \quad \text{and}\\ \Big|\sum_{j\neq j'}^{n}e_je_{j'}\sum_{s=i_*+1}^{d}\frac{\lambda_s z_{sj}z_{sj'}}{n\lambda_1}\Big| &\leq \Big\{\sum_{j\neq j'}^{n}e_j^2e_{j'}^2\Big\}^{1/2}\Big\{\sum_{j\neq j'}^{n}\Big(\sum_{s=i_*+1}^{d}\frac{\lambda_s z_{sj}z_{sj'}}{n\lambda_1}\Big)^2\Big\}^{1/2}\\ &= o_p(1)\end{aligned}$$

as $d \to \infty$ either when n is fixed or $n \to \infty$. Thus, we claim that

$$\boldsymbol{e}_n^T\frac{\boldsymbol{X}^T\boldsymbol{X}}{(n-1)\lambda_1}\boldsymbol{e}_n = \boldsymbol{e}_n^T\frac{\sum_{s=1}^{i_*}\lambda_s\boldsymbol{z}_s\boldsymbol{z}_s^T}{(n-1)\lambda_1}\boldsymbol{e}_n + \frac{\kappa}{(n-1)\lambda_1} + o_p(1) \tag{A.2}$$

from the fact that $\sum_{s=i_*+1}^{d}\lambda_s/\{(n-1)\lambda_1\} = \kappa/\{(n-1)\lambda_1\} + o(1)$ when $n \to \infty$. Note that $\boldsymbol{e}_n^T\boldsymbol{P}_n = \boldsymbol{e}_n^T$ and $\boldsymbol{P}_n\boldsymbol{z}_s = \boldsymbol{z}_{os}$ for all s. Also, note that $\boldsymbol{z}_{os}^T\boldsymbol{z}_{os'}/n = o_p(1)$ for $s \neq s'$ as $n \to \infty$ from the fact that $E\{(\boldsymbol{z}_{os}^T\boldsymbol{z}_{os'}/n)^2\} = o(1)$ as $n \to \infty$. Then, by noting that $P(\lim_{d\to\infty}||\boldsymbol{z}_{o1}|| \neq 0) = 1$, $\liminf_{d\to\infty}\lambda_1/\lambda_2 > 1$ and $\boldsymbol{z}_{o1}^T\mathbf{1}_n = 0$, it holds that

$$\begin{aligned}\max_{\boldsymbol{e}_n}\Big\{\boldsymbol{e}_n^T\frac{\sum_{s=1}^{i_*}\lambda_s\boldsymbol{z}_s\boldsymbol{z}_s^T}{(n-1)\lambda_1}\boldsymbol{e}_n\Big\} &= \max_{\boldsymbol{e}_n}\Big\{\boldsymbol{e}_n^T\frac{\sum_{s=1}^{i_*}\lambda_s\boldsymbol{z}_{os}\boldsymbol{z}_{os}^T}{(n-1)\lambda_1}\boldsymbol{e}_n\Big\}\\ &= ||\boldsymbol{z}_{o1}/\sqrt{n-1}||^2 + o_p(1)\end{aligned} \tag{A.3}$$

as $d \to \infty$ either when n is fixed or $n \to \infty$. Note that $\hat{\boldsymbol{u}}_1^T \boldsymbol{1}_n = 0$ and $\hat{\boldsymbol{u}}_1^T \boldsymbol{P}_n = \hat{\boldsymbol{u}}_1^T$ when $\boldsymbol{S}_D \neq \boldsymbol{O}$. Then, from (A.2), (A.3) and $\boldsymbol{P}_n \boldsymbol{X}^T \boldsymbol{X} \boldsymbol{P}_n/(n-1) = \boldsymbol{S}_D$, under (A-ii) and (A-iii), we have that

$$\hat{\boldsymbol{u}}_1^T \frac{\boldsymbol{S}_D}{\lambda_1} \hat{\boldsymbol{u}}_1 = \hat{\boldsymbol{u}}_1^T \frac{\boldsymbol{X}^T \boldsymbol{X}}{(n-1)\lambda_1} \hat{\boldsymbol{u}}_1 = ||\boldsymbol{z}_{o1}/\sqrt{n-1}||^2 + \frac{\kappa}{(n-1)\lambda_1} + o_p(1) \quad \text{(A.4)}$$

as $d \to \infty$ either when n is fixed or $n \to \infty$. It concludes the result. □

Proof of Lemma 2.1. By using Markov's inequality, for any $\tau > 0$, under (A-ii) and (A-iii), we have that

$$\begin{aligned}
&P\Big\{\Big(\sum_{s=2}^{d} \frac{\lambda_s\{||\boldsymbol{z}_{os}||^2 - (n-1)\}}{(n-1)\lambda_1}\Big)^2 > \tau\Big\} \\
&= P\Big\{\Big(\sum_{s=2}^{d} \frac{\lambda_s\{(n-1)\sum_{k=1}^{n}(z_{sk}^2 - 1)/n - \sum_{k\neq k'}^{n} z_{sk}z_{sk'}/n\}}{(n-1)\lambda_1}\Big)^2 > \tau\Big\} \\
&= O\Big\{\frac{\sum_{r,s\geq 2}^{d} \lambda_r\lambda_s E\{(z_{rk}^2-1)(z_{sk}^2-1)\}}{n\lambda_1^2}\Big\} + O\{\delta_1/(n\lambda_1)^2\} \to 0
\end{aligned}$$

as $d \to \infty$ either when n is fixed or $n \to \infty$. Thus it holds that $\text{tr}(\boldsymbol{S}_D)/\lambda_1 = \kappa/\lambda_1 + ||\boldsymbol{z}_{o1}/\sqrt{n-1}||^2 + o_p(1)$ from the fact that $\text{tr}(\boldsymbol{S}_D) = \lambda_1||\boldsymbol{z}_{o1}||^2/(n-1) + \sum_{s=2}^{d} \lambda_s||\boldsymbol{z}_{os}||^2/(n-1)$. Then, from Proposition 2.1 and $\liminf_{d\to\infty} \kappa/\lambda_1 > 0$, we can claim the results. □

Proof of Theorem 2.1. When $n \to \infty$, we can claim the results from Theorems 4.1, 4.2 and Corollary 4.1 in Yata and Aoshima (2013). When n is fixed, we can claim the results from Theorem 3.1 and Corollary 3.1 in Ishii et al. (2014). □

Proof of Theorem 2.2. From Theorem 2.1 and Lemma 2.1, under (A-i) to (A-iii), it holds that

$$\begin{aligned}
&P\Big(\frac{\lambda_1}{\text{tr}(\boldsymbol{\Sigma})} \in \Big[\frac{(n-1)\tilde{\lambda}_1}{b\tilde{\kappa} + (n-1)\tilde{\lambda}_1}, \frac{(n-1)\tilde{\lambda}_1}{a\tilde{\kappa} + (n-1)\tilde{\lambda}_1}\Big]\Big) \\
&= P\Big(\frac{(n-1)\tilde{\lambda}_1}{b\tilde{\kappa} + (n-1)\tilde{\lambda}_1} \leq \frac{\lambda_1}{\text{tr}(\boldsymbol{\Sigma})} \leq \frac{(n-1)\tilde{\lambda}_1}{a\tilde{\kappa} + (n-1)\tilde{\lambda}_1}\Big) \\
&= P\Big(\frac{a\tilde{\kappa}}{(n-1)\tilde{\lambda}_1} \leq \frac{\kappa}{\lambda_1} \leq \frac{b\tilde{\kappa}}{(n-1)\tilde{\lambda}_1}\Big) = P\Big(a \leq (n-1)\frac{\tilde{\lambda}_1\kappa}{\lambda_1\tilde{\kappa}} \leq b\Big) \\
&= 1 - \alpha + o(1)
\end{aligned}$$

as $d \to \infty$ when n is fixed. It concludes the result. $\square$

Proof of Lemma 2.2. We write that

$$n||\bar{\boldsymbol{x}} - \boldsymbol{\mu}||^2 - \text{tr}(\boldsymbol{S}_D) = \sum_{s=1}^{d} \lambda_s \Big(n\bar{z}_s^2 - \sum_{j=1}^{n} \frac{(z_{sj} - \bar{z}_s)^2}{n-1} \Big).$$

Then, from (A.1) and $n\bar{z}_s^2 - \sum_{j=1}^{n}(z_{sj} - \bar{z}_s)^2/(n-1) = \sum_{j\neq j'}^{n} z_{sj}z_{sj'}/(n-1)$ for all s, under (A-ii), we have that

$$\{||\bar{\boldsymbol{x}} - \boldsymbol{\mu}||^2 - \text{tr}(\boldsymbol{S}_D)/n\}/\lambda_1 = \bar{z}_s^2 - ||\boldsymbol{z}_{o1}/\sqrt{n-1}||^2/n + o_p(1)$$

as $d \to \infty$ when n is fixed. It concludes the result. $\square$

Proof of Theorem 2.3. Under (A-i), we note that $\bar{z}_1$ and $\boldsymbol{z}_{o1}$ are independent, and $n\bar{z}_1^2$ is distributed as χ_1^2. Then, from Theorem 2.1 and Lemma 2.2, we can conclude the result. $\square$

Proofs of Lemmas 3.1 and 3.2. We note that $||\boldsymbol{z}_{o1}||^2/n = 1 + o_p(1)$ as $n \to \infty$. From (A.4), under (A-ii) and (A-iii), we have that

$$\hat{\boldsymbol{u}}_1^T\boldsymbol{z}_{o1}/||\boldsymbol{z}_{o1}|| = 1 + o_p(1) \tag{A.5}$$

as $d \to \infty$ either when n is fixed or $n \to \infty$, so that $\hat{\boldsymbol{u}}_1^T\boldsymbol{z}_{o1} = ||\boldsymbol{z}_{o1}|| + o_p(n^{1/2})$. Thus, we can claim the result of Lemma 3.2. On the other hand, with the help of Proposition 2.1, under (A-ii) and (A-iii), it holds that from (A.5)

$$\begin{aligned}\boldsymbol{h}_1^T\hat{\boldsymbol{h}}_1 = \frac{\boldsymbol{h}_1^T(\boldsymbol{X} - \overline{\boldsymbol{X}})\hat{\boldsymbol{u}}_1}{\{(n-1)\hat{\lambda}_1\}^{1/2}} = \frac{\lambda_1^{1/2}\boldsymbol{z}_{o1}^T\hat{\boldsymbol{u}}_1}{\{(n-1)\hat{\lambda}_1\}^{1/2}} &= \frac{||\boldsymbol{z}_{o1}|| + o_p(n^{1/2})}{\{||\boldsymbol{z}_{o1}||^2 + \kappa/\lambda_1 + o_p(n)\}^{1/2}} \\ &= \frac{1}{\{1 + \kappa/(\lambda_1||\boldsymbol{z}_{o1}||^2)\}^{1/2}} + o_p(1)\end{aligned}$$

as $d \to \infty$ either when n is fixed or $n \to \infty$. It concludes the result of Lemma 3.1. $\square$

Proof of Theorem 3.1. With the help of Theorem 2.1, under (A-ii) and (A-iii), we have that from (A.5)

$$\boldsymbol{h}_1^T\tilde{\boldsymbol{h}}_1 = \frac{\boldsymbol{h}_1^T(\boldsymbol{X} - \overline{\boldsymbol{X}})\hat{\boldsymbol{u}}_1}{\{(n-1)\tilde{\lambda}_1\}^{1/2}} = \frac{||\boldsymbol{z}_{o1}|| + o_p(n^{1/2})}{\{||\boldsymbol{z}_{o1}||^2 + o_p(n)\}^{1/2}} = 1 + o_p(1)$$

as $d \to \infty$ either when n is fixed or $n \to \infty$. It concludes the result. $\square$

Proof of Theorem 3.2. By combing Theorem 2.1 with Lemma 3.2, under (A-ii) and (A-iii), we have that

$$\tilde{s}_{1j}/\sqrt{\lambda_1} = \hat{u}_{1j}\sqrt{(n-1)\tilde{\lambda}_1/\lambda_1} = \hat{u}_{1j}||\boldsymbol{z}_{o1}|| + o_p(1) = z_{o1j} + o_p(1)$$

as $d \to \infty$ when n is fixed. By noting that $z_{o1j} = z_{1j} - \bar{z}_1$ and $\bar{z}_1$ is distributed as $N(0, 1/n)$ under (A-i), we have the results. $\square$

Proof of Corollary 4.1. From Theorem 2.1, the result is obtained straightforwardly. $\square$

Proof of Lemma 4.1. Let $\boldsymbol{Z}_i = [\boldsymbol{z}_{1(i)}, ..., \boldsymbol{z}_{d(i)}]^T$ be a sphered data matrix of π_i for $i = 1, 2$, where $\boldsymbol{z}_{j(i)} = (z_{j1(i)}, ..., z_{jn_i(i)})^T$. We assume $\boldsymbol{\mu}_1 = \boldsymbol{\mu}_2 = \boldsymbol{0}$ without loss of generality. Let $\beta_{st} = (\lambda_{s(1)}\lambda_{t(2)})^{1/2}\boldsymbol{h}_{s(1)}^T\boldsymbol{h}_{t(2)}$ for all s, t. Let $i_\star$ be a fixed constant such that $\sum_{s=i_\star+1}^d \lambda_{s(j)}^2/\lambda_{1(j)}^2 = o(1)$ as $d \to \infty$ for $j = 1, 2$. Note that $i_\star$ exists under (A-ii) for each π_i. We write that

$$\begin{aligned}\boldsymbol{X}_1^T\boldsymbol{X}_2 &= \sum_{s,t \le i_\star} \beta_{st}\boldsymbol{z}_{s(1)}\boldsymbol{z}_{t(2)}^T + \sum_{s,t \ge i_\star+1}^{d} \beta_{st}\boldsymbol{z}_{s(1)}\boldsymbol{z}_{t(2)}^T \\ &\quad + \sum_{s=i_\star+1}^{d}\sum_{t=1}^{i_\star} \beta_{st}\boldsymbol{z}_{s(1)}\boldsymbol{z}_{t(2)}^T + \sum_{s=1}^{i_\star}\sum_{t=i_\star+1}^{d} \beta_{st}\boldsymbol{z}_{s(1)}\boldsymbol{z}_{t(2)}^T.\end{aligned}$$

Note that

$$\begin{aligned}&E\Big\{\Big(\sum_{s=i_\star+1}^{d}\sum_{t=1}^{i_\star} \beta_{st}z_{sj(1)}z_{tj'(2)}\Big)^2\Big\} \\ &= \mathrm{tr}\Big(\sum_{s=i_\star+1}^{d} \lambda_{s(1)}\boldsymbol{h}_{s(1)}\boldsymbol{h}_{s(1)}^T \sum_{t=1}^{i_\star} \lambda_{t(2)}\boldsymbol{h}_{t(2)}\boldsymbol{h}_{t(2)}^T\Big) \le i_\star\lambda_{i_\star+1(1)}\lambda_{1(2)}\end{aligned}$$

for all j, j'. Also, note that

$$\begin{aligned}E\Big\{\Big(\sum_{s,t \ge i_\star+1}^{d} \beta_{st}z_{sj(1)}z_{tj'(2)}\Big)^2\Big\} &= \mathrm{tr}\Big(\sum_{s=i_\star+1}^{d} \lambda_{s(1)}\boldsymbol{h}_{s(1)}\boldsymbol{h}_{s(1)}^T \sum_{t=i_\star+1}^{d} \lambda_{t(2)}\boldsymbol{h}_{t(2)}\boldsymbol{h}_{t(2)}^T\Big) \\ &\le \Big(\sum_{s=i_\star+1}^{d} \lambda_{s(1)}^2 \sum_{t=i_\star+1}^{d} \lambda_{t(2)}^2\Big)^{1/2}\end{aligned}$$

for all j, j'. Then, by using Markov's inequality, for any $\tau > 0$, under (A-ii) for each π_i, we have that

$$P\Big\{\sum_{j=1}^{n_1}\sum_{j'=1}^{n_2}\Big(\sum_{s=i_\star+1}^{d}\sum_{t=1}^{i_\star}\frac{\beta_{st}z_{sj(1)}z_{tj'(2)}}{(n_1n_2\lambda_{1(1)}\lambda_{1(2)})^{1/2}}\Big)^2 > \tau\Big\} \to 0,$$

$$P\Big\{\sum_{j=1}^{n_1}\sum_{j'=1}^{n_2}\Big(\sum_{s=1}^{i_\star}\sum_{t=i_\star+1}^{d}\frac{\beta_{st}z_{sj(1)}z_{tj'(2)}}{(n_1n_2\lambda_{1(1)}\lambda_{1(2)})^{1/2}}\Big)^2 > \tau\Big\} \to 0$$

$$\text{and } P\Big\{\sum_{j=1}^{n_1}\sum_{j'=1}^{n_2}\Big(\sum_{s,t\ge i_\star+1}^{d}\frac{\beta_{st}z_{sj(1)}z_{tj'(2)}}{(n_1n_2\lambda_{1(1)}\lambda_{1(2)})^{1/2}}\Big)^2 > \tau\Big\} \to 0$$

as $d \to \infty$ either when n_i is fixed or $n_i \to \infty$ for $i = 1, 2$. Hence, similar to (A.2), it holds that

$$\frac{\boldsymbol{e}_{n_1}^T\boldsymbol{X}_1^T\boldsymbol{X}_2\boldsymbol{e}_{n_2}}{(\nu_1\nu_2\lambda_{1(1)}\lambda_{1(2)})^{1/2}} = \frac{\boldsymbol{e}_{n_1}^T\sum_{s,t\le i_\star}\beta_{st}\boldsymbol{z}_{s(1)}\boldsymbol{z}_{t(2)}^T\boldsymbol{e}_{n_2}}{(\nu_1\nu_2\lambda_{1(1)}\lambda_{1(2)})^{1/2}} + o_p(1).$$

Note that $\boldsymbol{e}_{n_i}^T\boldsymbol{P}_{n_i} = \boldsymbol{e}_{n_i}^T$ and $\boldsymbol{P}_{n_i}\boldsymbol{z}_{1(i)} = \boldsymbol{z}_{o1(i)}$ for $i = 1, 2$, where $\boldsymbol{z}_{o1(i)} = \boldsymbol{z}_{1(i)} - (\bar{z}_{1(i)}, ..., \bar{z}_{1(i)})^T$ and $\bar{z}_{1(i)} = n_i^{-1}\sum_{k=1}^{n_i} z_{1k(i)}$. Also, note that $\boldsymbol{X}_i\boldsymbol{P}_{n_i} = (\boldsymbol{X}_i - \overline{\boldsymbol{X}}_i)$ for $i = 1, 2$, where $\overline{\boldsymbol{X}}_i = [\bar{\boldsymbol{x}}_i, ..., \bar{\boldsymbol{x}}_i]$ and $\bar{\boldsymbol{x}}_i = \sum_{j=1}^{n_i}\boldsymbol{x}_{j(i)}/n_i$. Let $\hat{\boldsymbol{u}}_{1(i)}$ be the first (unit) eigenvector of $(\boldsymbol{X}_i - \overline{\boldsymbol{X}}_i)^T(\boldsymbol{X}_i - \overline{\boldsymbol{X}}_i)$ for $i = 1, 2$. Note that $\hat{\boldsymbol{u}}_{1(i)}^T\boldsymbol{P}_{n_i} = \hat{\boldsymbol{u}}_{1(i)}^T$ when $(\boldsymbol{X}_i - \overline{\boldsymbol{X}}_i)^T(\boldsymbol{X}_i - \overline{\boldsymbol{X}}_i) \neq \boldsymbol{O}$ for $i = 1, 2$. Then, under (A-ii) for each π_i, we have that

$$\frac{\hat{\boldsymbol{u}}_{1(1)}^T(\boldsymbol{X}_1 - \overline{\boldsymbol{X}}_1)^T(\boldsymbol{X}_2 - \overline{\boldsymbol{X}}_2)\hat{\boldsymbol{u}}_{1(2)}}{(\nu_1\nu_2\lambda_{1(1)}\lambda_{1(2)})^{1/2}} = \frac{\hat{\boldsymbol{u}}_{1(1)}^T\sum_{s,t\le i_\star}\beta_{st}\boldsymbol{z}_{os(1)}\boldsymbol{z}_{ot(2)}^T\hat{\boldsymbol{u}}_{1(2)}}{(\nu_1\nu_2\lambda_{1(1)}\lambda_{1(2)})^{1/2}} + o_p(1) \tag{A.6}$$

as $d \to \infty$ either when n_i is fixed or $n_i \to \infty$ for $i = 1, 2$. Note that $\tilde{\boldsymbol{h}}_{1(i)} = \{\nu_i\tilde{\lambda}_{1(i)}\}^{-1/2}(\boldsymbol{X}_i - \overline{\boldsymbol{X}}_i)\hat{\boldsymbol{u}}_{1(i)}$ for $i = 1, 2$. Also, note that $\boldsymbol{z}_{os(i)}^T\boldsymbol{z}_{os'(i)}/n_i = o_p(1)$ $(s \neq s')$ when $n_i \to \infty$ for $i = 1, 2$. Then, by combining (A.6) with Theorem 2.1 and (A.5), we can claim the result. □

Proofs of Theorems 4.1 and 4.2. By combining Theorem 2.1, Lemmas 2.1 and 4.1, we can claim the results. □

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