

Least Favorable Direction Test for Multivariate Analysis of Variance in High Dimension

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Abstract: This ~~paper~~ ^{study} considers ~~the problem of~~ multivariate ^{a high-dimensional} analysis of variance for normal samples in ~~the high dimension~~ medium sample size setting. When the sample dimension is larger than the sample size, the classical likelihood ratio test is not defined ^{, because} ~~since~~ the likelihood function is unbounded. Based on ~~the~~ ^{this} unboundedness ~~of the likelihood function~~, we propose a new test called the least favorable direction test. The asymptotic distributions of the test statistic are derived ^{for} ~~under~~ both nonspiked and spiked covariances. The local asymptotic power function of the test is also given. ^{results for the} The ~~asymptotic~~ power function and simulations show that the proposed test is particularly powerful under ^a ~~spiked~~ covariance.

Note 1

Key words and phrases: High dimensional data, least favorable direction test, multivariate analysis of variance, principal component analysis, spiked covariance.

1. Introduction

Suppose there are k ($k \geq 2$) independent samples of p -dimensional data. Within the i th sample ($1 \leq i \leq k$), the observations $\{X_{ij}\}_{j=1}^{n_i}$ are independent and identically distributed (i.i.d.) as $\mathcal{N}_p(\theta_i, \Sigma)$, which is a normal distribution with mean vector θ_i and common variance matrix Σ . We would like to test the following hypotheses:

$$H_0 : \theta_1 = \theta_2 = \cdots = \theta_k \quad \text{vs.} \quad H_1 : \theta_i \neq \theta_j \text{ for some } i \neq j. \quad (1.1)$$

This testing problem is known as a one-way multivariate analysis of variance (MANOVA) and has been well studied when p is small relative to N , where $N = \sum_{i=1}^k n_i$ is the total sample size.

Let $\mathbf{H} = \sum_{i=1}^k n_i (\bar{\mathbf{X}}_i - \bar{\mathbf{X}})(\bar{\mathbf{X}}_i - \bar{\mathbf{X}})^\top$ be the sum-of-squares between groups, and let $\mathbf{G} = \sum_{i=1}^k \sum_{j=1}^{n_i} (X_{ij} - \bar{\mathbf{X}}_i)(X_{ij} - \bar{\mathbf{X}}_i)^\top$ be the sum-of-squares within groups, where $\bar{\mathbf{X}}_i = n_i^{-1} \sum_{j=1}^{n_i} X_{ij}$ is the sample mean of group i and $\bar{\mathbf{X}} = N^{-1} \sum_{i=1}^k \sum_{j=1}^{n_i} X_{ij}$ is the pooled sample mean. There are four classical test statistics for hypotheses (1.1), all of which are based on the eigenvalues of $\mathbf{H}\mathbf{G}^{-1}$.

Wilks' Lambda:	$ \mathbf{G} + \mathbf{H} / \mathbf{G} $
Pillai trace:	$\text{tr}[\mathbf{H}(\mathbf{G} + \mathbf{H})^{-1}]$
(En-dash) Hotelling-Lawley trace:	$\text{tr}[\mathbf{H}\mathbf{G}^{-1}]$
Roy's maximum root:	$\lambda_1(\mathbf{H}\mathbf{G}^{-1})$

In some modern scientific applications, ~~people~~ ^{researchers} would like to test hypotheses (1.1) in ^a ~~high~~ ^{that is, where} dimensional setting, ~~i.e.,~~ ^{; see, for example,} ~~p is greater than N .~~ ~~See,~~ ^{none of the four classical test statistics are defined} ~~e.g.,~~ Verstyne et al. (2005) and Tsai and Chen (2009). However, ^{when} ~~$p \geq N$, the four classical test statistics are all not defined. Researchers~~ ^{. As a result, extensive research has been done on} ~~have done extensive work to study~~ the testing problem (1.1) in ^{high} ~~di-~~ ^{settings. Thus} ~~mensional setting.~~ So far, numerous tests have been proposed for the case ^{; see, for example,} ~~$k = 2$.~~ ~~See, e.g.,~~ Bai and Saranadasa (1996), Srivastava (2007), Chen and Qin (2010), Cai et al. (2014), ^{Tests} ~~and~~ ^{Some tests} ~~and~~ Feng et al. (2015). ^{proposed} ~~Some tests~~ have also been ^{general} ~~introduced~~ for the ^{general} ~~case of~~ ~~$k \geq 2$.~~ Schott (2007) modified ^{the} ~~the~~ Hotelling's Lawley trace and proposed the ^{following} ~~test statistic~~:

$$T_{Sc} = \frac{1}{\sqrt{N-1}} \left(\frac{1}{k-1} \text{tr}(\mathbf{H}) - \frac{1}{N-k} \text{tr}(\mathbf{G}) \right).$$

^{Here,} ~~Statistic~~ T_{Sc} is a ^{member} ~~representative~~ of the so-called sum-of-squares ^{the} ~~type~~ statistics ^{, because} ~~as~~ it is based on an estimation of ^{the} ~~squared~~ Euclidean norm $\sum_{i=1}^k n_i \|\theta_i - \bar{\theta}\|^2$, where $\bar{\theta} = N^{-1} \sum_{i=1}^k n_i \theta_i$. See Srivastava and Kubokawa (2013), Yamada and Himeno (2015), Hu et al. (2017), Zhang et al. (2017), Zhou et al. (2017), ^{Sum-of-squares} ~~and~~ ^{known to be} ~~and~~ Cao et al. (2019) for ~~some~~ other sum-of-squares ^{in the case of} ~~type~~ test statistics for ~~general~~ $k \geq 2$. ~~It is known that the sum of squares type tests are~~ ^{against} ~~particularly powerful~~ dense alternatives. In another work, Cai and

Xia (2014) proposed ~~a~~ ^{the} test statistic

$$T_{CX} = \max_{1 \leq i \leq p} \sum_{1 \leq j < l \leq k} \frac{n_j n_l}{n_j + n_l} \frac{(\Omega(\bar{\mathbf{X}}_j - \bar{\mathbf{X}}_l))_i^2}{\omega_{ii}},$$

where $\Omega = (\omega)_{ij} = \Sigma^{-1}$ is the precision matrix. When Ω is unknown, it is substituted by an estimator. Unlike T_{Sc} , ~~the test statistic~~ T_{CX} is an extreme ^{test statistic,} ~~value type one~~ ^{in the case of} and is ~~very~~ powerful ~~against~~ sparse alternatives.

Most existing sum-of-squares ~~type~~ test procedures require the condition $\text{tr}(\Sigma^4)/\text{tr}^2(\Sigma^2) \rightarrow 0$, which is equivalent to

$$\frac{\lambda_1}{\sqrt{\text{tr}(\Sigma^2)}} \rightarrow 0, \quad (1.2)$$

where λ_i is the i th largest eigenvalue of Σ , ^{for} $i = 1, \dots, p$. In fact, the ^{following} equivalence of these two conditions can be seen from the [:] inequalities

$$\frac{\lambda_1^4}{\text{tr}^2(\Sigma^2)} \leq \frac{\text{tr}(\Sigma^4)}{\text{tr}^2(\Sigma^2)} \leq \frac{\lambda_1^2 \text{tr}(\Sigma^2)}{\text{tr}^2(\Sigma^2)} = \frac{\lambda_1^2}{\text{tr}(\Sigma^2)}.$$

Condition (1.2) is reasonable if Σ is nonspiked [,] in the sense that it does not have significantly large eigenvalues. ~~In some important situations, however,~~ ^{However, in practice,} ~~variables are~~ ^{may be} heavily correlated with common factors, ~~and~~ ^{in which case,} the covariance matrix Σ is ~~thus~~ [,] spiked [,] in the sense that a few eigenvalues of Σ are significantly larger than the others (Fan et al., 2013; Cai et al., 2015; Wang and Fan, 2017). In such cases, condition (1.2) can be violated, ~~and~~ ^{and,} consequently, existing sum-of-squares type tests may not have ^{the} correct level. ~~Some~~ ^{Adjusted}

~~adjusted~~ sum-of-squares ~~type~~ test procedures have been proposed to solve ~~this~~ ^{; see, for example,} ~~the~~ problem. ~~See, e.g.,~~ Katayama et al. (2013), Ma et al. (2015), Zhang et al. (2017) and Wang and Xu (2019). However, the power behavior of these corrected tests may not be satisfactory.

Recently, Aoshima and Yata (2018) and Wang and Xu (2018) considered ^a ~~two~~ ^a ~~sample~~ mean testing problem under ~~the~~ ^{than that of} spiked covariance model. These tests have better power behavior ~~compared with~~ ^{studies} sum-of-squares ~~type~~ tests. However, both ~~papers~~ imposed strong conditions on the magnitude of p . For example, under the approximate factor model in Fan et al. (2013), the test in Aoshima and Yata (2018) requires $p/n \rightarrow 0$, ^{whereas} ~~while~~ the test in Wang and Xu (2018) requires that $p/n^2 \rightarrow 0$ and ^{that} ~~the~~ small eigenvalues of Σ are all equal.

The likelihood ratio test (LRT) method has been very successful in leading to satisfactory procedures in many specific problems. However, the LRT statistic for hypotheses (1.1), ^{that is,} ~~i.e.~~ ^{lambda} Wilks' ~~Lambda~~ statistic, is not defined for $p > N - k$. In ^a ~~high~~ ^{neither the} dimensional setting, ~~both~~ ^a sum-of-squares ~~type statistics and~~ ^{nor the} extreme value ~~type~~ statistics are ~~not~~ based on ^a likelihood function. This motivates us to construct a likelihood-based test in ^a ~~high~~ dimensional setting. In a recent work, Zhao and Xu (2016) proposed a generalized likelihood ratio test in the context of ^a ~~one~~ ^a ~~sample~~ mean vector test.

They used a least favorable argument to construct a generalized likelihood ratio test statistic. Their simulation results showed that their test ~~has~~ ^{exhibits} good power performance, especially when the variables are correlated. However, ~~this phenomenon is not theoretically proved.~~ ^{they do not provide a theoretical proof}

~~We~~
~~In this paper, we~~ propose a generalized likelihood ratio test statistic for hypotheses (1.1), ^{the} ~~called~~ least favorable direction (LFD) test statistic, which is a generalization of the test in Zhao and Xu (2016). We give the asymptotic distributions of the test statistic under both nonspiked and spiked covariances. An adaptive LFD test procedure is constructed by consistently detecting ^{the} ~~unknown~~ covariance structure and estimating ^{the} ~~unknown~~ parameters. The asymptotic local power function of the LFD test is also given. Our theoretical results show that the LFD test is particularly powerful under ^a ~~the~~ spiked covariance. This explains the simulation results of Zhao and Xu (2016). ^{Extending} ~~Compared with~~ the work of Zhao and Xu (2016), our main contribution is that we ^{provide} ~~give~~ a thorough theoretical analysis of the LFD test. ^{This} ~~Our~~ ^{falls within a high-dimensional} ~~theoretical analysis fall into the high dimension~~ medium sample size setting, where both $n, p \rightarrow \infty$, but $p/n \rightarrow \infty$ (see Aoshima et al. (2018), Section 5). To prove our main results, we carefully study the high-order asymptotic behavior of the eigenvalues and eigenspaces of the sample covariance matrix. These results are also of independent ^{interest} ~~interests~~. We further compare

the proposed test procedure with existing tests ~~by~~ ^{using} simulations. ~~It is shown~~ ^{Here, we show} that the LFD test ~~has comparable~~ ^{exhibits comparable with that of} behavior ~~to~~ ^{compared} existing sum-of-squares tests under ~~the~~ ^a nonspiked covariance, while significantly ~~outperforms~~ ^{outperforming} competing tests under ~~the~~ ^a spiked covariance.

The rest of the paper is organized as follows. In Section 2, we propose the LFD test statistic and derive its explicit forms. The asymptotic distributions of the LFD test statistic under ~~both~~ nonspiked and spiked covariances are given in Section 3. Based on these theoretical results, an adaptive LFD test procedure is proposed. Section 4 complements our study with numerical simulations. ~~In Section 5, we give a short discussion.~~ ^{concludes the paper} Finally, the proofs are gathered in the ~~supplementary material.~~ ^{Supplementary Material}

2. Least favorable direction test

~~We introduce some notations.~~ ^{first introduce some necessary notation} Define the $p \times N$ pooled sample matrix \mathbf{X} as

$$\mathbf{X} = (X_{11}, X_{12}, \dots, X_{1n_1}, X_{21}, X_{22}, \dots, X_{2n_2}, \dots, X_{k1}, X_{k2}, \dots, X_{kn_k}).$$

The sum-of-squares within groups \mathbf{G} can be written as $\mathbf{G} = \mathbf{X}(\mathbf{I}_N - \mathbf{J}\mathbf{J}^\top)\mathbf{X}^\top$,

where

$$\mathbf{J} = \begin{pmatrix} \frac{1}{\sqrt{n_1}}\mathbf{1}_{n_1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \frac{1}{\sqrt{n_2}}\mathbf{1}_{n_2} & \mathbf{0} \\ \vdots & \vdots & \vdots \\ \mathbf{0} & \mathbf{0} & \frac{1}{\sqrt{n_k}}\mathbf{1}_{n_k} \end{pmatrix}$$

is an $N \times k$ matrix and $\mathbf{1}_{n_i}$ is an n_i -dimensional vector with all elements equal to $\frac{1}{\sqrt{n_i}}$, $i = 1, \dots, k$. Let $n = N - k$ be the degrees of freedom of \mathbf{G} .

Construct an $N \times n$ matrix $\tilde{\mathbf{J}}$ as

$$\tilde{\mathbf{J}} = \begin{pmatrix} \tilde{\mathbf{J}}_1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \tilde{\mathbf{J}}_2 & \mathbf{0} \\ \vdots & \vdots & \vdots \\ \mathbf{0} & \mathbf{0} & \tilde{\mathbf{J}}_k \end{pmatrix},$$

where $\tilde{\mathbf{J}}_i$ is an $n_i \times (n_i - 1)$ matrix defined as

$$\tilde{\mathbf{J}}_i = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \cdots & \frac{1}{\sqrt{(n_i-2)(n_i-1)}} & \frac{1}{\sqrt{(n_i-1)n_i}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \cdots & \frac{1}{\sqrt{(n_i-2)(n_i-1)}} & \frac{1}{\sqrt{(n_i-1)n_i}} \\ 0 & -\frac{2}{\sqrt{6}} & \cdots & \vdots & \vdots \\ \vdots & \vdots & \cdots & -\frac{n_i-2}{\sqrt{(n_i-2)(n_i-1)}} & \frac{1}{\sqrt{(n_i-1)n_i}} \\ 0 & 0 & \cdots & 0 & -\frac{n_i-1}{\sqrt{(n_i-1)n_i}} \end{pmatrix}.$$

The matrix $\tilde{\mathbf{J}}$ is a column orthogonal matrix satisfying $\tilde{\mathbf{J}}^\top \tilde{\mathbf{J}} = \mathbf{I}_n$ and $\tilde{\mathbf{J}}\tilde{\mathbf{J}}^\top = \mathbf{I}_N - \mathbf{J}\mathbf{J}^\top$. Define $\mathbf{Y} = \mathbf{X}\tilde{\mathbf{J}}$. Then \mathbf{G} can be written as

$$\mathbf{G} = \mathbf{Y}\mathbf{Y}^\top.$$

The sum-of-squares between groups \mathbf{H} can be written as

$$\mathbf{H} = \mathbf{X}(\mathbf{J}\mathbf{J}^\top - \frac{1}{N}\mathbf{1}_N\mathbf{1}_N^\top)\mathbf{X}^\top = \mathbf{X}\mathbf{J}(\mathbf{I}_k - \frac{1}{N}\mathbf{J}^\top\mathbf{1}_N\mathbf{1}_N^\top\mathbf{J})\mathbf{J}^\top\mathbf{X}^\top.$$

By some matrix algebra, we have $\mathbf{I}_k - N^{-1}\mathbf{J}^\top\mathbf{1}_N\mathbf{1}_N^\top\mathbf{J} = \mathbf{C}\mathbf{C}^\top$ where \mathbf{C} is a $k \times (k-1)$ matrix defined as $\mathbf{C} = \mathbf{C}_1\mathbf{C}_2$, and

$$\mathbf{C}_1 = \begin{pmatrix} \sqrt{n_1} & \sqrt{n_1} & \cdots & \sqrt{n_1} & \sqrt{n_1} \\ -\frac{n_1}{\sqrt{n_2}} & \sqrt{n_2} & \cdots & \sqrt{n_2} & \sqrt{n_2} \\ 0 & -\frac{n_1+n_2}{\sqrt{n_3}} & \cdots & \vdots & \vdots \\ \vdots & \vdots & \cdots & -\frac{\sum_{i=1}^{k-2} n_i}{\sqrt{n_{k-1}}} & \sqrt{n_{k-1}} \\ 0 & 0 & \cdots & 0 & -\frac{\sum_{i=1}^{k-1} n_i}{\sqrt{n_k}} \end{pmatrix},$$

$$\mathbf{C}_2 = \begin{pmatrix} \frac{n_1(n_1+n_2)}{n_2} & 0 & \cdots & 0 \\ 0 & \frac{(\sum_{i=1}^2 n_i)(\sum_{i=1}^3 n_i)}{n_3} & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & \frac{(\sum_{i=1}^{k-1} n_i)(\sum_{i=1}^k n_i)}{n_k} \end{pmatrix}^{-\frac{1}{2}}.$$

Then \mathbf{H} can be written as

$$\mathbf{H} = \mathbf{X}\mathbf{J}\mathbf{C}\mathbf{C}^\top\mathbf{J}^\top\mathbf{X}^\top.$$

Define $\Theta = (\sqrt{n_1}\theta_1, \dots, \sqrt{n_k}\theta_k)$. Then, the null hypothesis H_0 is equivalent to $\Theta\mathbf{C} = \mathbf{O}_{p \times (k-1)}$, where $\mathbf{O}_{p \times (k-1)}$ is a $p \times (k-1)$ matrix with all entries zero.

Thus, the hypotheses (1.1) are equivalent to

$$H_0 : \Theta\mathbf{C} = \mathbf{O}_{p \times (k-1)} \quad \text{vs.} \quad H_1 : \Theta\mathbf{C} \neq \mathbf{O}_{p \times (k-1)}.$$

The In low dimensional setting, the testing problem (1.1) is well studied. A classical test statistic is Roy's maximum root, which is constructed by Roy (1953) using his well-known union intersection principle. The key idea is to decompose data \mathbf{X} into a set of univariate data $\{\mathbf{X}_a = a^\top \mathbf{X} : a \in \mathbb{R}^p, a^\top a = 1\}$. This induces a decomposition of the null hypothesis and the alternative hypotheses hypothesis:

$$H_0 = \bigcap_{a \in \mathbb{R}^p, a^\top a = 1} H_{0a} \quad \text{vs.} \quad H_1 = \bigcup_{a \in \mathbb{R}^p, a^\top a = 1} H_{1a},$$

where $H_{0a} : a^\top \Theta\mathbf{C} = \mathbf{O}_{1 \times (k-1)}$ and $H_{1a} : a^\top \Theta\mathbf{C} \neq \mathbf{O}_{1 \times (k-1)}$. Let $L_0(a)$ and $L_1(a)$ be the maximum likelihood of \mathbf{X}_a under H_{0a} and H_{1a} , respectively.

For each a satisfying $a^\top a = 1$, the component LRT statistic

$$\frac{L_1(a)}{L_0(a)} = \left(\frac{a^\top (\mathbf{G} + \mathbf{H})a}{a^\top \mathbf{G}a} \right)^{N/2}$$

can be used to test H_{0a} versus H_{1a} . Using the union intersection principle, Roy proposed the test statistic $\max_{a^\top a = 1} L_1(a)/L_0(a) = (1 + \lambda_1(\mathbf{H}\mathbf{G}^{-1}))^{N/2}$, where $\lambda_i(\cdot)$ denotes the i th largest eigenvalue. This statistic is an increasing function of Roy's maximum root.

From a likelihood point of view, ~~the~~ log likelihood ratio is an estimator of the Kullback-Leibler divergence between the true distribution and the null distribution. Hence, the component LRT statistic $L_1(a)/L_0(a)$ characterizes the discrepancy between the true ~~distribution~~ and the null distribution along the direction a . This motivates us to consider the direction

$$a^* = \arg \max_{a^\top a = 1} \frac{L_1(a)}{L_0(a)}, \quad (2.1)$$

which ~~can~~ hopefully ~~achieve~~ yields the largest discrepancy between the true ~~distribution~~ and the null distribution. Thus, H_{0a^*} is the component null hypothesis ~~most~~ least likely to be ~~not~~ true. We ~~shall~~ call a^* the least favorable direction.

Note that

~~Roy's maximum root is in fact~~ the component LRT statistic along the least favorable direction.

Unfortunately, Roy's maximum root can only be defined when $n \geq p$, and hence cannot ~~be used in~~ a high-dimensional setting. In what follows, we assume $p > n$. In this case, the set

$$\mathcal{A} \stackrel{\text{def}}{=} \{a : L_1(a) = +\infty, a^\top a = 1\} = \{a : a^\top \mathbf{G}a = 0, a^\top a = 1\}$$

~~is not empty since~~ ~~because~~ \mathbf{G} is singular. Consequently, the right hand side of (2.1) is not well defined ~~since~~ ~~because~~ the ratio involves infinity. Hence, we need a new definition for ~~the~~ ~~a~~ LFD in high-dimensional setting. Define

$$\mathcal{B} = \{a : L_0(a) = +\infty, a^\top a = 1\} = \{a : a^\top (\mathbf{G} + \mathbf{H})a = 0, a^\top a = 1\}.$$

Note

~~It can be seen~~ that $\mathcal{B} \subset \mathcal{A}$. Moreover, by the independence of \mathbf{G} and \mathbf{H} , with probability ~~1~~^{one}, we have $\mathcal{A} \cap \mathcal{B}^c \neq \emptyset$. Then[,] for any direction a , there are three possible scenarios: $L_1(a) < +\infty$ and $L_0(a) < +\infty$; $L_1(a) = +\infty$ and $L_0(a) < +\infty$; ^{and} $L_1(a) = +\infty$ and $L_0(a) = +\infty$. To ~~maximize~~^{maximize} the discrepancy between $L_1(a)$ and $L_0(a)$, one may consider the direction ~~a~~ ^{a} such that $L_1(a) = +\infty$ and $L_0(a) < +\infty$. This suggests that the least favorable direction a^* , which hopefully maximizes the discrepancy between $L_1(a)$ and $L_0(a)$, should be defined as $a^* = \arg \min_{a \in \mathcal{A} \cap \mathcal{B}^c} L_0(a)$. Equivalently,

$$a^* = \arg \min_{a \in \mathcal{A} \cap \mathcal{B}^c} L_0(a) = \arg \max_{a^\top a=1, a^\top \mathbf{G} a=0} a^\top \mathbf{H} a.$$

Based on a^* and the likelihood $L_0(a)$, we propose a new test statistic[,]

$$T(\mathbf{X}) = a^{*T} \mathbf{H} a^* = \max_{a^\top a=1, a^\top \mathbf{G} a=0} a^\top \mathbf{H} a.$$

^{sufficiently}

The null hypothesis is rejected when $T(\mathbf{X})$ is ~~large enough~~^{sufficiently}. We ~~shall~~ call $T(\mathbf{X})$ the LFD test statistic. ^{Because} ~~Since~~ the least favorable direction a^* is obtained from the component likelihood function, the statistic $T(\mathbf{X})$ is also a generalized likelihood ratio test statistic.

Now[,] we derive the explicit forms of the LFD test statistic. Let $\mathbf{Y} = \mathbf{U}_\mathbf{Y} \mathbf{D}_\mathbf{Y} \mathbf{V}_\mathbf{Y}^\top$ be the singular value decomposition of \mathbf{Y} , where $\mathbf{U}_\mathbf{Y}$ and $\mathbf{V}_\mathbf{Y}$ are $p \times \min(n, p)$ and $n \times \min(n, p)$ column orthogonal matrices, respectively, and $\mathbf{D}_\mathbf{Y}$ is a $\min(n, p) \times \min(n, p)$ diagonal matrix ^{, with} ~~whose~~ diagonal elements

comprising

are the non-increasingly ordered singular values of \mathbf{Y} . If $p > n$, let $\mathbf{P}_\mathbf{Y} =$

$\mathbf{U}_\mathbf{Y}\mathbf{U}_\mathbf{Y}^\top$ be the projection matrix onto the column space of \mathbf{Y} . Then, Lemma

1 in ~~the Supplementary Material~~ implies that, for $p > n$,

$$T(\mathbf{X}) = \lambda_1(\mathbf{C}^\top \mathbf{J}^\top \mathbf{X}^\top (\mathbf{I}_p - \mathbf{P}_\mathbf{Y}) \mathbf{X} \mathbf{J} \mathbf{C}). \quad (2.2)$$

Although

~~While~~ (2.2) is convenient for theoretical analysis, it is not convenient for computation. When $p > N$, another simple form of $T(\mathbf{X})$ can be used for computation. If $p > N$, then $\mathbf{X}^\top \mathbf{X}$ is invertible. By the relationship

$$\begin{aligned} \begin{pmatrix} \mathbf{J}^\top \mathbf{X}^\top \mathbf{X} \mathbf{J} & \mathbf{J}^\top \mathbf{X}^\top \mathbf{X} \tilde{\mathbf{J}} \\ \tilde{\mathbf{J}}^\top \mathbf{X}^\top \mathbf{X} \mathbf{J} & \tilde{\mathbf{J}}^\top \mathbf{X}^\top \mathbf{X} \tilde{\mathbf{J}} \end{pmatrix}^{-1} &= \left(\begin{pmatrix} \mathbf{J}^\top \\ \tilde{\mathbf{J}}^\top \end{pmatrix} \mathbf{X}^\top \mathbf{X} \begin{pmatrix} \mathbf{J} & \tilde{\mathbf{J}} \end{pmatrix} \right)^{-1} \\ &= \begin{pmatrix} \mathbf{J}^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{J} & \mathbf{J}^\top (\mathbf{X}^\top \mathbf{X})^{-1} \tilde{\mathbf{J}} \\ \tilde{\mathbf{J}}^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{J} & \tilde{\mathbf{J}}^\top (\mathbf{X}^\top \mathbf{X})^{-1} \tilde{\mathbf{J}} \end{pmatrix} \end{aligned}$$

the and matrix inverse formula, we have that

$$\begin{aligned} (\mathbf{J}^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{J})^{-1} &= \mathbf{J}^\top \mathbf{X}^\top \mathbf{X} \mathbf{J} - \mathbf{J}^\top \mathbf{X}^\top \mathbf{X} \tilde{\mathbf{J}} (\tilde{\mathbf{J}}^\top \mathbf{X}^\top \mathbf{X} \tilde{\mathbf{J}})^{-1} \tilde{\mathbf{J}}^\top \mathbf{X}^\top \mathbf{X} \mathbf{J} \\ &= \mathbf{J}^\top \mathbf{X}^\top (\mathbf{I}_p - \mathbf{P}_\mathbf{Y}) \mathbf{X} \mathbf{J}. \end{aligned}$$

Thus,

$$T(\mathbf{X}) = \lambda_1(\mathbf{C}^\top (\mathbf{J}^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{J})^{-1} \mathbf{C}). \quad (2.3)$$

Compared with (2.2), the expression (2.3) ~~doesn't~~ involve $\mathbf{P}_\mathbf{Y}$ and is more convenient for computation.

In the case of $k = 2$, it can be seen that the least favorable direction is proportional to $(\mathbf{I}_p - \mathbf{P}_Y)(\bar{\mathbf{X}}_1 - \bar{\mathbf{X}}_2)$ and the LFD test statistic has expression

$$T(\mathbf{X}) = \frac{n_1 n_2}{n_1 + n_2} \|(\mathbf{I}_p - \mathbf{P}_Y)(\bar{\mathbf{X}}_1 - \bar{\mathbf{X}}_2)\|^2.$$

In this case, the least favorable direction coincides with the maximal data piling direction proposed by Ahn and Marron (2010).

3. Theoretical analysis

We now ~~turn to the analysis of~~ the asymptotic distributions of the LFD test statistic. The normality of the observations is an important assumption for our results, ~~and will be~~ ^{is} assumed throughout this section. We ~~shall give~~ ^{present} theoretical results ~~under~~ ^{for} both nonspiked and spiked covariances. Based on these results, ~~an~~ ^{we construct} adaptive test with ~~asymptotically correct level~~ ^{an} ~~can be~~ ^{In addition} constructed. ~~Also,~~ ^{the} these results allow us to derive the local asymptotic power function of LFD test.

3.1 Nonspiked covariance

In this subsection, we establish the asymptotic distribution of $T(\mathbf{X})$ under ~~a~~ ^a the nonspiked covariance. Let \mathbf{W}_{k-1} be a $(k-1) \times (k-1)$ symmetric random matrix ~~whose~~ ^{in which the} entries above the main diagonal are ~~iid~~ ^{i.i.d.} $\mathcal{N}(0, 1)$ random variables, ~~and the~~ ^{i.i.d.} entries on the diagonal are ~~iid~~ $\mathcal{N}(0, 2)$ random variables.

The following theorem establishes the asymptotic distribution of the LFD test statistic.

Theorem 1. Suppose as $n, p \rightarrow \infty$, condition (1.2) holds. Furthermore, suppose ~~that~~ $n\lambda_1/\text{tr}(\Sigma) \rightarrow 0$ and $\lambda_1 - \lambda_p = O(n^{-1}\sqrt{\text{tr}(\Sigma^2)})$. Then, under the local alternative hypothesis $\|\mathbf{C}^\top \Theta^\top \Theta \mathbf{C}\| = O(\sqrt{\text{tr}(\Sigma^2)})$,

$$\frac{T(\mathbf{X}) - (\text{tr}(\Sigma) - n \text{tr}(\Sigma^2)/\text{tr}(\Sigma))}{\sqrt{\text{tr}(\Sigma^2)}} \sim \lambda_1 \left(\mathbf{W}_{k-1} + \frac{\mathbf{C}^\top \Theta^\top \Theta \mathbf{C}}{\sqrt{\text{tr}(\Sigma^2)}} \right) + o_P(1),$$

where \sim means having the same distribution.

Remark 1. The condition $n\lambda_1/\text{tr}(\Sigma) \rightarrow 0$ implies $p/n \rightarrow \infty$. Hence, $T(\mathbf{X})$ is well defined for large n . The condition $\lambda_1 - \lambda_p = O(n^{-1}\sqrt{\text{tr}(\Sigma^2)})$ requires that the range of the eigenvalues of Σ ~~is not~~ too large.

To centralize $T(\mathbf{X})$ under the conditions of Theorem 1, ~~the parameters~~ $\text{tr}(\Sigma)$ and $\text{tr}(\Sigma^2)$ ~~should be estimated~~. Let $\hat{\Sigma} = n^{-1}\mathbf{G} = n^{-1}\mathbf{Y}\mathbf{Y}^\top$ be the sample covariance matrix. We use the following simple estimators

$$\widehat{\text{tr}(\Sigma)} = \text{tr}(\hat{\Sigma}), \quad \widehat{\text{tr}(\Sigma^2)} = \text{tr}(\hat{\Sigma}^2) - n^{-1} \text{tr}^2(\hat{\Sigma}).$$

Define

$$Q_1 = \frac{T(\mathbf{X}) - \left(\widehat{\text{tr}(\Sigma)} - n \widehat{\text{tr}(\Sigma^2)} / \widehat{\text{tr}(\Sigma)} \right)}{\sqrt{\widehat{\text{tr}(\Sigma^2)}}}.$$

Let $F_1(x)$ be the cumulative distribution function of $\lambda_1(\mathbf{W}_{k-1})$. Then, we reject the null hypothesis if $Q_1 > F_1^{-1}(1 - \alpha)$. The following corollary

gives the asymptotic local power function of the proposed test under ~~the~~^a nonspiked covariance.

Corollary 1. *Under the conditions of Theorem 1,*

$$\begin{aligned} & \Pr(Q_1 > F_1^{-1}(1 - \alpha)) \\ &= \Pr\left(\lambda_1 \left(\mathbf{W}_{k-1} + \frac{\mathbf{C}^\top \boldsymbol{\Theta}^\top \boldsymbol{\Theta} \mathbf{C}}{\sqrt{\text{tr}(\boldsymbol{\Sigma}^2)}}\right) > F_1^{-1}(1 - \alpha)\right) + o(1). \end{aligned}$$

Corollary 1 shows that under ~~the~~^a nonspiked covariance, the LFD test ~~has similar~~^{exhibits similar to that of} power behavior ~~to~~ existing sum-of-squares ~~type~~ tests. In fact, if $k = 2$, the asymptotic local power function given by Corollary 1 is equal to the asymptotic local power function of the tests in Bai and Saranadasa (1996) and Chen and Qin (2010).

3.2 Spiked covariance

Now^a we derive the asymptotic results under ~~the~~ spiked covariance, which ~~is~~^{is} ~~are much~~ more involved than the nonspiked case. Let $\boldsymbol{\Sigma} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^\top$ denote the eigenvalue decomposition of $\boldsymbol{\Sigma}$, where $\boldsymbol{\Lambda} = \text{diag}(\boldsymbol{\lambda}_1, \dots, \boldsymbol{\lambda}_p)$ and \mathbf{U} is an orthogonal matrix. Suppose that $\boldsymbol{\Sigma}$ has r spiked eigenvalues, where $1 \leq r \leq p$ can also vary as $n, p \rightarrow \infty$. We ~~shall~~ first assume the spiked number ~~We later adapt the analysis for~~ r is known. ~~Adaptation to unknown r will be considered latter.~~ Denote $\boldsymbol{\Lambda}_1 = \text{diag}(\boldsymbol{\lambda}_1, \dots, \boldsymbol{\lambda}_r)$ and $\boldsymbol{\Lambda}_2 = \text{diag}(\boldsymbol{\lambda}_{r+1}, \dots, \boldsymbol{\lambda}_p)$. Correspondingly, we

denote $\mathbf{U} = (\mathbf{U}_1, \mathbf{U}_2)$ where \mathbf{U}_1 and \mathbf{U}_2 are the first r columns and the last $p - r$ columns of \mathbf{U} . Then $\Sigma = \mathbf{U}_1 \Lambda_1 \mathbf{U}_1^\top + \mathbf{U}_2 \Lambda_2 \mathbf{U}_2^\top$.

First, we shall derive the asymptotic properties of the eigenvalues and eigenspaces of the sample covariance matrix $\hat{\Sigma}$ since they play a key role in our later analysis. The following proposition gives the asymptotic behavior of $\lambda_1(\hat{\Sigma}), \dots, \lambda_r(\hat{\Sigma})$ and $\sum_{i=r+1}^n \lambda_i(\hat{\Sigma})$.

Proposition 1. Suppose that $r \leq n$. Then uniformly for $i = 1, \dots, r$,

$$\lambda_i(\hat{\Sigma}) = \lambda_i + n^{-1} \text{tr}(\Lambda_2) + O_P \left(\lambda_i \sqrt{\frac{r}{n}} + \sqrt{\frac{\text{tr}(\Lambda_2^2)}{n}} + \lambda_{r+1} \right)$$

and

$$\sum_{i=r+1}^n \lambda_i(\hat{\Sigma}) = \left(1 - \frac{r}{n}\right) \text{tr}(\Lambda_2) + O_P \left(r \sqrt{\frac{\text{tr}(\Lambda_2^2)}{n}} + r \lambda_{r+1} \right).$$

Recent works have examined

Remark 2. Recently, the asymptotic behavior of the spiked eigenvalues of the sample covariance matrix is actively studied. See, e.g., Yata and Aoshima (2013), Shen et al. (2016), Wang and Fan (2017), Cai et al. (2019).

An important improvement of Proposition 1 over existing results is that Proposition 1 does not impose any conditions on the structure of Σ , but still gives the correct convergence rate.

Based on Proposition 1, we propose the following estimators of $\text{tr}(\Lambda_2)$

and $\lambda_1, \dots, \lambda_r$

$$\widehat{\text{tr}(\Lambda_2)} = \left(1 - \frac{r}{n}\right)^{-1} \sum_{i=r+1}^n \lambda_i(\hat{\Sigma}), \quad \hat{\lambda}_i = \lambda_i(\hat{\Sigma}) - n^{-1} \widehat{\text{tr}(\Lambda_2)}, \quad i = 1, \dots, r.$$

we propose the following

, which we use in our later analysis:

Moreover, ~~our latter analysis requires an estimator of $\text{tr}(\Lambda_2^2)$. We propose the following estimator of $\text{tr}(\Lambda_2^2)$,~~

$$\widehat{\text{tr}(\Lambda_2^2)} = \sum_{i=r+1}^n \left(\lambda_i(\hat{\Sigma}) - n^{-1} \widehat{\text{tr}(\Lambda_2)} \right)^2.$$

The following proposition gives the convergence rate of these estimators.

Proposition 2. Suppose ~~that~~ $r = o(n)$. Then, uniformly for $i = 1, \dots, r$,

$$\hat{\lambda}_i = \lambda_i + O_P \left(\lambda_i \sqrt{\frac{r}{n}} + \sqrt{\frac{\text{tr}(\Lambda_2^2)}{n}} + \lambda_{r+1} \right)$$

and

$$\begin{aligned} \widehat{\text{tr}(\Lambda_2)} &= \text{tr}(\Lambda_2) + O_P \left(r \sqrt{\frac{\text{tr}(\Lambda_2^2)}{n}} + r \lambda_{r+1} \right), \\ \widehat{\text{tr}(\Lambda_2^2)} &= \text{tr}(\Lambda_2^2) + O_P \left(\frac{r \text{tr}(\Lambda_2^2)}{n} + r \lambda_{r+1}^2 \right). \end{aligned}$$

Remark 3. Our estimators of $\lambda_1, \dots, \lambda_r$ and $\text{tr}(\Lambda_2)$ are similar to some existing estimators, ~~e.g.~~, the noise-reduction estimators ~~in~~ Yata and Aoshima (2012) and the estimators ~~in~~ Wang and Fan (2017). However, their theoretical results require that r is fixed, p is not large and Σ satisfies certain spiked covariance models.

Remark 4. The estimation of $\text{tr}(\Lambda_2^2)$ is relatively unexplored. Recently, Aoshima and Yata (2018) proposed an estimator of $\text{tr}(\Lambda_2^2)$ ~~by using~~ ^{based on} the cross-data-matrix methodology. They also proved the consistency of their estimator. ~~Their~~ ^{However, their} method relies, ~~however,~~ on an arbitrary split of the data into two samples of equal size.

Next, ~~we~~ ^{we} consider the asymptotic behavior of the eigenspaces of $\hat{\Sigma}$. Let $\mathbf{U}_{\mathbf{Y},1}$ denote the first r columns of $\mathbf{U}_{\mathbf{Y}}$. Then, ~~the~~ ^{the} columns of $\mathbf{U}_{\mathbf{Y},1}$ are the principal eigenvectors of $\hat{\Sigma}$, and $\mathbf{P}_{\mathbf{Y},1} = \mathbf{U}_{\mathbf{Y},1}\mathbf{U}_{\mathbf{Y},1}^\top$ is the projection matrix onto the rank r principal subspace of $\hat{\Sigma}$. The properties of $\mathbf{P}_{\mathbf{Y},1}$ ~~and~~ ^{the} individual principal eigenvectors have been ~~extensively studied.~~ ^{studied} See Cai et al. (2015), Shen et al. (2016), ~~Wang and Fan (2017)~~ ^{and} and the references therein. ~~The existing~~ ^{Existing} results include the consistency of the principal subspace and the high-order asymptotic behavior of the individual principal eigenvectors. However, these results are not ~~enough~~ ^{sufficient} for our ~~latter~~ analysis. The following proposition gives the high-order asymptotic behavior of $\mathbf{P}_{\mathbf{Y},1}$. To the best of our knowledge, ~~such result has never appeared~~ ^{this is a novel result} in the literature ~~before.~~ ^{i.i.d.}

Write $\mathbf{Y} = \mathbf{U}\Lambda^{1/2}\mathbf{Z}$, where \mathbf{Z} is a $p \times n$ random matrix with ~~iid~~ ^{i.i.d.} $\mathcal{N}(0, 1)$ entries. Then, ~~$\mathbf{Y} = \mathbf{U}_1\Lambda_1^{1/2}\mathbf{Z}_1 + \mathbf{U}_2\Lambda_2^{1/2}\mathbf{Z}_2$~~ ^{$\mathbf{Y} = \mathbf{U}_1\Lambda_1^{1/2}\mathbf{Z}_1 + \mathbf{U}_2\Lambda_2^{1/2}\mathbf{Z}_2$} , where \mathbf{Z}_1 and \mathbf{Z}_2 are the first r rows ~~and~~ ^{the} last $p - r$ rows ~~of~~ ^{, respectively,} \mathbf{Z} .

Proposition 3. Suppose ~~that~~ $r = o(n)$, $\text{tr}(\Lambda_2)/(n\lambda_r) \rightarrow 0$ ~~and~~ ^{and} $r\lambda_{r+1}/\text{tr}(\Lambda_2) \rightarrow$

0. Then,

$$\left\| \mathbf{P}_{\mathbf{Y},1} - \mathbf{P}_{\mathbf{Y},1}^\dagger \right\| = O_P \left(\frac{\text{tr}(\Lambda_2)}{n\lambda_r} + \frac{\lambda_{r+1}}{\lambda_r} \right),$$

where $\|\cdot\|$ is the spectral norm, $\mathbf{P}_{\mathbf{Y},1}^\dagger = \mathbf{U}_1 \mathbf{U}_1^\top + \mathbf{U}_1 \mathbf{Q}^\top \mathbf{U}_2^\top + \mathbf{U}_2 \mathbf{Q} \mathbf{U}_1^\top$ and $\mathbf{Q} = \Lambda_2^{1/2} \mathbf{Z}_2 \mathbf{Z}_1^\top (\mathbf{Z}_1 \mathbf{Z}_1^\top)^{-1} \Lambda_1^{-1/2}$.

Remark 5. The condition $\text{tr}(\Lambda_2)/(n\lambda_r) \rightarrow 0$ is commonly adopted in the studies on study of the principal subspaces. In fact, when this condition is violated, the principal subspace loses will lose its relation to the rank- r eigenspace of Σ ; see, for example, See, e.g., Nadler (2008).

Remark 6. Several Recently, some high-order Davis-Kahan theorems have been for example, lished, e.g., Lemma 2 in Koltchinskii and Lounici (2016) and Lemma 2 in Fan et al. (2019). These general results explicitly characterize characterizes the linear term and the high-order error on the rank- r eigenspace, owing due to matrix perturbation. Applying the By applying these results to $\hat{\Sigma}$ and Σ , we one can obtain similar results those given in ; however, the above results to Proposition 3. Compared with Proposition 3, however, the results so require require obtained are slightly weaker and requires stronger conditions.

If $p > n$, let $\mathbf{U}_{\mathbf{Y},2}$ be the $r+1$ to n th columns of $\mathbf{U}_{\mathbf{Y}}$. Then $\mathbf{P}_{\mathbf{Y},2} = \mathbf{U}_{\mathbf{Y},2} \mathbf{U}_{\mathbf{Y},2}^\top$ is the projection matrix onto the eigenspace spanned by the $r+1$ to n th eigenvectors of $\hat{\Sigma}$. Our later latter analysis also requires the asymptotic have properties of $\mathbf{P}_{\mathbf{Y},2}$, which has not been considered in the literature. Let

$\mathbf{V}_{\mathbf{Z}_1} = \mathbf{Z}_1^\top (\mathbf{Z}_1 \mathbf{Z}_1^\top)^{-1/2}$. Then $\mathbf{V}_{\mathbf{Z}_1} \mathbf{V}_{\mathbf{Z}_1}^\top = \mathbf{Z}_1^\top (\mathbf{Z}_1 \mathbf{Z}_1^\top)^{-1} \mathbf{Z}_1$ is the projection matrix onto the row space of \mathbf{Z}_1 . Let $\tilde{\mathbf{V}}_{\mathbf{Z}_1}$ be an $n \times (n-r)$ column orthogonal matrix that satisfies $\tilde{\mathbf{V}}_{\mathbf{Z}_1} \tilde{\mathbf{V}}_{\mathbf{Z}_1}^\top = \mathbf{I}_n - \mathbf{V}_{\mathbf{Z}_1} \mathbf{V}_{\mathbf{Z}_1}^\top$. The following proposition gives the asymptotic behavior of $\mathbf{P}_{\mathbf{Y},2}$.

Proposition 4. Suppose that $r = o(n)$, $\text{tr}(\Lambda_2) \lambda_1 / (n \lambda_r^2) \rightarrow 0$ and $n \lambda_{r+1} / \text{tr}(\Lambda_2) \rightarrow 0$. Then

$$\left\| \mathbf{P}_{\mathbf{Y},2} - \mathbf{P}_{\mathbf{Y},2}^\dagger \right\| = O_P \left(\sqrt{\frac{\text{tr}(\Lambda_2) \lambda_1}{n \lambda_r^2}} + \sqrt{\frac{n \lambda_{r+1}}{\text{tr}(\Lambda_2)}} \right),$$

where $\mathbf{P}_{\mathbf{Y},2}^\dagger = (\text{tr}(\Lambda_2))^{-1} \mathbf{U}_2 \Lambda_2^{1/2} \mathbf{Z}_2 \tilde{\mathbf{V}}_{\mathbf{Z}_1} \tilde{\mathbf{V}}_{\mathbf{Z}_1}^\top \mathbf{Z}_2^\top \Lambda_2^{1/2} \mathbf{U}_2^\top$.

Remark 7. The condition $\text{tr}(\Lambda_2) \lambda_1 / (n \lambda_r^2) \rightarrow 0$ is stronger than the condition $\text{tr}(\Lambda_2) / (n \lambda_r) \rightarrow 0$ in Proposition 3. These two conditions are equivalent if λ_1 and λ_r are of the same order.

Now we are ready to derive the asymptotic properties of $T(\mathbf{X})$ under the spiked covariance. Let \mathbf{W}_{k-1}^* be a $(k-1) \times (k-1)$ symmetric random matrix distributed as $\text{Wishart}(r, \mathbf{I}_{k-1})$ and is independent of \mathbf{W}_{k-1} , where $\text{Wishart}(m, \Psi)$ is the Wishart distribution with parameter Ψ and m degrees of freedom. The following theorem gives the asymptotic distribution of $T(\mathbf{X})$ under the null and the local alternative hypotheses.

Theorem 2. Suppose that $r = o(\sqrt{n})$, $r \text{tr}(\Lambda_2) \lambda_1 / (n \lambda_r^2) \rightarrow 0$, $rn \lambda_{r+1} / \text{tr}(\Lambda_2) \rightarrow 0$, $r \lambda_{r+1} / \sqrt{\text{tr}(\Lambda_2^2)} \rightarrow 0$ and $\lambda_{r+1} - \lambda_p = O(n^{-1} \sqrt{\text{tr}(\Lambda_2^2)})$. Then

(i) under the null hypothesis $\Theta \mathbf{C} = \mathbf{O}_{p \times (k-1)}$,

$$\begin{aligned} & \frac{T(\mathbf{X}) - ((1 + r/n) \text{tr}(\Lambda_2) - n \text{tr}(\Lambda_2^2) / \text{tr}(\Lambda_2))}{\sqrt{rn^{-2} \text{tr}^2(\Lambda_2) + \text{tr}(\Lambda_2^2)}} \\ & \sim \lambda_1 \left(\frac{n^{-1} \text{tr}(\Lambda_2)}{\sqrt{rn^{-2} \text{tr}^2(\Lambda_2) + \text{tr}(\Lambda_2^2)}} (\mathbf{W}_{k-1}^* - r \mathbf{I}_{k-1}) \right. \\ & \quad \left. + \frac{\sqrt{\text{tr}(\Lambda_2^2)}}{\sqrt{rn^{-2} \text{tr}^2(\Lambda_2) + \text{tr}(\Lambda_2^2)}} \mathbf{W}_{k-1} \right) + o_P(1); \end{aligned}$$

(ii) if $r \rightarrow \infty$ or $\text{tr}(\Lambda_2)/(n\sqrt{\text{tr}(\Lambda_2^2)}) \rightarrow 0$, then under the local alternative

$$\text{hypothesis } \|\mathbf{C}^\top \Theta^\top \Theta \mathbf{C}\| = O(\sqrt{rn^{-2} \text{tr}^2(\Lambda_2) + \text{tr}(\Lambda_2^2)}),$$

$$\begin{aligned} & \frac{T(\mathbf{X}) - ((1 + r/n) \text{tr}(\Lambda_2) - n \text{tr}(\Lambda_2^2) / \text{tr}(\Lambda_2))}{\sqrt{rn^{-2} \text{tr}^2(\Lambda_2) + \text{tr}(\Lambda_2^2)}} \\ & \sim \lambda_1 \left(\frac{n^{-1} \text{tr}(\Lambda_2)}{\sqrt{rn^{-2} \text{tr}^2(\Lambda_2) + \text{tr}(\Lambda_2^2)}} (\mathbf{W}_{k-1}^* - r \mathbf{I}_{k-1}) \right. \\ & \quad + \frac{\sqrt{\text{tr}(\Lambda_2^2)}}{\sqrt{rn^{-2} \text{tr}^2(\Lambda_2) + \text{tr}(\Lambda_2^2)}} \mathbf{W}_{k-1} \\ & \quad \left. + \frac{\mathbf{C}^\top \Theta^\top \mathbf{U}_2 \mathbf{U}_2^\top \Theta \mathbf{C}}{\sqrt{rn^{-2} \text{tr}^2(\Lambda_2) + \text{tr}(\Lambda_2^2)}} \right) + o_P(1). \end{aligned}$$

Remark 8. Suppose the approximate factor model in Fan et al. (2013)

holds. That is, r is fixed, $\lambda_1, \dots, \lambda_r$ diverge at rate $O(p)$ and $\lambda_{r+1}, \dots, \lambda_p$

are bounded. Then the conditions of Theorem 2 become $p/n \rightarrow \infty$ and

$\lambda_{r+1} - \lambda_p = O(\sqrt{p}/n)$. Hence Theorem 2 holds for ~~ultra-high dimensional~~ ^{ultrahigh-dimensional}

data. In contrast, ~~recently proposed~~ ^{recent} tests ~~under~~ ^{for} the spiked covariance model

can only be used for lower-dimensional data. In fact, under the approximate

factor model in Fan et al. (2013), Aoshima and Yata (2018) requires $p/n \rightarrow$

and 0, while Wang and Xu (2018) requires $p/n^2 \rightarrow 0$ and $\boldsymbol{\lambda}_{r+1} = \cdots = \boldsymbol{\lambda}_p$.

Note

We note that if $k = 2$ and $p/n^2 \rightarrow 0$, then the coefficient of $\mathbf{W}_{k-1}^* - r\mathbf{I}_{k-1}$ is negligible, and, as a result, $T(\mathbf{X})$ is asymptotically normally distributed.

Thus, Theorem 2 gives the high-order behavior of $T(\mathbf{X})$.

Now, we formulate a test procedure with an asymptotically correct level.

Define the standardized statistic as

$$Q_2 = \frac{T(\mathbf{X}) - \left((1 + r/n) \widehat{\text{tr}(\boldsymbol{\Lambda}_2)} - n \widehat{\text{tr}(\boldsymbol{\Lambda}_2^2)} / \widehat{\text{tr}(\boldsymbol{\Lambda}_2)} \right)}{\sqrt{rn^{-2}(\widehat{\text{tr}(\boldsymbol{\Lambda}_2)})^2 + \widehat{\text{tr}(\boldsymbol{\Lambda}_2^2)}}}.$$

Let $F_2(x; \text{tr}(\boldsymbol{\Lambda}_2), \text{tr}(\boldsymbol{\Lambda}_2^2))$ be the cumulative distribution function of

$$\lambda_1 \left(\frac{n^{-1} \text{tr}(\boldsymbol{\Lambda}_2)}{\sqrt{rn^{-2} \text{tr}^2(\boldsymbol{\Lambda}_2) + \text{tr}(\boldsymbol{\Lambda}_2^2)}} (\mathbf{W}_{k-1}^* - r\mathbf{I}_{k-1}) + \frac{\sqrt{\text{tr}(\boldsymbol{\Lambda}_2^2)}}{\sqrt{rn^{-2} \text{tr}^2(\boldsymbol{\Lambda}_2) + \text{tr}(\boldsymbol{\Lambda}_2^2)}} \mathbf{W}_{k-1} \right).$$

Then, we reject the null hypothesis if

$$Q_2 > F_2^{-1} \left(1 - \alpha; \widehat{\text{tr}(\boldsymbol{\Lambda}_2)}, \widehat{\text{tr}(\boldsymbol{\Lambda}_2^2)} \right).$$

The following corollary shows that this test procedure has an asymptotically correct level, as well as giving the asymptotic local power function.

Corollary 2. Suppose the conditions of Theorem 2 hold. Then,

(i) under the null hypothesis $\boldsymbol{\Theta}\mathbf{C} = \mathbf{O}_{p \times (k-1)}$,

$$\Pr \left(Q_2 > F_2^{-1} \left(1 - \alpha; \widehat{\text{tr}(\boldsymbol{\Lambda}_2)}, \widehat{\text{tr}(\boldsymbol{\Lambda}_2^2)} \right) \right) = \alpha + o(1);$$

(ii) if $r \rightarrow \infty$ or $\text{tr}(\mathbf{\Lambda}_2)/(n\sqrt{\text{tr}(\mathbf{\Lambda}_2^2)}) \rightarrow 0$, then under the local alternative

$$\text{hypothesis } \|\mathbf{C}^\top \mathbf{\Theta}^\top \mathbf{\Theta} \mathbf{C}\| = O(\sqrt{rn^{-2} \text{tr}^2(\mathbf{\Lambda}_2) + \text{tr}(\mathbf{\Lambda}_2^2)}),$$

$$\begin{aligned} & \Pr \left(Q_2 > F_2^{-1} \left(1 - \alpha; \widehat{\text{tr}(\mathbf{\Lambda}_2)}, \widehat{\text{tr}(\mathbf{\Lambda}_2^2)} \right) \right) \\ &= \Pr \left(\lambda_1 \left(\frac{n^{-1} \text{tr}(\mathbf{\Lambda}_2)}{\sqrt{rn^{-2} \text{tr}^2(\mathbf{\Lambda}_2) + \text{tr}(\mathbf{\Lambda}_2^2)}} (\mathbf{W}_{k-1}^* - r \mathbf{I}_{k-1}) \right. \right. \\ & \quad \left. \left. + \frac{\sqrt{\text{tr}(\mathbf{\Lambda}_2^2)}}{\sqrt{rn^{-2} \text{tr}^2(\mathbf{\Lambda}_2) + \text{tr}(\mathbf{\Lambda}_2^2)}} \mathbf{W}_{k-1} \right. \right. \\ & \quad \left. \left. + \frac{\mathbf{C}^\top \mathbf{\Theta}^\top \mathbf{U}_2 \mathbf{U}_2^\top \mathbf{\Theta} \mathbf{C}}{\sqrt{rn^{-2} \text{tr}^2(\mathbf{\Lambda}_2) + \text{tr}(\mathbf{\Lambda}_2^2)}} \right) \right. \\ & \quad \left. > F_2^{-1} \left(1 - \alpha; \text{tr}(\mathbf{\Lambda}_2), \text{tr}(\mathbf{\Lambda}_2^2) \right) \right) + o(1). \end{aligned}$$

To gain some insight into the asymptotic behavior of $T(\mathbf{X})$, we consider $k = 2$ and compare the ~~LFD~~ test with ~~the tests in~~ Bai and Saranadasa (1996) and Chen and Qin (2010). Corollary 2 implies that if

$$\liminf_{n \rightarrow \infty} \frac{\mathbf{C}^\top \mathbf{\Theta}^\top \mathbf{U}_2 \mathbf{U}_2^\top \mathbf{\Theta} \mathbf{C}}{\sqrt{rn^{-2} \text{tr}^2(\mathbf{\Lambda}_2) + \text{tr}(\mathbf{\Lambda}_2^2)}} > 0,$$

then the LFD test has nontrivial power asymptotically. In contrast, if

$$\limsup_{n \rightarrow \infty} \frac{\mathbf{C}^\top \mathbf{\Theta}^\top \mathbf{\Theta} \mathbf{C}}{\sqrt{\text{tr}(\mathbf{\Sigma}^2)}} = 0,$$

then the tests in Bai and Saranadasa (1996) and Chen and Qin (2010) ~~has~~

trivial power asymptotically. To compare $\mathbf{C}^\top \mathbf{\Theta}^\top \mathbf{U}_2 \mathbf{U}_2^\top \mathbf{\Theta} \mathbf{C}$ and $\mathbf{C}^\top \mathbf{\Theta}^\top \mathbf{\Theta} \mathbf{C}$,

we temporarily place a prior on $\mathbf{\Theta}$. Suppose ~~that~~ $\sqrt{n_i} \theta_i$ has prior distribution $\mathcal{N}_p(\mathbf{0}_p, \psi \mathbf{I}_p)$, ~~for~~ $i = 1, 2$. Then $\psi^{-1} \mathbf{C}^\top \mathbf{\Theta}^\top \mathbf{\Theta} \mathbf{C}$ ~~is distributed as~~ χ^2 distribution with p degrees of freedom. On the other hand, $\psi^{-1} \mathbf{C}^\top \mathbf{\Theta}^\top \mathbf{U}_2 \mathbf{U}_2^\top \mathbf{\Theta} \mathbf{C}$

3.2 Spiked covariance

follows a ~~is distributed as~~ χ^2 distribution with $p - r$ degrees of freedom. ~~Then~~ we have

$$\frac{\mathbf{C}^\top \boldsymbol{\Theta}^\top \mathbf{U}_2 \mathbf{U}_2^\top \boldsymbol{\Theta} \mathbf{C}}{\mathbf{C}^\top \boldsymbol{\Theta}^\top \boldsymbol{\Theta} \mathbf{C}} \xrightarrow{P} 1.$$

Therefore, on

~~So in~~ average, the signal contained in $\mathbf{C}^\top \boldsymbol{\Theta}^\top \mathbf{U}_2 \mathbf{U}_2^\top \boldsymbol{\Theta} \mathbf{C}$ is roughly the same as that in $\mathbf{C}^\top \boldsymbol{\Theta}^\top \boldsymbol{\Theta} \mathbf{C}$. Now, we compare the asymptotic variance. It is not hard to see that

$$\frac{rn^{-2} \text{tr}^2(\boldsymbol{\Lambda}_2) + \text{tr}(\boldsymbol{\Lambda}_2^2)}{\text{tr}(\boldsymbol{\Sigma}^2)} \rightarrow 0.$$

That is, the asymptotic variance of $T(\mathbf{X})$ is much smaller than ~~those of~~ the tests in Bai and Saranadasa (1996) and Chen and Qin (2010). To appreciate this ~~phenomenon~~, note that in the expression (2.2), $(\mathbf{I}_p - \mathbf{P}_Y) \mathbf{X} \mathbf{J} \mathbf{C} | \mathbf{P}_Y \sim \mathcal{N}_p(\mathbf{0}_p, (\mathbf{I}_p - \mathbf{P}_Y) \boldsymbol{\Sigma} (\mathbf{I}_p - \mathbf{P}_Y))$. ~~But~~ $\mathbf{I}_p - \mathbf{P}_Y$ tends to be orthogonal to $\mathbf{U}_1 \mathbf{U}_1^\top$ which is the projection matrix onto the eigenspace corresponding to the leading eigenvalues of $\boldsymbol{\Sigma}$. Hence the projection by $\mathbf{I}_p - \mathbf{P}_Y$ helps reduce the variance of $\mathbf{X} \mathbf{J} \mathbf{C}$.

Thus, if $\boldsymbol{\Theta}$ satisfies

$$\liminf_{n \rightarrow \infty} \frac{\mathbf{C}^\top \boldsymbol{\Theta}^\top \boldsymbol{\Theta} \mathbf{C}}{\sqrt{rn^{-2} \text{tr}^2(\boldsymbol{\Lambda}_2) + \text{tr}(\boldsymbol{\Lambda}_2^2)}} > 0, \quad \limsup_{n \rightarrow \infty} \frac{\mathbf{C}^\top \boldsymbol{\Theta}^\top \boldsymbol{\Theta} \mathbf{C}}{\sqrt{\text{tr}(\boldsymbol{\Sigma}^2)}} = 0,$$

then

the LFD test has nontrivial power ~~while~~ ~~the tests in~~ Bai and Saranadasa (1996) and Chen and Qin (2010) ~~has~~ trivial power. Hence the LFD test tends to be more powerful than ~~the tests in~~ Bai and Saranadasa (1996)

and Chen and Qin (2010).

In practice, ~~one~~ ^{we} may not know ~~whether~~ ^{whether} the covariance matrix is spiked. ~~Furthermore, even if we know that it~~ ^{Furthermore, even if we know that it} ~~Even if it is known that the covariance matrix~~ ^{Even if it is known that the covariance matrix} is spiked, the spike number r ~~Therefore, we~~ ^{Therefore, we} may be unknown. ~~So we would like to~~ ^{So we would like to} propose an adaptive test procedure. ~~while~~ ^{, and} Note that Theorem 1 requires $n\lambda_1/\text{tr}(\Sigma) \rightarrow 0$ ~~while~~ ^{, and} Theorem 2 requires $\text{tr}(\Lambda_2)/n\lambda_r \rightarrow 0$ and $n\lambda_{r+1}/\text{tr}(\Lambda_2) \rightarrow 0$. This motivates us to consider the following adaptive test procedure. Let $\tau > 1$ be a hyperparameter. If

$$\frac{n\lambda_1(\hat{\Sigma})}{\text{tr}(\hat{\Sigma})} < \tau,$$

then we reject the null hypothesis if $Q_1 > F^{-1}(1 - \alpha)$. Otherwise, we reject the null hypothesis if $Q_2 > F_2^{-1}(1 - \alpha; \widehat{\text{tr}(\Lambda_2)}, \widehat{\text{tr}(\Lambda_2^2)})$, where the unknown r is substituted by the estimator

$$\hat{r} = \min \left\{ 1 \leq i < n : \frac{n\lambda_{i+1}(\hat{\Sigma})}{\sum_{j=i+1}^n \lambda_j(\hat{\Sigma})} < \tau \right\}.$$

We have the following proposition.

Proposition 5. *Let $\tau > 1$ be a constant.*

(i) *Under the conditions of Theorem 1,*

$$\Pr \left(\frac{n\lambda_1(\hat{\Sigma})}{\text{tr}(\hat{\Sigma})} < \tau \right) \rightarrow 1;$$

(ii) *Under the conditions of Theorem 2,*

$$\Pr \left(\frac{n\lambda_1(\hat{\Sigma})}{\text{tr}(\hat{\Sigma})} < \tau \right) \rightarrow 0, \quad \Pr(\hat{r} = r) \rightarrow 1.$$

Proposition 5 implies that the spiked covariance structure can be ~~consistently detected~~. ~~Therefore,~~ So the proposed adaptive LFD test procedure can indeed adapt to the unknown covariance structure.

4. Numerical study

In this section, we compare the numerical performance of the adaptive LFD test procedure with ~~some existing tests, including~~ ^{that of} the MANOVA tests in Schott (2007), Cai and Xia (2014), Hu et al. (2017), and Zhang et al. (2017). These competing tests are denoted by Sc, CX, HBWW, and ZGZ, respectively. Throughout the simulations, we take the nominal test level $\alpha = 0.05$ and the group number $k = 3$. For the adaptive LFD test, we take $\tau = 5$. For CX, we use their oracle procedure. All ~~the~~ simulation results are based on 5000 replications.

First, we simulate the empirical level and power under various models of Σ and Θ . To characterize the signal strength, we define ^{the} signal-to-noise ratio (SNR) as

$$\text{SNR} = \frac{\mathbf{C}^\top \Theta^\top \Theta \mathbf{C}}{\sqrt{\text{tr}(\Sigma^2)}}.$$

We consider four models for Σ , where the first two ~~of them~~ are nonspiked, and the last two ~~of them~~ are spiked.

- Model I: $\Sigma = \mathbf{I}_p$.

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- Model II: $\Sigma = (\sigma_{ij})$ where $\sigma_{ij} = 0.6^{|i-j|}$.
 - Model III: $\Sigma = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top$ where \mathbf{U} is a $p \times p$ orthogonal matrix generated from Haar distribution and $\mathbf{\Lambda} = \text{diag}(3p, 2p, p, 1, \dots, 1)$.
 - Model IV: $\Sigma = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top + \mathbf{A}\mathbf{A}^\top$ where \mathbf{U} is a $p \times p$ orthogonal matrix generated from Haar distribution, $\mathbf{\Lambda} = \text{diag}(p, p, 1, \dots, 1)$ and \mathbf{A} is a $p \times p$ matrix whose elements are independently generated from Bernoulli distribution with success probability 0.01.

Under the null hypothesis, we shall always take $\theta_1 = \dots = \theta_k = \mathbf{0}_p$. We consider two different structures of alternative hypotheses: the nonsparse alternative and the sparse alternative. In the nonsparse case, we take $\theta_1 = \kappa \mathbf{1}_p$, $\theta_2 = -\kappa \mathbf{1}_p$ and $\theta_3 = \mathbf{0}_p$, where κ is selected to make the SNR equal to specific values. In the sparse case, we take $\theta_1 = \kappa(\mathbf{1}_{p/5}^\top, \mathbf{0}_{4p/5}^\top)^\top$, $\theta_2 = \kappa(\mathbf{0}_{p/5}^\top, \mathbf{1}_{p/5}^\top, \mathbf{0}_{3p/5}^\top)^\top$ and $\theta_3 = \mathbf{0}_p$. Again, κ is selected to make the SNR equal to specific values. The simulation results are summarized in Figures 1–4, and show that in all scenarios, the empirical sizes of the LFD test are reasonably close to the nominal level 0.05. Under model I and model II, where the covariance matrices are nonspiked, the empirical power of the LFD test is slightly lower than the sum-of-squares type tests, but is higher than the CX test. Under model III and model IV, where the covariance

matrices are spiked, the empirical power of the LFD test is significantly higher than ~~the~~ ^{that of} sum-of-squares ~~type~~ tests. ~~Also,~~ ^{In addition} the LFD test ~~offers~~ ^{exhibits} higher empirical power than ~~the~~ ^{that of} CX test in most cases, except for model IV with sparse means. These simulation results verify our theoretical results that the LFD test is particularly powerful under ~~the~~ ^a spiked covariance.

In our second simulation study, we ~~would like to~~ investigate the effect of correlations between ~~variables~~ ^{the} variables. We consider ~~the~~ ^a compound symmetry structure ^{one,} that is, the diagonal elements of Σ are ~~1~~ and the off-diagonal elements are ρ with $0 \leq \rho < 1$. The parameter ρ characterizes the correlations between ~~variables~~ ^{the} variables. We take $\theta_1 = \kappa(\mathbf{1}_{p/5}^\top, \mathbf{0}_{4p/5}^\top)^\top$, $\theta_2 = \kappa(\mathbf{0}_{p/5}^\top, \mathbf{1}_{p/5}^\top, \mathbf{0}_{3p/5}^\top)^\top$ and $\theta_3 = \mathbf{0}_p$, where κ is selected such that $\mathbf{C}^\top \Theta^\top \Theta \mathbf{C} / (\sum_{i=2}^p \lambda_i^2)^{1/2} = 5$. Figure 5 plots the empirical ~~powers of~~ ^{power for} various tests versus ρ . We can see that the empirical power of the LFD test ~~holds~~ ^{remains} nearly constant as ρ varies, ^{whereas} ~~while~~ ^{power of the} the empirical ~~powers of~~ competing sum-of-squares ~~type~~ tests ~~decrease~~ ^{decreases} rapidly as ρ increases. When ρ is ~~non zero~~ ^{nonzero}, the LFD test outperforms ~~com-~~ ^{the} peting tests significantly.

5. Concluding remarks

~~In this paper, using~~ ^{Using} the idea of ~~least favorable direction~~ ^a least favorable direction, we ~~proposed~~ ^{have} ~~the~~ ^{an} LFD test for MANOVA in ~~high-dimensional~~ ^a high-dimensional setting. We ~~derived~~ ^{have} the asymp-

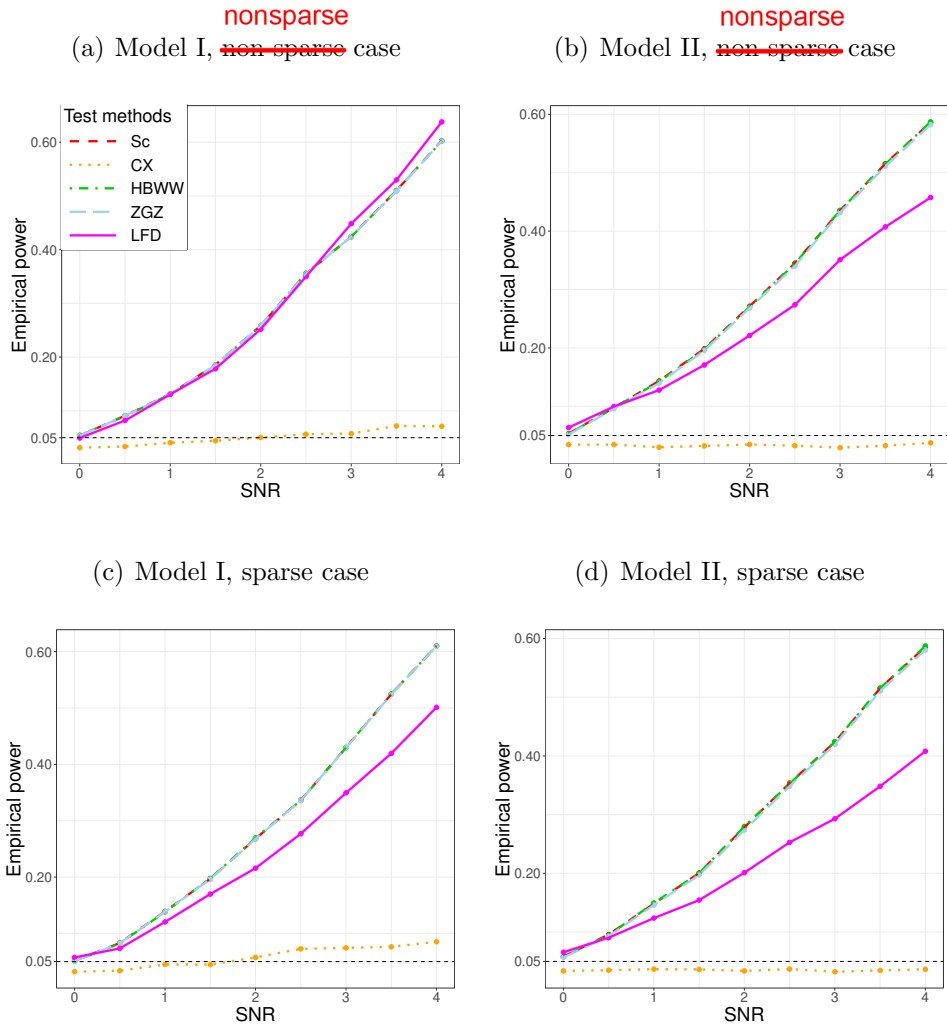


Figure 1: Empirical ~~sizes~~ size and ~~powers~~ power of tests under model I and model II;

$n_1 = n_2 = n_3 = 20, p = 300$.

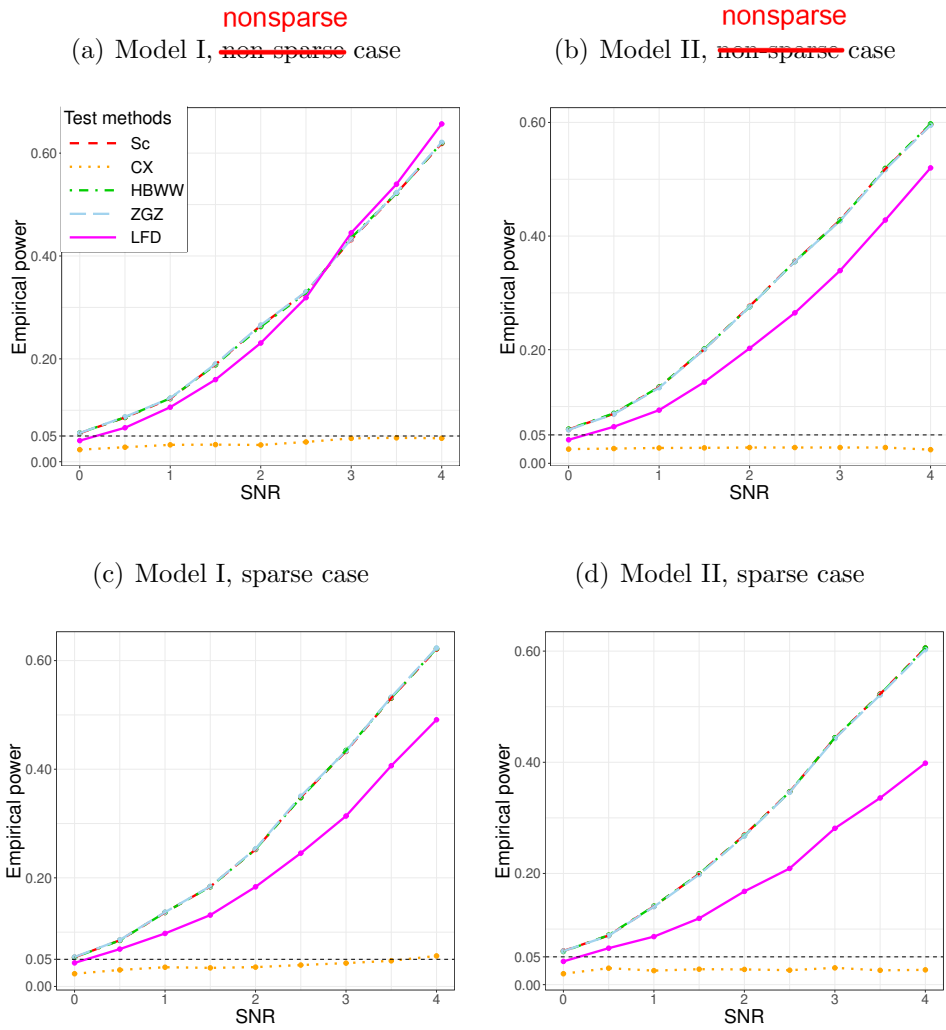


Figure 2: Empirical ~~sizes~~ size and ~~powers~~ power of tests under model I and model II;

$$n_1 = n_2 = n_3 = 25, p = 800.$$

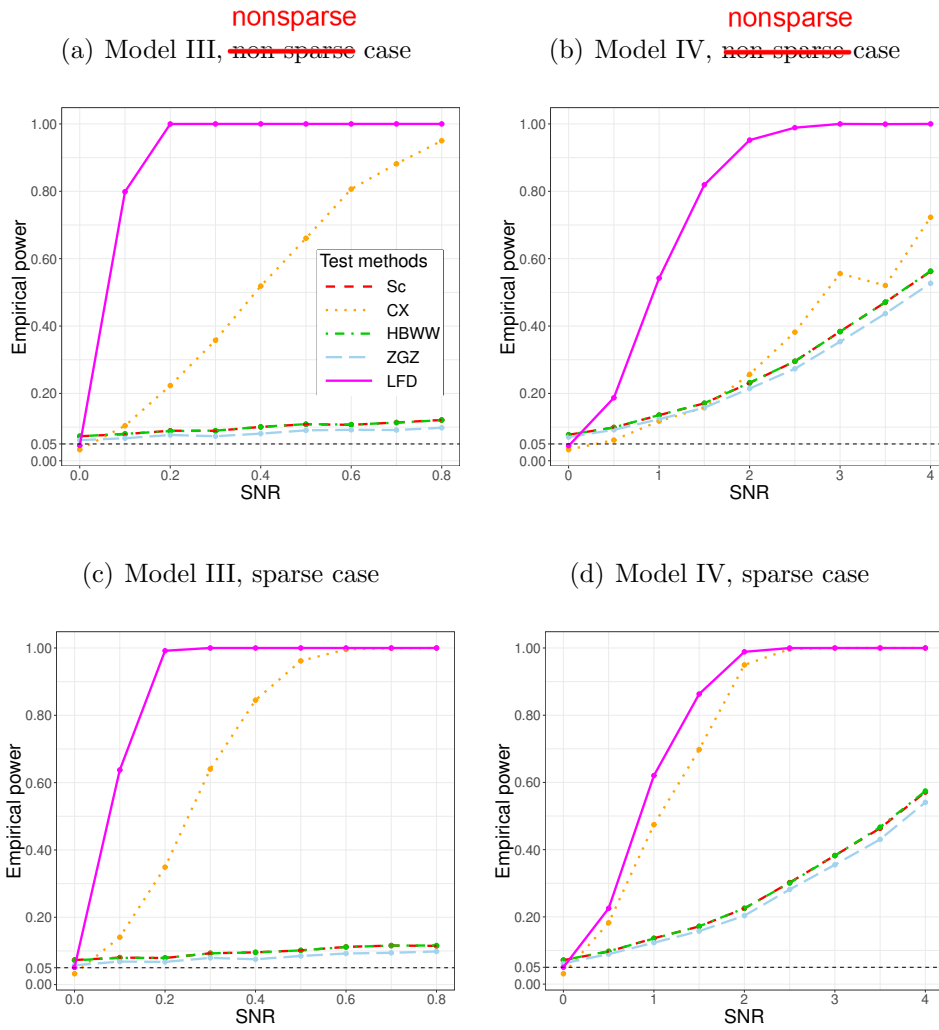


Figure 3: Empirical ~~sizes~~ ^{size} and ~~powers~~ ^{power} of tests under model III and model ~~IV~~ ^{IV}. $n_1 = n_2 = n_3 = 20$, $p = 300$.

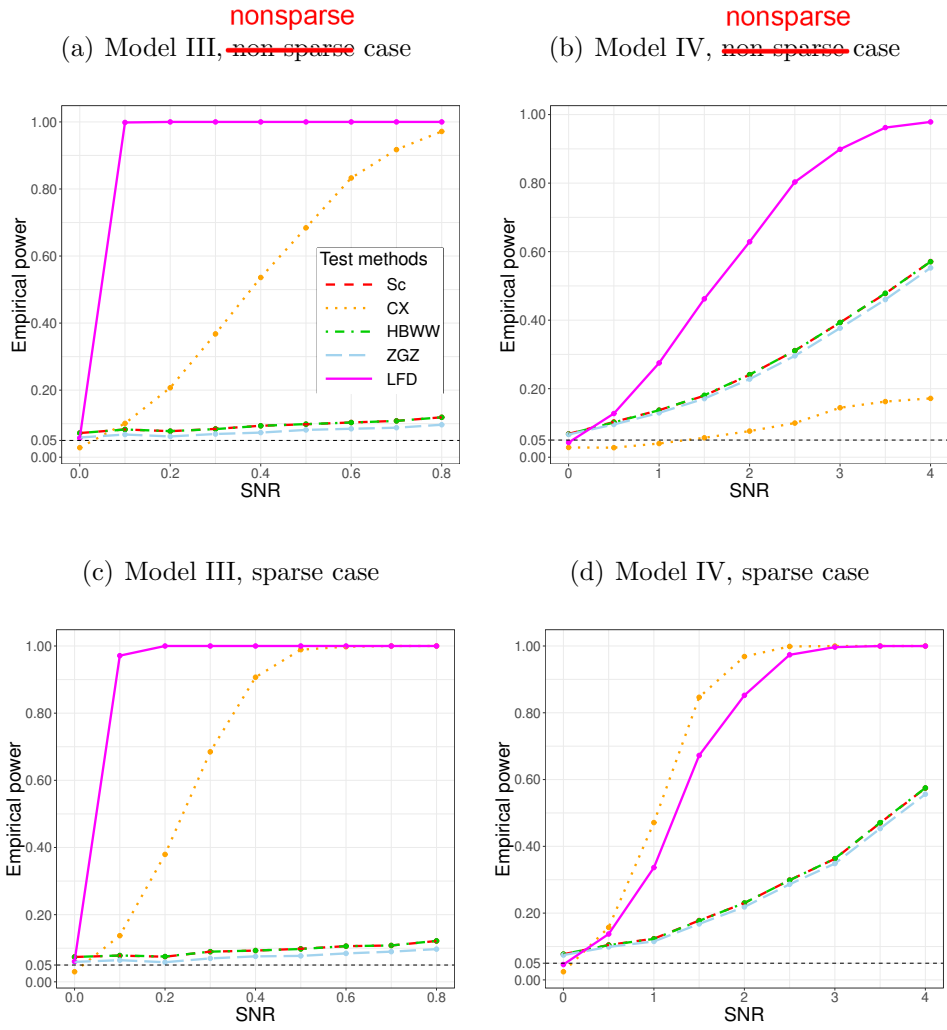


Figure 4: Empirical ~~sizes~~ ^{size} and ~~powers~~ ^{power} of tests under model III and model ~~IV~~ ^{IV}. $n_1 = n_2 = n_3 = 25$, $p = 800$.

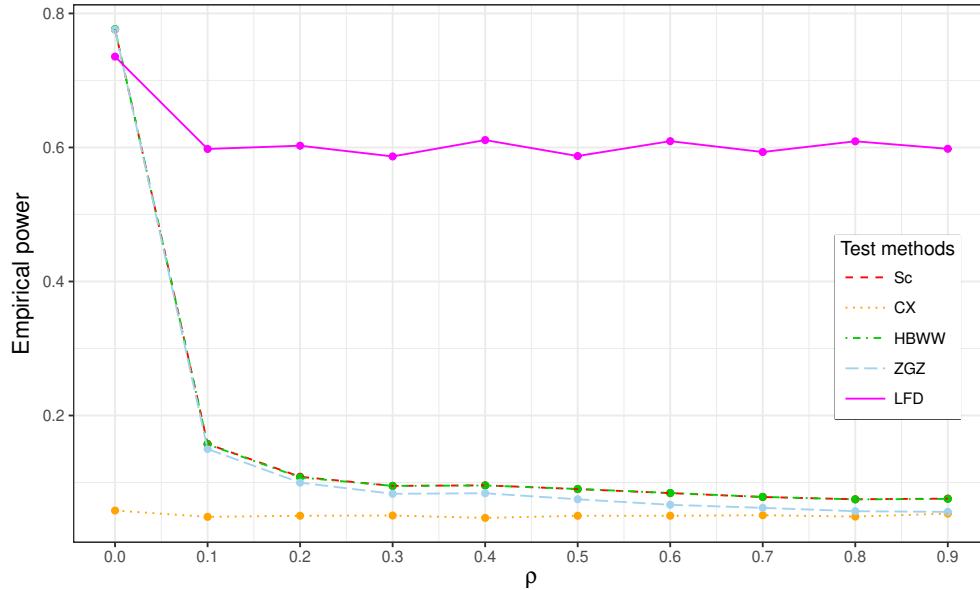


Figure 5: Empirical ^{power} powers of tests; $n_1 = n_2 = n_3 = 35$, $p = 1000$.

for totic distribution of the LFD test statistic ~~under~~ both nonspiked and spiked covariances. The asymptotic local power functions are also given. ~~From our~~ ^{The results of} ~~theoretical~~ ^{show} ~~theoretic~~ ^{exhibits} results and simulation studies, ~~it is seen~~ that the LFD test ~~has~~ ^{comparable with that of} comparable power behavior ~~to~~ ^{and} existing tests when the covariance matrix is nonspiked, ~~while~~ ^{and} tends to be much more powerful than existing tests when the covariance matrix is spiked.

~~There are several~~ ^{Several} interesting, but challenging problems ~~yet to be solved~~ ^{remain}. First, for the case ~~where the~~ ^{of an unknown} covariance structure ~~is unknown~~, we proposed an adaptive LFD test procedure by consistently detecting ~~unknown~~ ^{the} covariance structure and estimating the unknown r . However, this procedure

~~Determining~~
 relies on a hyperparameter τ . ~~How to choose~~ an optimal τ remains an interesting problem. Second, our theoretical results rely on the normality of the observations. In fact, our proofs ~~utilize~~ ^{use} the independence of \mathbf{XJC} and \mathbf{Y} . Note that \mathbf{XJC} and $\mathbf{Y} = \mathbf{X}\tilde{\mathbf{J}}$ are both ~~the~~ linear combinations of ~~independent~~ random vectors X_{ij} . ^{independent}, ^{where this independence is known to characterize} ~~It is known that the independence of~~ ~~linear combinations of independent random variables essentially character-~~ ~~ize~~ the normality of the variables (see, e.g., Kagan et al. (1973), Section 3.1). Hence our strategy is not feasible without the normality assumption. It is unclear whether the ~~conclusions~~ ^{conclusions} of our theorems hold without ~~normal~~ ^{this} assumption. Third, our theoretical results require $p/n \rightarrow \infty$. In fact, the asymptotic behavior of $T(\mathbf{X})$ will be different in the regime where $p/n \rightarrow$ constant. Random matrix theory may be useful to investigate the asymptotic behavior of $T(\mathbf{X})$ in this regime. We leave these topics for future research.

^{Material} Supplementary ~~Materials~~

^{Supplementary Material}
 The online ~~supplementary material~~ presents proofs of the propositions and theorems.

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