# A GENERALIZED LIKELIHOOD RATIO TEST FOR MULTIVARIATE ANALYSIS OF VARIANCE IN HIGH DIMENSION

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Abstract: This paper considers the problem of multivariate analysis of variance for normal samples. When the sample dimension is larger than the sample size, the classical likelihood ratio test is not defined since the likelihood function is unbounded. Although the unboundedness of the likelihood function causes some trouble, it contains important information based on which we propose a generalized likelihood ratio test. The asymptotic null distribution of the test statistic is derived and the local asymptotic power function is given. Our theoretical framework allows the covariance matrix to have a few large eigenvalues which can characterize the strong correlations between variables. Our theoretical results and simulations show that the proposed test has particular high power when there are strong correlations between variables.

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

### 1. Introduction

Suppose there are k ( $k \geq 2$ ) groups of p dimensional data. Within the ith group ( $1 \leq i \leq k$ ), we have observations  $\{X_{ij}\}_{j=1}^{n_i}$  which are independent and identically distributed (i.i.d.) as  $N_p(\xi_i, \Sigma)$ , the p dimensional normal distribution with mean vector  $\xi_i$  and common variance matrix  $\Sigma$ . We would like to test the hypotheses

$$H_0: \xi_1 = \xi_2 = \dots = \xi_k \quad \text{v.s.} \quad H_1: \xi_i \neq \xi_j \text{ for some } i \neq j.$$
 (1.1)

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

Let  $\mathbf{H} = \sum_{i=1}^k n_i (\bar{\mathbf{X}}_i - \bar{\mathbf{X}}) (\bar{\mathbf{X}}_i - \bar{\mathbf{X}})^T$  be the sum-of-squares between groups and  $\mathbf{G} = \sum_{i=1}^k \sum_{j=1}^{n_i} (X_{ij} - \bar{\mathbf{X}}_i) (X_{ij} - \bar{\mathbf{X}}_i)^T$  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 hypothesis (1.1), which are all based on the eigenvalues of  $\mathbf{H}\mathbf{G}^{-1}$ .

Wilks' Lambda:  $|\mathbf{G} + \mathbf{H}|/|\mathbf{G}|$ 

Pillai trace:  $tr[\mathbf{H}(\mathbf{G} + \mathbf{H})^{-1}]$ 

Hotelling-Lawley trace:  $tr[\mathbf{H}\mathbf{G}^{-1}]$ 

Roy's maximum root:  $\lambda_{\max}(\mathbf{H}\mathbf{G}^{-1})$ 

In some modern scientific applications, people would like to test hypothesis (1.1) in high dimensional setting, i.e., p is greater than n. See, for example, Verstynen et al. (2005) and Tsai and Chen (2009). However, when  $p \geq n$ , the four classical test statistics are not defined. Researchers have done extensive work to study the testing problem (1.1) in high dimensional setting. So far, most tests are designed for two sample case, i.e., k=2. See, for example, Bai and Saranadasa (1996), Srivastava (2007), Chen and Qin (2010), Cai et al. (2013) and Feng et al. (2014). For multiple sample case, Schott (2007) modified Hotelling-Lawley trace and proposed the test statistic

$$T_{SC} = \frac{1}{\sqrt{n-1}} \left( \frac{1}{k-1} \operatorname{tr} \left( \mathbf{H} \right) - \frac{1}{n-k} \operatorname{tr} \left( \mathbf{G} \right) \right).$$

Statistic  $T_{SC}$  is a representative of the so-called sum-of-squares type statistics as it is based on an estimation of squared Euclidean norm  $\sum_{i=1}^{k} n_i \|\xi_i - \bar{\xi}\|^2$ , where  $\bar{\xi} = n^{-1} \sum_{i=1}^{k} n_i \xi_i$ . See Srivastava and Kubokawa (2013), Yamada and Himeno (2015) and Bu Zhou (2017) for some other sum-of-squares type test statistics.

In another work, Cai and Xia (2014) proposed a test statistic

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

Where  $\Omega = (\omega)_{ij} = \Sigma^{-1}$  is the precision matrix. When  $\Omega$  is unknown, they

substitute it by an estimator  $\hat{\Omega}$ . Unlike  $T_{SC}$ ,  $T_{CX}$  is an extreme value type statistic.

Note that both sum-of-squares type statistics and extreme value type statistics are not based on likelihood function. While the likelihood ratio test (LRT), i.e., Wilks' Lambda, is not defined for p > n - k, it remains a problem how to construct likelihood-based tests in high dimensional setting. In a recent work, Zhao and Xu (2016) proposed a generalized likelihood ratio test in the context of one-sample mean vector test. They found that the unboundedness of likelihood function contains useful information. Based on this, they used a least favorable argument to construct a generalized likelihood ratio test statistic. Their simulation results showed that their test has good power performance, especially when the variables are correlated.

Following Zhao and Xu (2016)'s methodology, we propose a generalized likelihood ratio test statistic for hypotheses (1.1). To understand the behavior of the new test, we derive the asymptotic distribution of the test statistic. Our theoretical framework allows the covariance matrix to have r significantly large eigenvalues. This covariance structure, known as spiked covariance, can characterize the strong correlations between variables. See, for example, Fan et al. (2008), Cai et al. (2013), Shen et al. (2013) and Ma et al. (2015). The asymptotic distribution of the proposed test statistic in-

volves some unknown parameters. We give estimators of these parameters and formulate a test with correct level asymptotically. Based on the theoretical results, the asymptotic local power function of the new test can be derived. While the asymptotic powers of most existing tests are negatively affected by the large eigenvalues of the covariance matrix, the asymptotic power of the new test doesn't depend on the large eigenvalues of the covariance matrix. Hence the new test is particularly powerful when there are strong correlations between variables. We also conduct a simulation study to examine the numerical performance of the test.

The rest of the paper is organized as follows. In Section 2, we review some existing tests and propose a new test. Section 3 concerns the theoretical properties of the proposed test. Section 4 complements our study with some numerical simulations. In Section 5, we give a short discussion. Finally, the proofs are gathered in the Appendix.

# 2. Methodology

### 2.1 Existing methods

To facilitate the discussion, we introduce some notations. Let

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

be the pooled sample matrix. The sum-of-squares within groups G can be written as  $G = X(I_n - JJ^T)X^T$  where

$$\mathbf{J} = egin{pmatrix} rac{1}{\sqrt{n_1}} \mathbf{1}_{n_1} & \mathbf{0} & \mathbf{0} \ & \mathbf{0} & rac{1}{\sqrt{n_2}} \mathbf{1}_{n_2} & \mathbf{0} \ & dots & dots & dots \ & \mathbf{0} & \mathbf{0} & rac{1}{\sqrt{n_k}} \mathbf{1}_{n_k} \end{pmatrix},$$

and  $\mathbf{1}_{n_i}$  is an  $n_i$ -dimensional vector with all elements equal to 1. Construct a matrix  $\tilde{\mathbf{J}}$  as

$$ilde{\mathbf{J}} = egin{pmatrix} ilde{\mathbf{J}}_1 & \mathbf{0} & \mathbf{0} \ 0 & ilde{\mathbf{J}}_2 & \mathbf{0} \ dots & dots & dots \ \mathbf{0} & \mathbf{0} & ilde{\mathbf{J}}_k \end{pmatrix},$$

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

$$\tilde{\mathbf{J}}_{i} = \begin{pmatrix}
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \cdots & \frac{1}{\sqrt{(n_{i}-2)(n_{i}-1)}} & \frac{1}{\sqrt{(n_{i}-1)n_{i}}} \\
-\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \cdots & \frac{1}{\sqrt{(n_{i}-2)(n_{i}-1)}} & \frac{1}{\sqrt{(n_{i}-1)n_{i}}} \\
0 & -\frac{2}{\sqrt{6}} & \cdots & \vdots & \vdots \\
\vdots & \vdots & \cdots & -\frac{n_{i}-2}{\sqrt{(n_{i}-2)(n_{i}-1)}} & \frac{1}{\sqrt{(n_{i}-1)n_{i}}} \\
0 & 0 & \cdots & 0 & -\frac{n_{i}-1}{\sqrt{(n_{i}-1)n_{i}}}
\end{pmatrix}$$

Then  $\tilde{\mathbf{J}}$  is an  $n \times (n - k)$  orthogonal matrix satisfying  $\tilde{\mathbf{J}}^T \tilde{\mathbf{J}} = \mathbf{I}_{n-k}$  and  $\tilde{\mathbf{J}} \tilde{\mathbf{J}}^T = \mathbf{I}_n - \mathbf{J} \mathbf{J}^T$ . Let  $\mathbf{Y} = \mathbf{X} \tilde{\mathbf{J}}$ . Then  $\mathbf{G}$  has representation

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

On the other hand, the sum-of-squares between groups H satisfies

$$\mathbf{H} = \mathbf{X}(\mathbf{J}\mathbf{J}^T - \frac{1}{n}\mathbf{1}_n\mathbf{1}_n^T)\mathbf{X}^T = \mathbf{X}\mathbf{J}(\mathbf{I}_k - \frac{1}{n}\mathbf{J}^T\mathbf{1}_n\mathbf{1}_n^T\mathbf{J})\mathbf{J}^T\mathbf{X}^T.$$

We can write  $\mathbf{I}_k - \frac{1}{n} \mathbf{J}^T \mathbf{1}_n \mathbf{1}_n^T \mathbf{J} = \mathbf{C} \mathbf{C}^T$  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  $\mathbf{H}$  has representation

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

Define  $\Xi = (\sqrt{n_1}\xi_1, \dots, \sqrt{n_k}\xi_k)$  and the null hypothesis  $H_0$  is equivalent to  $\Xi \mathbf{C} = \mathbf{O}_{p \times (k-1)}$ , where  $\mathbf{O}_{p \times (k-1)}$  is a  $p \times (k-1)$  matrix with all elements equal to 0. Thus the problem becomes testing hypotheses

$$H_0: \Xi \mathbf{C} = \mathbf{O}_{p \times (k-1)}$$
 v.s.  $H_1: \Xi \mathbf{C} \neq \mathbf{O}_{p \times (k-1)}$ 

based on data matrix  $\mathbf{X}$  when p is larger.

In low dimensional setting, the testing problem (1.1) is well studied. The difficulty occurs when  $p \geq n$ , where the four classical test statistics can not be defined. To construct test statistic in high dimensional setting, a simple idea is to reduce the problem (1.1) to a class of univariate problems. Following this idea, a general strategy to propose a test statistic can be summarized as three steps.

1. Construct a class of projected univariate data  $\{X_{\gamma} : \gamma \in \Gamma\}$  which contains all the information of data X. This induces a decomposition of the null hypothesis and the alternative hypothesis:

$$H_0 = \bigcap_{\gamma \in \Gamma} H_{0\gamma}$$
 v.s.  $H_1 = \bigcup_{\gamma \in \Gamma} H_{1\gamma}$ .

- 2. Construct a test statistic  $T_{\gamma}$  for  $H_{0\gamma}$  against  $H_{1\gamma}$  such that  $H_{0\gamma}$  is rejected if  $T_{\gamma}$  is large.
- 3. Summarize the component test statistics  $\{T_{\gamma}: \gamma \in \Gamma\}$  into a global test statistic.

It turns out that many tests in the literature can be derived by the above strategy. While the LRT may be the best choice of univariate problems in step 2, there are more choices in step 1 and step 3. In step 3, Roy's union intersection principle suggests using  $\max_{\gamma \in \Gamma} T_{\gamma}$  as a global test statistic (Roy, 1953), while another choice is to integrate  $T_{\gamma}$  according to some measure  $\mu(\gamma)$  and use  $\int_{\gamma} T_{\gamma} \mu(d\gamma)$  as global test statistic. For step 1, we consider two different constructions of data projection.

(i) Consider the class of univariate data  $\{\mathbf{X}_i = e_i^T \mathbf{X} : i = 1, ..., p\}$ , where  $e_i$  is the *i*th standard basis in  $\mathbb{R}^p$ . Hence  $H_0 = \bigcap_{i=1}^p H_{0i}$  and  $H_1 = \bigcup_{i=1}^p H_{1i}$ , where

$$H_{0i}: e_i^T \Xi \mathbf{C} = \mathbf{O}_{1 \times (k-1)}$$
 and  $H_{1a}: e_i^T \Xi \mathbf{C} \neq \mathbf{O}_{1 \times (k-1)}$ .

(ii) Consider the class of univariate data  $\{\mathbf{X}_a = a^T\mathbf{X} : i = 1, a \in \mathbb{R}^p, a^Ta = 1\}$ . Hence  $H_0 = \bigcap_{a \in \mathbb{R}^p, a^Ta = 1} H_{0a}$  and  $H_1 = \bigcup_{a \in \mathbb{R}^p, a^Ta = 1} H_{1a}$ , where

 $H_{0a}: a^T \Xi \mathbf{C} = \mathbf{O}_{1 \times (k-1)}$  and  $H_{1a}: a^T \Xi \mathbf{C} \neq \mathbf{O}_{1 \times (k-1)}$ .

First, we consider the construction (i) in step 1. Suppose component test statistics

$$T_i = (k-1)^{-1} e_i^T \mathbf{H} e_i - (n-k)^{-1} e_i^T \mathbf{G} e_i \quad i = 1, \dots, p$$

are used in step 2, and in step 3 we integrate  $T_i$  according to the uniform measure on  $1, \ldots, p$ . Then the resulting statistic is  $p^{-1} \sum_{i=1}^{p} T_i$  which is equivalent to  $T_{SC}$ . If instead the likelihood ratio test statistic  $e_i^T \mathbf{H} e_i / e_i^T \mathbf{G} e_i$  is used in step 2, one obtains a scalar invariant test statistic which is a direct generalization of Srivastava (2009)'s test. On the other hand, by using data  $\Omega^{-1}\mathbf{X}$  and component test statistics

$$T_i^* = \sum_{1 \le i \le l \le k} \frac{n_j n_l}{n_j + n_l} \frac{(\Omega(\bar{\mathbf{X}}_j - \bar{\mathbf{X}}_l))_i^2}{\omega_{ii}},$$

we have  $T_{CX} = \max_{1 \leq i \leq p} T_i^*$ . Here the component test statistic  $T_i^*$  is similar to likelihood ratio tests.

While many existing tests can be derived by the construction (i) in step 1, this construction has limitation in that it relies on the choice of an orthogonal basis of  $\mathbb{R}^p$ . In fact, test statistics resulting from this construction mostly requires certain prior information about the covariance matrix. For example, Schott (2007) requires that  $\operatorname{tr}(\Sigma^{2j})/p \to \tau_j \in (0, \infty), j = 1, 2$ , and Cai and Xia (2014) requires a consistent estimator of  $\Omega$ .

Next, we consider using construction (ii) in step 1, which does not rely on the basis of  $\mathbb{R}^p$ . Suppose the likelihood ratio test statistic  $T_a = a^T \mathbf{H} a / a^T \mathbf{G} a$  is used in step 2. If we use the integrating strategy in step 3 and choose  $\mu$  equal to the uniform distribution on the sphere, then the test

statistic becomes

$$\int_{a^T a = 1} \frac{a^T \mathbf{H} a}{a^T \mathbf{G} a} \, \mu(da).$$

Although it is hard to give an explicit form of the integration, we can approximate it by random projection. More specifically, one can randomly generate unit vectors  $a_1, \ldots, a_M$  and the statistics can be approximated by  $M^{-1} \sum_{i=1}^{M} a_i^T \mathbf{H} a_i / a_i^T \mathbf{G} a_i$ . This statistic is well defined in high dimensional setting. A similar method is proposed by Lopes et al. (2015) for k=2 from a different point of view. Their analysis and simulations show that such random projection method has relatively good performance especially when variables are correlated. On the other hand, if  $n-k \geq p$ , Roy's union intersection principle can be used in step 3, the resulting statistic is the well-known Roy's maximum root:

$$\max_{a^T a=1} T_a = \lambda_{\max}(\mathbf{H}\mathbf{G}^{-1}).$$

In fact, this statistic is first derived in Roy (1953) as an example of his union intersection principle.

### 2.2 A new test statistic

Roy's maximum root is constructed from the component statistics  $\{T_a: a^T a = 1\}$ . It doesn't require prior knowledge of covariance matrix and is

widely used in practice. Let  $L_0(a)$  and  $L_1(a)$  be the maximum likelihood of  $\mathbf{X}_a$  under  $H_{0a}$  and  $H_{1a}$ , respectively. The log likelihood ratio

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

is an increasing function of  $T_a$ . From a likelihood point view, log likelihood ratio is an estimator of the Kullback-Leibler divergence between the true distribution and the null distribution. Hence the component LRT statistic characterizes the discrepancy between  $H_{0a}$  and  $H_{1a}$ . By maximizing  $\log(L_1(a)/L_0(a))$ , one obtains component hypothesis  $H_{0a^*}$ , where  $a^* = \arg\max_{a^Ta=1}(L_1(a)/L_0(a))$ . We shall call  $a^*$  the least favorable direction since  $H_{0a^*}$  is the component null hypothesis most likely to be not true. Since Roy's maximum root equals to  $T_{a^*}$ , it is the component LRT statistic along the least favorable direction.

Roy's maximum root can only be defined when  $n-k \ge p$ , hence can not be used in the high dimensional setting. In what follows, we shall assume p > n-k. In this case, Roy's maximum root is not defined since

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

is not empty. Note that

$${a: L_0(a) < +\infty, a^T a = 1} = {a: a^T (\mathbf{G} + \mathbf{H}) a \neq 0, a^T a = 1}.$$

By the independence of **G** and **H**, with probability 1, we have  $\mathcal{A} \cap \{a : L_0(a) < +\infty, a^T a = 1\} \neq \emptyset$ . 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  $a^* = \arg\min_{a \in \mathcal{A}} L_0(a)$ . Equivalently,

$$a^* = \underset{a \in \mathcal{A}}{\operatorname{arg \, min}} L_0(a) = \underset{a^T a = 1, a^T G a = 0}{\operatorname{arg \, max}} a^T \mathbf{H} a.$$

This motivates us to propose a new test statistic as

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

We reject the null hypothesis if  $T(\mathbf{X})$  is large enough. Since  $a^*$  is obtained from likelihood function, the statistic  $T(\mathbf{X})$  can be regarded as a generalized likelihood ratio test statistic. The idea of generalized likelihood ratio test is first proposed by Zhao and Xu (2016).

Now we derive the explicit forms of the test statistic. Let  $\mathbf{Y} = \mathbf{U}_{\mathbf{Y}} \mathbf{D}_{\mathbf{Y}} \mathbf{V}_{\mathbf{Y}}^T$  be the singular value decomposition of  $\mathbf{Y}$ , where  $\mathbf{U}_{\mathbf{Y}}$  and  $\mathbf{V}_{\mathbf{Y}}$  are  $p \times (n-k)$  and  $(n-k) \times (n-k)$  both column orthogonal matrices,  $\mathbf{D}_{Y}$  is an  $(n-k) \times (n-k)$  diagonal matrix. Let  $\mathbf{P}_{\mathbf{Y}} = \mathbf{U}_{\mathbf{Y}} \mathbf{U}_{\mathbf{Y}}^T$  be the projection matrix on the column space of  $\mathbf{Y}$ . Then Proposition 4 in Appendix implies that

$$T(\mathbf{X}) = \lambda_{\max} (\mathbf{C}^T \mathbf{J}^T \mathbf{X}^T (\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}}) \mathbf{X} \mathbf{J} \mathbf{C}). \tag{2.2}$$

Next, we derive another simple form of  $T(\mathbf{X})$ . By the relationship

$$\begin{pmatrix} \mathbf{J}^T \mathbf{X}^T \mathbf{X} \mathbf{J} & \mathbf{J}^T \mathbf{X}^T \mathbf{X} \tilde{\mathbf{J}} \\ \tilde{\mathbf{J}}^T \mathbf{X}^T \mathbf{X} \mathbf{J} & \tilde{\mathbf{J}}^T \mathbf{X}^T \mathbf{X} \tilde{\mathbf{J}} \end{pmatrix}^{-1} = \begin{pmatrix} \begin{pmatrix} \mathbf{J}^T \\ \tilde{\mathbf{J}}^T \end{pmatrix} \mathbf{X}^T \mathbf{X} \begin{pmatrix} \mathbf{J} & \tilde{\mathbf{J}} \end{pmatrix} \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{J}^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{J} & \mathbf{J}^T (\mathbf{X}^T \mathbf{X})^{-1} \tilde{\mathbf{J}} \\ \tilde{\mathbf{J}}^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{J} & \tilde{\mathbf{J}}^T (\mathbf{X}^T \mathbf{X})^{-1} \tilde{\mathbf{J}} \end{pmatrix}$$

and matrix inverse formula, we have that

$$\left(\mathbf{J}^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{J}\right)^{-1} = \mathbf{J}^T\mathbf{X}^T\mathbf{X}\mathbf{J} - \mathbf{J}^T\mathbf{X}^T\mathbf{X}\tilde{\mathbf{J}} \left(\tilde{\mathbf{J}}^T\mathbf{X}^T\mathbf{X}\tilde{\mathbf{J}}\right)^{-1}\tilde{\mathbf{J}}^T\mathbf{X}^T\mathbf{X}\mathbf{J} = \mathbf{J}^T\mathbf{X}^T(\mathbf{I}_p - \mathbf{P_Y})\mathbf{X}\mathbf{J}.$$

Thus,

$$T(\mathbf{X}) = \lambda_{\max} \Big( \mathbf{C}^T (\mathbf{J}^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{J})^{-1} \mathbf{C} \Big).$$
 (2.3)

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

### 3. Main results

To understand the statistical properties of  $T(\mathbf{X})$ , we derive the asymptotic distribution of  $T(\mathbf{X})$ . We are especially interested in the case when variables are correlated. For some real world problems, variables are heavily correlated with common factors, then the covariance matrix  $\Sigma$  is spiked in the sense that a few eigenvalues of  $\Sigma$  are significantly larger than the others (Fan et al., 2008; Cai et al., 2013; Shen et al., 2013; Ma et al., 2015). To characterize this correlation pattern, we make the following assumption for the eigenvalues of  $\Sigma$ .

**Assumption 1.** Let  $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p$  be the eigenvalues of  $\Sigma$ . Suppose the first r  $(r \geq 0)$  eigenvalues are significantly larger than the others. We assume r = o(n). We assume  $c_1 \geq \lambda_{r+1} \geq \ldots \geq \lambda_p \geq c_2$  for some positive absolute constants  $c_1$  and  $c_2$ . If  $r \neq 0$ , we assume

$$\frac{\boldsymbol{\lambda}_r n}{p} \to \infty, \quad \frac{\boldsymbol{\lambda}_1^2 p r^2}{\boldsymbol{\lambda}_r^2 n^2} \to 0 \quad \frac{\log \boldsymbol{\lambda}_r}{n} \to 0.$$

Remark 1. The spiked covariance model is commonly assumed in the study of PCA theory. Most existing works assumed r is fixed. Here we allow r to vary as a smaller order of n. The condition  $\lambda_r n/p \to \infty$  requires  $\lambda_r$  to be much larger than p/n. This is satisfied, for example, for the factor model adopted by Ma et al. (2015). The harshest condition is  $\lambda_1^2 p r^2/(\lambda_r^2 n^2) \to 0$ . If  $\lambda_1$  and  $\lambda_r$  are of the same order and r is fixed, this condition is equivalent to  $p/n^2 \to 0$ . We require this condition since the PCA consistency results are not valid when p is too large. See, for example, (Cai et al., 2013). If r > 0, this condition is unavoidable and the asymptotic behavior of  $T(\mathbf{X})$  is different if this condition is violated.

To establish the asymptotic distribution of  $T(\mathbf{X})$  under Assumption 1, we need following notations. Let  $\mathbf{W}_{k-1}$  be a  $(k-1) \times (k-1)$  symmetric random matrix whose entries above the main diagonal are i.i.d. N(0,1)and the entries on the diagonal are i.i.d. N(0,2). Let  $\mathbf{\Sigma} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$  denote the eigenvalue decomposition of  $\mathbf{\Sigma}$ , where  $\mathbf{\Lambda} = \operatorname{diag}(\boldsymbol{\lambda}_1, \dots, \boldsymbol{\lambda}_p)$ . We denote  $\mathbf{U} = (\mathbf{U}_1, \mathbf{U}_2)$  where  $\mathbf{U}_1$  is  $p \times r$  and  $\mathbf{U}_2$  is  $p \times (p - r)$ . Denote  $\mathbf{\Lambda}_1 = \operatorname{diag}(\boldsymbol{\lambda}_1, \dots, \boldsymbol{\lambda}_r)$  and  $\mathbf{\Lambda}_2 = \operatorname{diag}(\boldsymbol{\lambda}_{r+1}, \dots, \boldsymbol{\lambda}_p)$ . Then  $\mathbf{\Sigma} = \mathbf{U}_1 \mathbf{\Lambda}_1 \mathbf{U}_1^T + \mathbf{U}_2 \mathbf{\Lambda}_2 \mathbf{U}_2^T$ .

The following theorem establishes the asymptotic distribution of  $T(\mathbf{X})$ .

**Theorem 1.** Under Assumption 1, suppose  $p/n \to \infty$  and

$$\operatorname{tr}\left(\mathbf{\Lambda}_{2}-\frac{1}{p-r}\operatorname{tr}(\mathbf{\Lambda}_{2})\mathbf{I}_{p-r}\right)^{2}=o\left(\frac{p}{n}\right).$$

Then under local alternative hypothesis

$$\frac{1}{\sqrt{p}} \|\Xi \mathbf{C}\|_F^2 = O(1),$$

we have

$$\frac{T(\mathbf{X}) - \frac{p - r - n + k}{p - r} \operatorname{tr}(\mathbf{\Lambda}_2)}{\sqrt{\operatorname{tr}(\mathbf{\Lambda}_2^2)}} \sim \lambda_{\max} \left( \mathbf{W}_{k-1} + \frac{1}{\sqrt{\operatorname{tr}(\mathbf{\Lambda}_2^2)}} \mathbf{C}^T \mathbf{\Xi}^T (\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}}) \mathbf{\Xi} \mathbf{C} \right) + o_P(1),$$

where  $\sim$  means they have the same distribution.

To gain some insight into the asymptotic behavior of  $T(\mathbf{X})$ , suppose the null hypothesis holds and k=2, then Theorem 1 implies that

$$\frac{T(\mathbf{X}) - \frac{p-r-n+k}{p-r}\operatorname{tr}(\mathbf{\Lambda}_2)}{\sqrt{2\operatorname{tr}(\mathbf{\Lambda}_2^2)}} \xrightarrow{\mathcal{L}} N(0,1).$$

The asymptotic variance of  $T(\mathbf{X})$  is  $2\operatorname{tr}(\mathbf{\Lambda}_2^2)$ . If r=0, this equals to  $2\operatorname{tr}(\mathbf{\Sigma}^2)$  which is the asymptotic variance of Bai and Saranadasa (1996)

and Chen and Qin (2010)'s statistic. While for r > 0,  $2 \operatorname{tr}(\Lambda_2^2)$  is smaller than  $2 \operatorname{tr}(\Sigma^2)$ . In fact, if  $\liminf_{n \to \infty} \lambda_1/p \in (0, +\infty]$ , we have

$$\liminf_{n\to\infty}\frac{2\operatorname{tr}(\boldsymbol{\Sigma}^2)}{2\operatorname{tr}(\boldsymbol{\Lambda}_2^2)}\in(1,+\infty].$$

The reason for this is because the projection  $\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}}$  appeared in expression (2.2) can remove large variance terms of  $\mathbf{XJC}$ .

To formulate a test procedure with asymptotic correct level,  $\operatorname{tr}(\Lambda_2)$  and  $\operatorname{tr}(\Lambda_2^2)$  should be estimated. Since they rely on the unknown parameter r, we use the following statistic to estimate r:

$$\hat{r} = \begin{cases} \arg\max_{1 \le i \le n-k-1} \frac{\lambda_i(\mathbf{Y}^T \mathbf{Y})}{\lambda_{i+1}(\mathbf{Y}^T \mathbf{Y})} \ge \gamma_n & \text{if } \max_{1 \le i \le n-k-1} \frac{\lambda_i(\mathbf{Y}^T \mathbf{Y})}{\lambda_{i+1}(\mathbf{Y}^T \mathbf{Y})} \ge \gamma_n \\ 0 & \text{otherwise} \end{cases}$$

where  $\gamma_n$  is slowly tends to  $+\infty$  as  $n \to \infty$ . The following proposition establishes the consistency of  $\hat{r}$ .

**Proposition 1.** Suppose  $p/n \to \infty$ , r = o(n),  $\lambda_r n/p \to \infty$  and  $c_1 \ge \lambda_{r+1} \ge \ldots \ge \lambda_p \ge c_2$ . If  $\gamma_n \to \infty$  and  $\gamma_n = o(n\lambda_r/p)$ , then  $\Pr(\hat{r} = r) \to 1$ .

**Remark 2.** For the factor model adopted by Ma et al. (2015),  $\lambda_r$  is of order p. Then we can take  $\gamma_n = \sqrt{n}$ .

We use the following statistic to estimate  $tr(\Lambda_2)$ :

$$\widehat{\operatorname{tr}(\boldsymbol{\Lambda}_2)} = \frac{1}{n-k} \sum_{i=\hat{r}+1}^{n-k} \lambda_i(\mathbf{Y}^T \mathbf{Y}).$$

**Proposition 2.** Under the assumptions of Theorem 1, suppose  $\gamma_n \to \infty$  and  $\gamma_n = o(n\lambda_r/p)$ , then

$$\widehat{\operatorname{tr}(\boldsymbol{\Lambda}_2)} = \operatorname{tr}(\boldsymbol{\Lambda}_2) + o_P(\sqrt{p}).$$

To estimate  $\operatorname{tr}(\mathbf{\Lambda}_2^2)$ , we use the idea of leave-two-out. Let  $\mathbf{Y}_{(i,j)}$  be the matrix obtained by deleting the ith and jth columns from  $\mathbf{Y}$ . Let  $\mathbf{Y}_{(i,j)} = \mathbf{U}_{\mathbf{Y};(i,j)} \mathbf{D}_{\mathbf{Y};(i,j)} \mathbf{V}_{\mathbf{Y};(i,j)}^T$  be the singular value decomposition of  $\mathbf{Y}_{(i,j)}$ . Here  $\mathbf{U}_{\mathbf{Y};(i,j)}$  is  $p \times (n-k-2)$ . Let  $\tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}$  be a  $p \times (p-n+k+2)$  orthogonal matrix satisfying  $\tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^T = \mathbf{I}_p - \mathbf{U}_{\mathbf{Y};(i,j)} \mathbf{U}_{\mathbf{Y};(i,j)}^T$ .

Let  $w_{ij}$  be the (i,j)th element of  $\mathbf{Y}^T \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^T \mathbf{Y}$ . Define

$$\widehat{\operatorname{tr}(\Lambda_2^2)} = \frac{2}{(n-k)(n-k-1)} \sum_{1 \le i < j \le n-k} w_{ij}^2.$$

We use  $\widehat{\operatorname{tr}(\boldsymbol{\Lambda}_2^2)}$  to estimate  $\operatorname{tr}(\boldsymbol{\Lambda}_2^2)$ . The following proposition shows that  $\widehat{\operatorname{tr}(\boldsymbol{\Lambda}_2^2)}$  is a ratio consistent estimator.

Proposition 3. Under the assumptions of Theorem 1, we have

$$\frac{\widehat{\operatorname{tr}(\boldsymbol{\Lambda}_2^2)}}{\operatorname{tr}(\boldsymbol{\Lambda}_2^2)} \xrightarrow{P} 1.$$

Now we can construct a test procedure with asymptotic correct level  $\alpha$ .

Let

$$Q = \frac{T(\mathbf{X}) - \frac{p - \hat{r} - n + k}{p - \hat{r}} \widehat{\operatorname{tr}(\boldsymbol{\Lambda}_2)}}{\sqrt{\widehat{\operatorname{tr}(\boldsymbol{\Lambda}_2^2)}}}.$$

Let F(x) be the cumulative distribution function of  $\lambda_{\max}(\mathbf{W}_{k-1})$ . We reject the null hypothesis if  $Q > F^{-1}(1-\alpha)$ .

Theorem 1, Proposition 2 and Proposition 3 implies that the resulting test procedure has asymptotic correct level under the assumptions of Theorem 1. And by Theorem 1, the asymptotic local power function of the proposed test procedure is

$$\Pr\left(\lambda_{\max}\left(\mathbf{W}_{k-1} + \frac{1}{\sqrt{\operatorname{tr}(\mathbf{\Lambda}_2^2)}}\mathbf{C}^T \mathbf{\Xi}^T (\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}}) \mathbf{\Xi} \mathbf{C}\right) \ge F_{\mathbf{W}}^{-1}(1 - \alpha)\right).$$

If k = 2, the asymptotic local power function of Bai and Saranadasa (1996) and Chen and Qin (2010)'s method can be written as

$$\Pr\left(\lambda_{\max}\left(\mathbf{W}_1 + \frac{1}{\sqrt{\operatorname{tr}(\mathbf{\Sigma}^2)}}\mathbf{C}^T \mathbf{\Xi}^T \mathbf{\Xi}\mathbf{C}\right) \ge F_{\mathbf{W}}^{-1}(1-\alpha)\right).$$

Hence the asymptotic relative efficiency between our method and Bai and Saranadasa (1996) and Chen and Qin (2010)'s method is

$$\sqrt{\frac{\operatorname{tr}(\mathbf{\Sigma}^2)}{\operatorname{tr}(\mathbf{\Lambda}_2^2)}} \frac{\mathbf{C}^T \mathbf{\Xi}^T (\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}}) \mathbf{\Xi} \mathbf{C}}{\mathbf{C}^T \mathbf{\Xi}^T \mathbf{\Xi} \mathbf{C}}.$$

There's a random term  $\mathbf{P}_{\mathbf{Y}}$  in the expression. To gain some insight into this, suppose, for example,  $\sqrt{n_i}\xi_i$  is from prior distribution  $N_p(0, \psi \mathbf{I}_p)$ , i = 1, ..., k. Then  $\psi^{-1}\mathbf{C}^T \Xi^T \Xi \mathbf{C}$  is distributed as Wishart<sub>k-1</sub>( $p, \mathbf{I}_{k-1}$ ), the k-1 dimensional Wishart distribution with degree of freedom p and parameter  $\mathbf{I}_{k-1}$ . On the other hand,  $\mathbf{C}^T \Xi^T (\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}}) \Xi \mathbf{C}$  is distributed as

Wishart<sub>k-1</sub> $(p - n + k, \mathbf{I}_{k-1})$ . In this case, we have

$$\frac{\mathbf{C}^T \Xi^T (\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}}) \Xi \mathbf{C}}{\mathbf{C}^T \Xi^T \Xi \mathbf{C}} \xrightarrow{P} 1.$$

Thus, when

$$\liminf_{n\to\infty}\frac{\mathrm{tr}(\mathbf{\Sigma}^2)}{\mathrm{tr}(\mathbf{\Lambda}_2^2)}\in(1,+\infty],$$

the new test tends to be more powerful than Chen and Qin (2010)'s test.

### 4. Numerical study

### 4.1 Permutation method

Most existing test can not be used under spiked covariance model since spiked covariance model violated their assumption. To compare the new test with other tests, we use permutation method to determine the critical value in our simulation.

Permutation method is a powerful tool to determine the critical value of a test statistic. The test procedure resulting from permutation method is exact as long as the null distribution of observations are exchangeable (Romano, 1990). The major down-side to permutation method is that it can be computationally intensive. Fortunately, for the test statistic proposed in this paper, the permutation method can be computationally fast. By

expression (2.3), a permuted statistic can be written as

$$T(\mathbf{X}\Gamma) = \lambda_{\max} \Big( \mathbf{C}^T (\mathbf{J}^T \Gamma^T (\mathbf{X}^T \mathbf{X})^{-1} \Gamma \mathbf{J})^{-1} \mathbf{C} \Big), \tag{4.4}$$

where  $\Gamma$  is an  $n \times n$  permutation matrix. Note that  $(\mathbf{X}^T\mathbf{X})^{-1}$ , the most time-consuming component, can be calculated aforehand. The permutation procedure for our statistic can be summarized as:

- 1. Calculate  $T(\mathbf{X})$  according to (2.3), hold intermediate result  $(\mathbf{X}^T\mathbf{X})^{-1}$ .
- 2. For a large M, independently generate M random permutation matrix  $\Gamma_1, \ldots, \Gamma_M$  and calculate  $T(\mathbf{X}\Gamma_1), \ldots, T(\mathbf{X}\Gamma_M)$  according to (4.4).
- 3. Calculate the *p*-value by  $\tilde{p} = (M+1)^{-1} \left[1 + \sum_{i=1}^{M} I\{T(\mathbf{X}\Gamma_i) \geq T(\mathbf{X})\}\right]$ . Reject the null hypothesis if  $\tilde{p} \leq \alpha$ .

Here M is the permutation times. It can be seen that step 1 and step 2 cost  $O(n^2p + n^3)$  and  $O(n^2M)$  operations respectively. In large sample or high dimensional setting, step 2 has a negligible effect on total computational complexity.

### 4.2 Simulation results

In this section, we evaluate the empirical power performance of the new test. Define signal-to-noise ratio (SNR) as

$$SNR = \frac{\|\Xi \mathbf{C}\|_F^2}{\sqrt{\Lambda_2^2}}.$$

We use SNR to characterize the signal strength. Since the critical values of most existing tests can not guarantee correct test level under spiked covariance model, we use permutation method to determine the critical value in the simulations.

In our first simulation study, we take k=3. For comparison, we also carry out simulations for the test of Cai and Xia (2014) and the test of Schott (2007). We denote these two tests by CX and SC, respectively. We take r=2 and  $\Sigma=\mathrm{diag}(1.5p,p,1,1,\ldots,1)$ . We consider two structure of alternative hypotheses: the non-sparse alternative and the sparse alternative. In the non-sparse case, we set  $\xi_1=\kappa 1_p$ ,  $\xi_2=-\kappa 1_p$  and  $\xi_3=\mathbf{0}_p$ , where  $\kappa$  is selected to make the SNR equal to the given value. In the sparse case, we set  $\xi_1=\kappa(1_{p/5}^T,0_{4p/5}^T)^T$ ,  $\xi_2=\kappa(\mathbf{0}_{p/5}^T,1_{p/5}^T,\mathbf{0}_{3p/5}^T)^T$  and  $\xi_3=\mathbf{0}_p$ . Again,  $\kappa$  is selected to make the SNR equal to the given value. The empirical power is computed based on 1000 simulations. The simulation results are summarized in Tables 1-4. It can be seen from the results that the pro-

posed test outperforms the other two tests for both non-sparse and sparse alternatives. This verifies our theoretical results that the new test performs well under spiked covariance.

In our second simulation study, we would like to investigate the effect of correlations between variables. We take k=2 so that we can compare our test with some existing two sample tests. For comparison, we carry out simulations for the test of Srivastava (2007), Chen and Qin (2010), Cai et al. (2013) and Feng et al. (2014). We shall denote these tests SR, CQ, CLX and FZWZ, respectively. Let the diagonal elements of  $\Sigma$  be 1 and the offdiagonal elements of  $\Sigma$  be  $\rho$  where  $0 \le \rho < 1$ . The parameter  $\rho$  characterizes the correlations between variables. We set  $\xi_1 = \kappa(\mathbf{1}_{p/2}^T, -\mathbf{1}_{p/2}^T)^T$  and  $\xi_2 =$  $\mathbf{0}_p$ , where  $\kappa$  is selected such that SNR equals to 5. Figure 1 plots the empirical power versus  $\rho$ , where empirical power is computed based on 1000 simulations. We can see that the empirical power of the proposed test holds nearly constant as  $\rho$  varies while the empirical powers of Chen and Qin (2010) and Feng et al. (2014)'s tests decrease as  $\rho$  increases. When  $\rho$ is small, the new test has reasonable performance. When  $\rho$  is larger than 0.1, the new test outperforms all other tests.

Table 1: Empirical powers of tests under non-sparse alternative.  $\alpha = 0.05$ ,  $k = 3, n_1 = n_2 = n_3 = 10$ .

SNR	p = 50			p = 75			p = 100		
	CX	SC	NEW	CX	SC	NEW	CX	SC	NEW
0	0.047	0.044	0.052	0.051	0.050	0.051	0.059	0.047	0.047
1	0.074	0.056	0.074	0.089	0.050	0.089	0.062	0.062	0.093
2	0.120	0.045	0.133	0.090	0.040	0.119	0.071	0.049	0.127
3	0.107	0.046	0.197	0.118	0.057	0.242	0.102	0.057	0.220
4	0.160	0.062	0.271	0.131	0.057	0.328	0.146	0.053	0.339
5	0.207	0.064	0.386	0.149	0.052	0.458	0.146	0.067	0.484
6	0.199	0.061	0.485	0.192	0.047	0.583	0.160	0.057	0.588
7	0.234	0.071	0.577	0.221	0.074	0.685	0.185	0.057	0.707
8	0.266	0.072	0.648	0.263	0.078	0.775	0.201	0.062	0.829
9	0.319	0.081	0.718	0.245	0.068	0.838	0.230	0.064	0.896
10	0.304	0.075	0.784	0.297	0.089	0.904	0.288	0.062	0.913

Table 2: Empirical powers of tests under non-sparse alternative.  $\alpha=0.05,$   $\underline{k=3,\,n_1=n_2=n_3=25}.$ 

SNR	p = 100			p = 150			p = 200		
	CX	SC	NEW	CX	SC	NEW	CX	SC	NEW
0	0.045	0.041	0.054	0.052	0.046	0.043	0.048	0.043	0.049
1	0.074	0.061	0.099	0.054	0.056	0.082	0.057	0.061	0.107
2	0.092	0.066	0.128	0.086	0.050	0.146	0.079	0.065	0.174
3	0.097	0.070	0.207	0.094	0.058	0.258	0.087	0.053	0.307
4	0.117	0.050	0.249	0.116	0.053	0.375	0.127	0.061	0.412
5	0.147	0.057	0.334	0.139	0.058	0.535	0.122	0.034	0.570
6	0.204	0.057	0.444	0.169	0.070	0.666	0.139	0.055	0.738
7	0.215	0.065	0.523	0.190	0.054	0.774	0.165	0.061	0.847
8	0.247	0.074	0.618	0.200	0.064	0.851	0.181	0.055	0.915
9	0.274	0.073	0.650	0.229	0.059	0.915	0.212	0.052	0.943
10	0.291	0.069	0.729	0.245	0.064	0.930	0.225	0.051	0.977

Table 3: Empirical powers of tests under sparse alternative.  $\alpha=0.05,$   $\underline{k=3,\,n_1=n_2=n_3=10}.$ 

SNR	p = 50			p = 75			p = 100		
	CX	SC	NEW	CX	SC	NEW	CX	SC	NEW
0	0.038	0.043	0.037	0.046	0.058	0.059	0.049	0.044	0.047
1	0.064	0.054	0.076	0.067	0.061	0.088	0.066	0.053	0.084
2	0.101	0.052	0.097	0.085	0.048	0.114	0.111	0.058	0.114
3	0.144	0.060	0.169	0.132	0.050	0.188	0.112	0.049	0.166
4	0.181	0.060	0.220	0.161	0.052	0.239	0.157	0.063	0.249
5	0.236	0.063	0.295	0.194	0.061	0.313	0.216	0.057	0.311
6	0.285	0.070	0.333	0.253	0.065	0.419	0.243	0.060	0.398
7	0.344	0.081	0.425	0.299	0.061	0.506	0.291	0.066	0.543
8	0.401	0.082	0.513	0.363	0.077	0.620	0.299	0.065	0.611
9	0.455	0.079	0.600	0.407	0.067	0.667	0.392	0.060	0.709
10	0.522	0.076	0.641	0.467	0.086	0.784	0.417	0.071	0.766

Table 4: Empirical powers of tests under sparse alternative.  $\alpha=0.05,$   $\underline{k=3,\,n_1=n_2=n_3=25}.$ 

SNR	p = 100			p = 150			p = 200		
	CX	SC	NEW	CX	SC	NEW	CX	SC	NEW
0	0.068	0.051	0.051	0.046	0.053	0.043	0.065	0.049	0.052
1	0.074	0.049	0.062	0.062	0.046	0.109	0.084	0.048	0.103
2	0.100	0.060	0.123	0.064	0.055	0.149	0.093	0.055	0.155
3	0.105	0.048	0.157	0.104	0.054	0.228	0.114	0.065	0.270
4	0.152	0.064	0.246	0.133	0.056	0.320	0.129	0.054	0.303
5	0.194	0.054	0.280	0.190	0.036	0.419	0.151	0.048	0.434
6	0.232	0.059	0.311	0.210	0.057	0.500	0.203	0.051	0.553
7	0.298	0.061	0.405	0.246	0.054	0.586	0.220	0.057	0.661
8	0.367	0.061	0.477	0.314	0.051	0.707	0.261	0.077	0.765
9	0.405	0.064	0.499	0.351	0.057	0.783	0.275	0.064	0.823
10	0.455	0.067	0.587	0.405	0.061	0.828	0.367	0.059	0.900

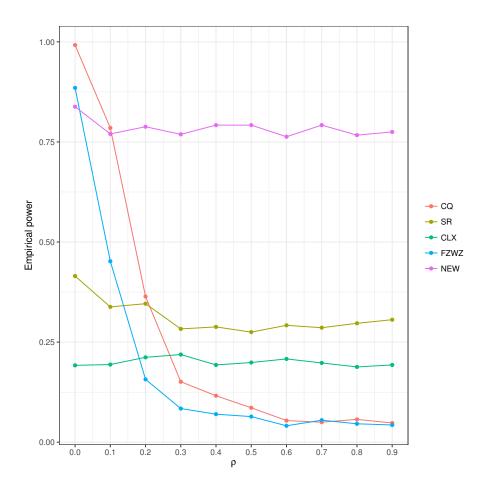


Figure 1: The empirical powers of tests.  $\alpha=0.05,\ k=2,\ n_1=n_2=20,$  p=150.

# 5. Concluding remarks

In this paper, using the idea of least favorable direction, we proposed a generalized likelihood ratio test for MANOVA in high dimensional setting. We derive the asymptotic distribution of the new test statistic. We also give the asymptotic local power function. Our theoretic work and simulation studies show that when the covariance matrix is spiked, the proposed test tends to be more powerful than existing tests.

Our proof relies on the normality of the observations. It remains a question that if the theorems are still valid without normal assumption. Moreover, we assumed p doesn't grow too fast. Without prior knowledge of  $\Sigma$ , this condition is unavoidable since when p is large, it's impossible to consistently estimate the principal space. See, for example, Cai et al. (2013). On the other hand, if we know some prior knowledge of  $\Sigma$ , for example,  $\Sigma$  is sparse, it's possible to construct a better test. We leave it for future research.

# Appendix

**Proposition 4.** Suppose  $\mathbf{A}$  is a  $p \times r$  matrix with rank r and  $\mathbf{B}$  is a  $p \times p$  non-zero semi-definite matrix. Denote by  $\mathbf{A} = \mathbf{U}_{\mathbf{A}} \mathbf{D}_{\mathbf{A}} \mathbf{V}_{\mathbf{A}}^T$  the singular value decomposition of  $\mathbf{A}$ , where  $\mathbf{U}_{\mathbf{A}}$  and  $\mathbf{V}_{\mathbf{A}}$  are  $p \times r$  and  $r \times r$  column

orthogonal matrix,  $\mathbf{D}_{\mathbf{A}}$  is a  $r \times r$  diagonal matrix. Let  $\mathbf{P}_{\mathbf{A}} = \mathbf{U}_{\mathbf{A}} \mathbf{U}_{\mathbf{A}}^T$  be the projection on the column space of  $\mathbf{A}$ . Then

$$\max_{a^T a = 1, a^T \mathbf{A} \mathbf{A}^T a = 0} a^T \mathbf{B} a = \lambda_{\max} (\mathbf{B} (\mathbf{I}_p - \mathbf{P}_{\mathbf{A}})).$$
 (5.5)

*Proof.* Note that  $a^T \mathbf{A} \mathbf{A}^T a = 0$  is equivalent to  $\mathbf{P}_{\mathbf{A}} a = 0$  which in turn is equivalent to  $a = (\mathbf{I}_p - \mathbf{P}_{\mathbf{A}})a$ . Then

$$\max_{a^T a = 1, a^T \mathbf{A} \mathbf{A}^T a = 0} a^T \mathbf{B} a = \max_{a^T a = 1, \mathbf{P}_{\mathbf{A}} a = 0} a^T (\mathbf{I}_p - \mathbf{P}_{\mathbf{A}}) \mathbf{B} (\mathbf{I}_p - \mathbf{P}_{\mathbf{A}}) a, \tag{5.6}$$

which is obviously no greater than  $\lambda_{\max} ((\mathbf{I} - \mathbf{P_A}) \mathbf{B} (\mathbf{I} - \mathbf{P_A}))$ . To prove that they are equal, without loss of generality, we can assume  $\lambda_{\max} ((\mathbf{I} - \mathbf{P_A}) \mathbf{B} (\mathbf{I} - \mathbf{P_A})) > 0$ . Let  $\alpha_1$  be one eigenvector corresponding to the largest eigenvalue of  $(\mathbf{I} - \mathbf{P_A}) \mathbf{B} (\mathbf{I} - \mathbf{P_A})$ . Since  $(\mathbf{I} - \mathbf{P_A}) \mathbf{B} (\mathbf{I} - \mathbf{P_A}) \mathbf{P_A} = (\mathbf{I} - \mathbf{P_A}) \mathbf{B} (\mathbf{P_A} - \mathbf{P_A}) = \mathbf{O}_{p \times p}$  and  $\mathbf{P_A}$  is symmetric, the rows of  $\mathbf{P_A}$  are eigenvectors of  $(\mathbf{I} - \mathbf{P_A}) \mathbf{B} (\mathbf{I} - \mathbf{P_A})$  corresponding to eigenvalue 0. It follows that  $\mathbf{P_A} \alpha_1 = 0$ . Therefore,  $\alpha_1$  satisfies the constraint of (5.6) and (5.6) is no less than  $\lambda_{\max} ((\mathbf{I} - \mathbf{P_A}) \mathbf{B} (\mathbf{I} - \mathbf{P_A}))$ . The conclusion now follows by noting that  $\lambda_{\max} ((\mathbf{I} - \mathbf{P_A}) \mathbf{B} (\mathbf{I} - \mathbf{P_A})) = \lambda_{\max} (\mathbf{B} (\mathbf{I} - \mathbf{P_A}))$ .

**Lemma 1** (Davidson and Szarek (2001) Theorem II.7). Let **A** be  $m \times n$ 

with iid N(0,1) entries. If m > n, then for any t > 0,

$$\Pr(\sqrt{\lambda_1(\mathbf{A}\mathbf{A}^T)} > \sqrt{m} + \sqrt{n} + t) \le \exp(-t^2/2),$$

$$\Pr(\sqrt{\lambda_n(\mathbf{A}\mathbf{A}^T)} < \sqrt{m} - \sqrt{n} - t) \le \exp(-t^2/2).$$

Proves of the main results It can be seen that XJC is independent of Y. Since EY =  $\mathbf{O}_{p \times (n-k)}$ , we can write Y =  $\mathbf{U} \mathbf{\Lambda}^{1/2} \mathbf{G}_1$ , where  $\mathbf{G}_1$  is a  $p \times (n-k)$  matrix with i.i.d. N(0,1) entries. We write XJC =  $\mathbf{\Xi}\mathbf{C} + \mathbf{U}\mathbf{\Lambda}^{1/2}\mathbf{G}_2$ , where  $\mathbf{G}_2$  is a  $p \times (k-1)$  matrix with i.i.d. N(0,1) entries.

Then

$$\mathbf{C}^{T}\mathbf{J}^{T}\mathbf{X}^{T}(\mathbf{I}_{p} - \mathbf{P}_{\mathbf{Y}})\mathbf{X}\mathbf{J}\mathbf{C} = \mathbf{G}_{2}^{T}\boldsymbol{\Lambda}^{1/2}\mathbf{U}^{T}(\mathbf{I}_{p} - \mathbf{P}_{\mathbf{Y}})\mathbf{U}\boldsymbol{\Lambda}^{1/2}\mathbf{G}_{2} + \Xi\mathbf{C}^{T}(\mathbf{I}_{p} - \mathbf{P}_{\mathbf{Y}})\Xi\mathbf{C} + \Xi\mathbf{C}^{T}(\mathbf{I}_{p} - \mathbf{P}_{\mathbf{Y}})\mathbf{U}\boldsymbol{\Lambda}^{1/2}\mathbf{G}_{2} + \mathbf{G}_{2}^{T}\boldsymbol{\Lambda}^{1/2}\mathbf{U}^{T}(\mathbf{I}_{p} - \mathbf{P}_{\mathbf{Y}})\Xi\mathbf{C}.$$
(5.7)

The first term of (5.7) can be represented as

$$\mathbf{G}_{2}^{T} \mathbf{\Lambda}^{1/2} \mathbf{U}^{T} (\mathbf{I}_{p} - \mathbf{P}_{\mathbf{Y}}) \mathbf{U} \mathbf{\Lambda}^{1/2} \mathbf{G}_{2} = \sum_{i=1}^{p} \lambda_{i} (\mathbf{\Lambda}^{1/2} \mathbf{U}^{T} (\mathbf{I}_{p} - \mathbf{P}_{\mathbf{Y}}) \mathbf{U} \mathbf{\Lambda}^{1/2}) \eta_{i} \eta_{i}^{T},$$
(5.8)

where  $\eta_i \stackrel{i.i.d.}{\sim} N(0, \mathbf{I}_{k-1})$ .

Let  $\mathbf{G}_1 = (\mathbf{G}_{1A}^T, \mathbf{G}_{1B}^T)^T$ , where  $\mathbf{G}_{1A}$  is the first r rows of  $\mathbf{G}_1$  and  $\mathbf{G}_{1B}$  is the last p-r rows of  $\mathbf{G}_1$ . The following lemma gives the asymptotic property of  $\lambda_i(\mathbf{Y}^T\mathbf{Y})$ ,  $i=1,\ldots,r$ .

**Lemma 2.** Suppose  $p/n \to \infty$ , r = o(n),  $\lambda_r n/p \to \infty$  and  $c_1 \ge \lambda_{r+1} \ge \ldots \ge \lambda_p \ge c_2$ . Then

$$\sup_{1 \le i \le r} \left| \frac{\lambda_i(\mathbf{Y}^T \mathbf{Y})}{n \lambda_i} - 1 \right| \to 0, \tag{5.9}$$

$$\limsup_{n \to +\infty} \frac{\lambda_{r+1}(\mathbf{Y}^T \mathbf{Y})}{p} \le c_1, \tag{5.10}$$

$$\liminf_{n \to +\infty} \frac{\lambda_{n-k}(\mathbf{Y}^T \mathbf{Y})}{p} \ge c_2, \tag{5.11}$$

almost surely.

*Proof.* Note that

$$\mathbf{Y}^T\mathbf{Y} = \mathbf{G}_1^T \mathbf{\Lambda} \mathbf{G}_1 = \mathbf{G}_{1A}^T \mathbf{\Lambda}_1 \mathbf{G}_{1A} + \mathbf{G}_{1B}^T \mathbf{\Lambda}_2 \mathbf{G}_{1B}.$$

For  $1 \le i \le r$ , we have

$$\lambda_i(\mathbf{G}_{1A}^T \mathbf{\Lambda}_1 \mathbf{G}_{1A}) \le \lambda_i(\mathbf{Y}^T \mathbf{Y}) \le \lambda_i(\mathbf{G}_{1A}^T \mathbf{\Lambda}_1 \mathbf{G}_{1A}) + c_1 \lambda_1(\mathbf{G}_{1B}^T \mathbf{G}_{1B}). \quad (5.12)$$

Using Weyl's inequality, we can derive a lower bound for  $\lambda_i(\mathbf{G}_{1A}^T \mathbf{\Lambda}_1 \mathbf{G}_{1A})$ ,  $i = 1, \dots, r$ .

$$\lambda_{i}(\mathbf{G}_{1A}^{T}\mathbf{\Lambda}_{1}\mathbf{G}_{1A}) \geq \lambda_{i}(\mathbf{G}_{1A}^{T}\operatorname{diag}(\boldsymbol{\lambda}_{i}\mathbf{I}_{i}, \mathbf{O}_{(r-i)\times(r-i)})\mathbf{G}_{1A})$$

$$=\lambda_{i}\left(\boldsymbol{\lambda}_{i}\mathbf{G}_{1A}^{T}\mathbf{G}_{1A} - \boldsymbol{\lambda}_{i}\mathbf{G}_{1A}^{T}\operatorname{diag}(\mathbf{O}_{i\times i}, \mathbf{I}_{r-i})\mathbf{G}_{1A}\right)$$

$$\geq \lambda_{r}\left(\boldsymbol{\lambda}_{i}\mathbf{G}_{1A}^{T}\mathbf{G}_{1A}\right) + \lambda_{p+i-r}\left(-\boldsymbol{\lambda}_{i}\mathbf{G}_{1A}^{T}\operatorname{diag}(\mathbf{O}_{i\times i}, \mathbf{I}_{r-i})\mathbf{G}_{1A}\right)$$

$$=\boldsymbol{\lambda}_{i}\lambda_{r}(\mathbf{G}_{1A}\mathbf{G}_{1A}^{T}).$$
(5.13)

Similarly, we can obtain the upper bound.

$$\lambda_{i}(\mathbf{G}_{1A}^{T}\boldsymbol{\Lambda}_{1}\mathbf{G}_{1A})$$

$$=\lambda_{i}\Big(\mathbf{G}_{1A}^{T}\Big(\operatorname{diag}(\boldsymbol{\lambda}_{1},\ldots,\boldsymbol{\lambda}_{i-1},\mathbf{O}_{(r-i+1)\times(r-i+1)})+\operatorname{diag}(\mathbf{O}_{(i-1)\times(i-1)},\boldsymbol{\lambda}_{i},\ldots,\boldsymbol{\lambda}_{r})\Big)\mathbf{G}_{1A}\Big)$$

$$\leq\lambda_{1}(\mathbf{G}_{1A}^{T}\operatorname{diag}(\mathbf{O}_{(i-1)\times(i-1)},\boldsymbol{\lambda}_{i}\mathbf{I}_{r-i+1})\mathbf{G}_{1A})\leq\boldsymbol{\lambda}_{i}\lambda_{1}(\mathbf{G}_{1A}\mathbf{G}_{1A}^{T}).$$
(5.14)

The inequality (5.12), (5.13) and (5.14) implies that

$$\sup_{1 \le i \le r} \left| \frac{\lambda_i(\mathbf{Y}^T \mathbf{Y})}{n \boldsymbol{\lambda}_i} - 1 \right| \le \max \left( \left| \frac{\lambda_1(\mathbf{G}_{1A} \mathbf{G}_{1A}^T)}{n} - 1 \right|, \left| \frac{\lambda_r(\mathbf{G}_{1A} \mathbf{G}_{1A}^T)}{n} - 1 \right| \right) + \frac{c_1}{n \boldsymbol{\lambda}_r} \lambda_1(\mathbf{G}_{1B}^T \mathbf{G}_{1B}).$$

We only need to prove the right hand side converges to 0 almost surely.

By Lemma 1, for every t > 0, we have

$$\Pr\left(\sqrt{1 - \frac{k}{n}} - \sqrt{\frac{r}{n}} - \frac{t}{\sqrt{n}} \le \sqrt{\frac{\lambda_r(\mathbf{G}_{1A}\mathbf{G}_{1A}^T)}{n}} \le \sqrt{\frac{\lambda_1(\mathbf{G}_{1A}\mathbf{G}_{1A}^T)}{n}} \le \sqrt{1 - \frac{k}{n}} + \sqrt{\frac{r}{n}} + \frac{t}{\sqrt{n}}\right)$$

$$\ge 1 - 2\exp(-\frac{t^2}{2}).$$
(5.15)

Let  $t = n^{1/4}$ . Since r = o(n), we have

$$\sqrt{1-\frac{k}{n}} - \sqrt{\frac{r}{n}} - \frac{t}{\sqrt{n}} \to 1$$
 and  $\sqrt{1-\frac{k}{n}} + \sqrt{\frac{r}{n}} + \frac{t}{\sqrt{n}} \to 1$ .

This, together with Borel-Cantelli lemma, yields

$$\frac{\lambda_r(\mathbf{G}_{1A}\mathbf{G}_{1A}^T)}{n} \to 1 \quad \frac{\lambda_1(\mathbf{G}_{1A}\mathbf{G}_{1A}^T)}{n} \to 1,$$

almost surely. As for  $\lambda_1(\mathbf{G}_{1B}^T\mathbf{G}_{1B})$ , by Lemma 1, we have

$$\Pr\left(\frac{c_1}{n\lambda_r}\lambda_1(\mathbf{G}_{1B}\mathbf{G}_{1B}^T) \le \frac{c_1}{n\lambda_r}(\sqrt{n-k} + \sqrt{p-r} + t)^2\right) \ge 1 - \exp(-\frac{t^2}{2}).$$
(5.16)

Let  $t = n^{1/2}$ , since we have assumed  $\lambda_r n/p \to \infty$ , we have

$$\frac{c_1}{n\lambda_r}\lambda_1(\mathbf{G}_{1B}\mathbf{G}_{1B}^T) \to 0$$

almost surely. Then (5.9) follows.

Inequality (5.10) and (5.11) follows from the fact

$$\lambda_{r+1}(\mathbf{Y}^T\mathbf{Y}) \le \lambda_1(\mathbf{G}_{1B}^T\mathbf{\Lambda}_2\mathbf{G}_{1B}) \le c_1\lambda_1(\mathbf{G}_{1B}^T\mathbf{G}_{1B}),$$

$$\lambda_{n-k}(\mathbf{Y}^T\mathbf{Y}) \ge \lambda_{n-k}(\mathbf{G}_{1B}^T\mathbf{\Lambda}_2\mathbf{G}_{1B}) \ge c_2\lambda_{n-k}(\mathbf{G}_{1B}^T\mathbf{G}_{1B}),$$

and Lemma 1.  $\Box$ 

Let  $\mathbf{U}_{\mathbf{Y}} = (\mathbf{U}_{\mathbf{Y},1}, \mathbf{U}_{\mathbf{Y},2})$ , where  $\mathbf{U}_{\mathbf{Y},1}$  and  $\mathbf{U}_{\mathbf{Y},2}$  are the first r and last p-r columns of  $\mathbf{U}_{\mathbf{Y}}$  respectively.

**Lemma 3.** Under the assumptions of Lemma 2, we have

$$\lambda_{\max}(\mathbf{I}_r - \mathbf{U}_1^T \mathbf{U}_{\mathbf{Y},1} \mathbf{U}_{\mathbf{Y},1}^T \mathbf{U}_1) = O_P(\frac{p}{\lambda_r n}).$$

If in addition, we assume

$$\frac{\log \lambda_r}{n} \to 0, \tag{5.17}$$

then

$$E \lambda_{\max}(\mathbf{I}_r - \mathbf{U}_1^T \mathbf{U}_{\mathbf{Y},1} \mathbf{U}_{\mathbf{Y},1}^T \mathbf{U}_1) = O(\frac{p}{\lambda_r n}).$$

*Proof.* From  $\mathbf{U}\mathbf{\Lambda}^{1/2}\mathbf{G}_1\mathbf{G}_1^T\mathbf{\Lambda}^{1/2}\mathbf{U}^T = \mathbf{U}_{\mathbf{Y}}\mathbf{D}_{\mathbf{Y}}^2\mathbf{U}_{\mathbf{Y}}^T$ , we have

$$\begin{pmatrix} \boldsymbol{\Lambda}_1^{\frac{1}{2}}\mathbf{G}_{1A}\mathbf{G}_{1A}^T\boldsymbol{\Lambda}_1^{\frac{1}{2}} & \boldsymbol{\Lambda}_1^{\frac{1}{2}}\mathbf{G}_{1A}\mathbf{G}_{1B}^T\boldsymbol{\Lambda}_2^{\frac{1}{2}} \\ \boldsymbol{\Lambda}_2^{\frac{1}{2}}\mathbf{G}_{1B}\mathbf{G}_{1A}^T\boldsymbol{\Lambda}_1^{\frac{1}{2}} & \boldsymbol{\Lambda}_2^{\frac{1}{2}}\mathbf{G}_{1B}\mathbf{G}_{1B}^T\boldsymbol{\Lambda}_2^{\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} \mathbf{U}_1^T\mathbf{U}_{\mathbf{Y}}\mathbf{D}_{\mathbf{Y}}^2\mathbf{U}_{\mathbf{Y}}^T\mathbf{U}_1 & \mathbf{U}_1^T\mathbf{U}_{\mathbf{Y}}\mathbf{D}_{\mathbf{Y}}^2\mathbf{U}_{\mathbf{Y}}^T\mathbf{U}_2 \\ \mathbf{U}_2^T\mathbf{U}_{\mathbf{Y}}\mathbf{D}_{\mathbf{Y}}^2\mathbf{U}_{\mathbf{Y}}^T\mathbf{U}_1 & \mathbf{U}_2^T\mathbf{U}_{\mathbf{Y}}\mathbf{D}_{\mathbf{Y}}^2\mathbf{U}_{\mathbf{Y}}^T\mathbf{U}_2 \end{pmatrix}$$

It follows that

$$\boldsymbol{\Lambda}_{2}^{\frac{1}{2}}\mathbf{G}_{1B}\mathbf{G}_{1B}^{T}\boldsymbol{\Lambda}_{2}^{\frac{1}{2}}\geq \lambda_{r}(\mathbf{Y}^{T}\mathbf{Y})\mathbf{U}_{2}^{T}\mathbf{U}_{\mathbf{Y},1}\mathbf{U}_{\mathbf{Y},1}^{T}\mathbf{U}_{2}.$$

Hence

$$\lambda_1(\mathbf{U}_2^T \mathbf{U}_{\mathbf{Y},1} \mathbf{U}_{\mathbf{Y},1}^T \mathbf{U}_2) \le \frac{c_1}{\lambda_r(\mathbf{Y}^T \mathbf{Y})} \lambda_1(\mathbf{G}_{1B} \mathbf{G}_{1B}^T).$$
 (5.18)

By Lemma 1, for every t > 0, we have

$$\Pr\left(\frac{1}{p}(\sqrt{p-r}-\sqrt{n-k}-t)^2 \le \frac{1}{p}\lambda_1(\mathbf{G}_{1B}\mathbf{G}_{1B}^T) \le \frac{1}{p}(\sqrt{p-r}+\sqrt{n-k}+t)^2\right) \ge 1-2\exp(-\frac{t^2}{2}).$$
(5.19)

Let  $t = n^{1/2}$ , then Borel-Cantelli lemma implies that

$$\frac{1}{n}\lambda_1(\mathbf{G}_{1B}\mathbf{G}_{1B}^T) \to 1 \tag{5.20}$$

almost surely. Then (5.20), (5.18) and Lemma 2 implies that

$$\lambda_1(\mathbf{U}_2^T\mathbf{U}_{\mathbf{Y},1}\mathbf{U}_{\mathbf{Y},1}^T\mathbf{U}_2) = O_P(\frac{p}{\lambda_r n}).$$

The first conclusion then follows by the following simple relationship

$$\lambda_{\max}(\mathbf{U}_{2}^{T}\mathbf{U}_{\mathbf{Y},1}\mathbf{U}_{\mathbf{Y},1}^{T}\mathbf{U}_{2}) = \lambda_{\max}(\mathbf{U}_{\mathbf{Y},1}^{T}\mathbf{U}_{2}\mathbf{U}_{2}^{T}\mathbf{U}_{\mathbf{Y},1})$$

$$=\lambda_{\max}(\mathbf{U}_{\mathbf{Y},1}^{T}(\mathbf{I}_{p} - \mathbf{U}_{1}\mathbf{U}_{1}^{T})\mathbf{U}_{\mathbf{Y},1}) = \lambda_{\max}(\mathbf{I}_{r} - \mathbf{U}_{\mathbf{Y},1}^{T}\mathbf{U}_{1}\mathbf{U}_{1}^{T}\mathbf{U}_{\mathbf{Y},1})$$

$$=1 - \lambda_{\min}(\mathbf{U}_{\mathbf{Y},1}^{T}\mathbf{U}_{1}\mathbf{U}_{1}^{T}\mathbf{U}_{\mathbf{Y},1}) = 1 - \lambda_{\min}(\mathbf{U}_{1}^{T}\mathbf{U}_{\mathbf{Y},1}\mathbf{U}_{\mathbf{Y},1}^{T}\mathbf{U}_{1})$$

$$=\lambda_{\max}(\mathbf{I}_{r} - \mathbf{U}_{1}^{T}\mathbf{U}_{\mathbf{Y},1}\mathbf{U}_{\mathbf{Y},1}^{T}\mathbf{U}_{1}).$$

Next we prove the second conclusion of the lemma. In (5.15), (5.16) and (5.19), we take  $t = \sqrt{2 \log(\lambda_r n/p)}$ . Then these inequalities, (5.18) and condition (5.17) implies that

$$\lambda_1(\mathbf{U}_2^T\mathbf{U}_{\mathbf{Y},1}\mathbf{U}_{\mathbf{Y},1}^T\mathbf{U}_2) \le \frac{c^*p}{\boldsymbol{\lambda}_r n}$$

with probability at least  $1-3p/\lambda_r n$  for some constant  $c^*$ . Since  $\lambda_1(\mathbf{U}_2^T\mathbf{U}_{\mathbf{Y},1}\mathbf{U}_{\mathbf{Y},1}^T\mathbf{U}_2) \le 1$ , we have

$$\mathbb{E}\,\lambda_1(\mathbf{U}_2^T\mathbf{U}_{\mathbf{Y},1}\mathbf{U}_{\mathbf{Y},1}^T\mathbf{U}_2) \le \frac{c^*p}{\boldsymbol{\lambda}_r n}(1 - \frac{3p}{\boldsymbol{\lambda}_r n}) + \frac{3p}{\boldsymbol{\lambda}_r n} = O(\frac{p}{\boldsymbol{\lambda}_r n}).$$

This completes the proof.

**Lemma 4.** Under the assumptions of Lemma 2, we have the following upper and lower bound for  $\Lambda^{1/2}\mathbf{U}^T(\mathbf{I}_p - \mathbf{P_Y})\mathbf{U}\Lambda^{1/2}$ .

$$\lambda_i(\mathbf{\Lambda}^{1/2}\mathbf{U}^T(\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}})\mathbf{U}\mathbf{\Lambda}^{1/2}) \ge \boldsymbol{\lambda}_{i+n-k}, \quad i = 1, \dots, p-n+k,$$
 (5.21)

$$\lambda_i \left( \mathbf{\Lambda}^{1/2} \mathbf{U}^T (\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}}) \mathbf{U} \mathbf{\Lambda}^{1/2} \right) = O_P \left( \frac{\lambda_1 p}{\lambda_r n} \right) + c_1, \quad i = 1, \dots, r, \quad (5.22)$$

$$\lambda_i(\mathbf{\Lambda}^{1/2}\mathbf{U}^T(\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}})\mathbf{U}\mathbf{\Lambda}^{1/2}) \le \boldsymbol{\lambda}_i, \quad i = r + 1, \dots, p.$$
 (5.23)

Proof. The inequality (5.23) follows from the fact  $\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}} \leq \mathbf{I}_p$ . The inequality (5.21) follows from the fact that  $\operatorname{Rank}(\mathbf{P}_{\mathbf{Y}}) \leq n - k$  and Weyl's inequality. As for inequality (5.22), note that the positive eigenvalues of  $\mathbf{\Lambda}^{1/2}\mathbf{U}^T(\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}})\mathbf{U}\mathbf{\Lambda}^{1/2}$  equal to the positive eigenvalues of  $(\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}})\mathbf{U}\mathbf{\Lambda}\mathbf{U}^T(\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}})\mathbf{U}\mathbf{U}^T(\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}}$ 

 $P_Y$ ). We write  $(I_p - P_Y)U\Lambda U^T(I_p - P_Y)$  as the sum of two terms

$$(\mathbf{I}_{p}-\mathbf{P}_{\mathbf{Y}})\mathbf{U}\mathbf{\Lambda}\mathbf{U}^{T}(\mathbf{I}_{p}-\mathbf{P}_{\mathbf{Y}})$$

$$= (\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}})\mathbf{U}_1\mathbf{\Lambda}_1\mathbf{U}_1^T(\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}}) + (\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}})\mathbf{U}_2\mathbf{\Lambda}_2\mathbf{U}_2^T(\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}}) \stackrel{def}{=} \mathbf{R}_1 + \mathbf{R}_2.$$

Lemma 3 can be applied to control the largest eigenvalue of  $\mathbf{R}_1$ :

$$\lambda_1(\mathbf{R}_1) = \lambda_1(\mathbf{\Lambda}_1^{1/2}\mathbf{U}_1^T(\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}})\mathbf{U}_1\mathbf{\Lambda}_1^{1/2}) \le \lambda_1(\mathbf{\Lambda}_1^{1/2}\mathbf{U}_1^T(\mathbf{I}_p - \mathbf{U}_{\mathbf{Y},1}\mathbf{U}_{\mathbf{Y},1}^T)\mathbf{U}_1\mathbf{\Lambda}_1^{1/2})$$

$$\le \lambda_1\lambda_1(\mathbf{U}_1^T(\mathbf{I}_p - \mathbf{U}_{\mathbf{Y},1}\mathbf{U}_{\mathbf{Y},1}^T)\mathbf{U}_1) = \lambda_1\lambda_1(\mathbf{I}_r - \mathbf{U}_1^T\mathbf{U}_{\mathbf{Y},1}\mathbf{U}_{\mathbf{Y},1}^T\mathbf{U}_1) = O_P(\frac{\lambda_1p}{\lambda_rn}).$$

Thus, for  $i = 1, \ldots, r$ , we have

$$\lambda_i(\mathbf{\Lambda}^{1/2}\mathbf{U}^T(\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}})\mathbf{U}\mathbf{\Lambda}^{1/2}) \le \lambda_1(\mathbf{R}_1) + \lambda_1(\mathbf{R}_2) = O_P(\frac{\boldsymbol{\lambda}_1 p}{\boldsymbol{\lambda}_r n}) + c_1.$$

**Lemma 5.** Under the assumptions of Theorem 1, we have

$$\operatorname{tr}\left(\mathbf{\Lambda}^{1/2}\mathbf{U}^{T}(\mathbf{I}_{p}-\mathbf{P}_{\mathbf{Y}})\mathbf{U}\mathbf{\Lambda}^{1/2}\right) = \frac{p-r-n+k}{p-r}\operatorname{tr}(\mathbf{\Lambda}_{2}) + o_{P}(\sqrt{p}), \quad (5.24)$$

and

$$\operatorname{tr}\left(\mathbf{\Lambda}^{1/2}\mathbf{U}^{T}(\mathbf{I}_{p}-\mathbf{P}_{\mathbf{Y}})\mathbf{U}\mathbf{\Lambda}^{1/2}\right)^{2}=(1+o_{P}(1))\operatorname{tr}(\mathbf{\Lambda}_{2}^{2}).$$
 (5.25)

*Proof.* By Lemma 4, we have

$$\sum_{i=n-k+1}^{p} \boldsymbol{\lambda}_{i}^{2} \leq \operatorname{tr} \left( \boldsymbol{\Lambda}^{1/2} \mathbf{U}^{T} (\mathbf{I}_{p} - \mathbf{P}_{\mathbf{Y}}) \mathbf{U} \boldsymbol{\Lambda}^{1/2} \right)^{2} \leq r (O_{P} (\frac{\boldsymbol{\lambda}_{1} p}{\boldsymbol{\lambda}_{r} n}) + c_{1})^{2} + \sum_{i=r+1}^{p} \boldsymbol{\lambda}_{i}^{2}.$$

Hence

$$\left|\operatorname{tr}\left(\mathbf{\Lambda}^{1/2}\mathbf{U}^{T}(\mathbf{I}_{p}-\mathbf{P}_{\mathbf{Y}})\mathbf{U}\mathbf{\Lambda}^{1/2}\right)^{2}-\sum_{i=r+1}^{p}\boldsymbol{\lambda}_{i}^{2}\right|$$

$$\leq \max\left(\sum_{i=r+1}^{n-k}\boldsymbol{\lambda}_{i}^{2},r(O_{P}(\frac{\boldsymbol{\lambda}_{1}p}{\boldsymbol{\lambda}_{r}n})+c_{1})^{2}\right)$$

$$\leq r(O_{P}(\frac{\boldsymbol{\lambda}_{1}p}{\boldsymbol{\lambda}_{r}n})+c_{1})^{2}+O(n)=o_{P}(p).$$

Then (5.25) holds.

Now we prove (5.24). Note that

$$\operatorname{tr}\left(\boldsymbol{\Lambda}^{1/2}\mathbf{U}^{T}(\mathbf{I}_{p}-\mathbf{P}_{\mathbf{Y}})\mathbf{U}\boldsymbol{\Lambda}^{1/2}\right) = \operatorname{tr}\left(\boldsymbol{\Lambda}_{1}^{1/2}\mathbf{U}_{1}^{T}(\mathbf{I}_{p}-\mathbf{P}_{\mathbf{Y}})\mathbf{U}_{1}\boldsymbol{\Lambda}_{1}^{1/2}\right) + \operatorname{tr}\left(\boldsymbol{\Lambda}_{2}^{1/2}\mathbf{U}_{2}^{T}(\mathbf{I}_{p}-\mathbf{P}_{\mathbf{Y}})\mathbf{U}_{2}\boldsymbol{\Lambda}_{2}^{1/2}\right).$$

By Lemma 4, we have

$$\operatorname{tr}\left(\mathbf{\Lambda}_{1}^{1/2}\mathbf{U}_{1}^{T}(\mathbf{I}_{p}-\mathbf{P}_{\mathbf{Y}})\mathbf{U}_{1}\mathbf{\Lambda}_{1}^{1/2}\right)=O_{P}\left(\frac{\boldsymbol{\lambda}_{1}pr}{\boldsymbol{\lambda}_{r}n}\right)=o_{P}(\sqrt{p}).$$

The second term can be written as  $\operatorname{tr}\left(\mathbf{\Lambda}_{2}^{1/2}\mathbf{U}_{2}^{T}(\mathbf{I}_{p}-\mathbf{P}_{\mathbf{Y}})\mathbf{U}_{2}\mathbf{\Lambda}_{2}^{1/2}\right)=\operatorname{tr}(\mathbf{\Lambda}_{2})-$ 

 $\operatorname{tr}(\mathbf{P}_{\mathbf{Y}}\mathbf{U}_{2}\mathbf{\Lambda}_{2}\mathbf{U}_{2}^{T})$ . For  $\operatorname{tr}(\mathbf{P}_{\mathbf{Y}}\mathbf{U}_{2}\mathbf{\Lambda}_{2}\mathbf{U}_{2}^{T})$ , we have

$$\left|\operatorname{tr}(\mathbf{P}_{\mathbf{Y}}\mathbf{U}_{2}\boldsymbol{\Lambda}_{2}\mathbf{U}_{2}^{T})-\frac{n-k}{p-r}\operatorname{tr}(\boldsymbol{\Lambda}_{2})\right|=\left|\operatorname{tr}\left(\mathbf{P}_{\mathbf{Y}}\mathbf{U}\left(\boldsymbol{\Lambda}_{2}-\frac{1}{p-r}(\operatorname{tr}\boldsymbol{\Lambda}_{2})\mathbf{I}_{p-r}\right)\mathbf{U}^{T}\right)\right|$$

$$\leq\sqrt{\operatorname{tr}\left(\mathbf{P}_{\mathbf{Y}}^{2}\right)}\sqrt{\operatorname{tr}\left(\boldsymbol{\Lambda}_{2}-\frac{1}{p-r}\left(\operatorname{tr}\boldsymbol{\Lambda}_{2}\right)\mathbf{I}_{p-r}\right)^{2}}=\sqrt{(n-k)\operatorname{tr}\left(\boldsymbol{\Lambda}_{2}-\frac{1}{p-r}\left(\operatorname{tr}\boldsymbol{\Lambda}_{2}\right)\mathbf{I}_{p-r}\right)^{2}}=o(\sqrt{p}).$$

Hence

$$\operatorname{tr}\left(\boldsymbol{\Lambda}_{2}^{1/2}\mathbf{U}_{2}^{T}(\mathbf{I}_{p}-\mathbf{P}_{\mathbf{Y}})\mathbf{U}_{2}\boldsymbol{\Lambda}_{2}^{1/2}\right)=\frac{p-r-n+k}{p-r}\operatorname{tr}(\boldsymbol{\Lambda}_{2})+o(\sqrt{p}).$$

Then (5.24) holds.

Proof of Theorem 1. Lemma (4) implies that the first term of (5.7) satisfies the Lyapunov condition

$$\frac{\lambda_1 \left( \left( \mathbf{\Lambda}^{1/2} \mathbf{U}^T (\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}}) \mathbf{U} \mathbf{\Lambda}^{1/2} \right)^2 \right)}{\operatorname{tr} \left( \left( \mathbf{\Lambda}^{1/2} \mathbf{U}^T (\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}}) \mathbf{U} \mathbf{\Lambda}^{1/2} \right)^2 \right)} = \frac{\left( O_P \left( \frac{\mathbf{\lambda}_{1p}}{\mathbf{\lambda}_{rn}} \right) + c_1 \right)^2}{\left( 1 + o_P(1) \right) \operatorname{tr} (\mathbf{\Lambda}_2)} \xrightarrow{P} 0.$$

Apply Lyapunov central limit theorem conditioning on  $\mathbf{P}_{\mathbf{Y}}$ , we have

$$\left(\operatorname{tr}\left(\left(\mathbf{\Lambda}^{1/2}\mathbf{U}^{T}(\mathbf{I}_{p}-\mathbf{P}_{\mathbf{Y}})\mathbf{U}\mathbf{\Lambda}^{1/2}\right)^{2}\right)\right)^{-1/2}$$

$$\left(\mathbf{G}_{2}^{T}\mathbf{\Lambda}^{1/2}\mathbf{U}^{T}(\mathbf{I}_{p}-\mathbf{P}_{\mathbf{Y}})\mathbf{U}\mathbf{\Lambda}^{1/2}\mathbf{G}_{2}-\operatorname{tr}\left(\mathbf{\Lambda}^{1/2}\mathbf{U}^{T}(\mathbf{I}_{p}-\mathbf{P}_{\mathbf{Y}})\mathbf{U}\mathbf{\Lambda}^{1/2}\right)\mathbf{I}_{k-1}\right)\xrightarrow{\mathcal{L}}\mathbf{W}_{k-1}.$$

This, combined with Lemma 5 and Slutsky's theorem, yields

$$\frac{1}{\sqrt{\operatorname{tr}(\boldsymbol{\Lambda}_2^2)}} \left( \mathbf{G}_2^T \boldsymbol{\Lambda}^{1/2} \mathbf{U}^T (\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}}) \mathbf{U} \boldsymbol{\Lambda}^{1/2} \mathbf{G}_2 - \frac{p - r - n + k}{p - r} \operatorname{tr}(\boldsymbol{\Lambda}_2) \mathbf{I}_{k-1} \right) \xrightarrow{\mathcal{L}} \mathbf{W}_{k-1}.$$

Next we show that the cross term of (5.7) is negligible. Note that

$$E[\|\mathbf{C}^{T}\Xi^{T}(\mathbf{I}_{p} - \mathbf{P}_{Z\tilde{J}})\mathbf{U}\boldsymbol{\Lambda}^{1/2}\mathbf{G}_{2}\|_{F}^{2}|\mathbf{Y}]$$

$$= (k-1)\operatorname{tr}(\mathbf{C}^{T}\Xi^{T}(\mathbf{I}_{p} - \mathbf{P}_{\mathbf{Y}})\mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^{T}(\mathbf{I}_{p} - \mathbf{P}_{\mathbf{Y}})\Xi\mathbf{C})$$

$$\leq (k-1)\lambda_{1}((\mathbf{I}_{p} - \mathbf{P}_{\mathbf{Y}})\mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^{T}(\mathbf{I}_{p} - \mathbf{P}_{\mathbf{Y}}))\|\Xi\mathbf{C}\|_{F}^{2}$$

$$\leq (k-1)\lambda_{1}(\boldsymbol{\Lambda}^{1/2}\mathbf{U}^{T}(\mathbf{I}_{p} - \mathbf{P}_{\mathbf{Y}})\mathbf{U}\boldsymbol{\Lambda}^{1/2})\|\Xi\mathbf{C}\|_{F}^{2}$$

$$= (k-1)O_{P}(\frac{\lambda_{1}p}{\lambda_{r}n} + c_{1})\|\Xi\mathbf{C}\|_{F}^{2}$$

$$= (k-1)O_{P}(\frac{\lambda_{1}\sqrt{p}}{\lambda_{r}n} + \frac{c_{1}}{\sqrt{p}})\sqrt{p}\|\Xi\mathbf{C}\|_{F}^{2} = o_{P}(p),$$

where the last equality holds since we have assumed  $\frac{1}{\sqrt{p}} \|\Xi \mathbf{C}\|_F^2 = O(1)$ .

Hence 
$$\|\mathbf{C}^T \Xi^T (\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}}) \mathbf{U} \mathbf{\Lambda}^{1/2} \mathbf{G}_2 \|_F^2 = o_P(p)$$
. Now,

$$\frac{1}{\sqrt{\operatorname{tr}(\boldsymbol{\Lambda}_2^2)}} \left( \mathbf{C}^T \mathbf{Y}^T (\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}}) \mathbf{Y} \mathbf{C} - \frac{p-r-n+k}{p-r} \operatorname{tr}(\boldsymbol{\Lambda}_2) \mathbf{I}_{k-1} - \mathbf{C}^T \boldsymbol{\Xi}^T (\mathbf{I}_p - \mathbf{P}_{\mathbf{Y}}) \boldsymbol{\Xi} \mathbf{C} \right) \xrightarrow{\mathcal{L}} \mathbf{W}_{k-1}.$$

Equivalently,

$$\frac{1}{\sqrt{\operatorname{tr}(\mathbf{\Lambda}_{2}^{2})}} \left( \mathbf{C}^{T} \mathbf{Y}^{T} (\mathbf{I}_{p} - \mathbf{P}_{\mathbf{Y}}) \mathbf{Y} \mathbf{C} - \frac{p - r - n + k}{p - r} \operatorname{tr}(\mathbf{\Lambda}_{2}) \mathbf{I}_{k-1} \right) 
\sim \frac{1}{\sqrt{\operatorname{tr}(\mathbf{\Lambda}_{2}^{2})}} \mathbf{C}^{T} \Xi^{T} (\mathbf{I}_{p} - \mathbf{P}_{\mathbf{Y}}) \Xi \mathbf{C} + \mathbf{W}_{k-1} + o_{P}(1).$$

The conclusion follows by taking the maximum eigenvalue.

Proof of Proposition 1. First we consider the case of r > 0. By the construction of  $\hat{r}$ ,

$$\{\hat{r} = r\} \supseteq \{\frac{\lambda_r(\mathbf{Y}^T\mathbf{Y})}{\lambda_{r+1}(\mathbf{Y}^T\mathbf{Y})} \ge \gamma_n\} \cap \{\frac{\lambda_{r+1}(\mathbf{Y}^T\mathbf{Y})}{\lambda_{n-k}(\mathbf{Y}^T\mathbf{Y})} \le \gamma_n\}.$$

Suppose  $0 < \epsilon < 1$  is a fixed number. By assumption, there exists an  $n_0^*$ , for  $n \ge n_0^*$ ,  $\gamma_n \le (1 - \epsilon)n\lambda_r/(c_1p)$  and  $\gamma_n \ge (1 + \epsilon)c_1/c_2$ . Thus

$$\{\hat{r} = r\} \supseteq \{\frac{\lambda_r(\mathbf{Y}^T\mathbf{Y})}{\lambda_{r+1}(\mathbf{Y}^T\mathbf{Y})} \ge (1 - \epsilon)\frac{n\lambda_r}{c_1p}\} \cap \{\frac{\lambda_{r+1}(\mathbf{Y}^T\mathbf{Y})}{\lambda_{n-k}(\mathbf{Y}^T\mathbf{Y})} \le (1 + \epsilon)\frac{c_1}{c_2}\}.$$

Lemma 2 implies that almost surely, there exists an  $n_0$ , for  $n \geq n_0$ , we have

$$\frac{\lambda_r(\mathbf{Y}^T\mathbf{Y})}{\lambda_{r+1}(\mathbf{Y}^T\mathbf{Y})} \ge (1 - \epsilon) \frac{n\lambda_r}{c_1 p}, \quad \frac{\lambda_{r+1}(\mathbf{Y}^T\mathbf{Y})}{\lambda_{n-k}(\mathbf{Y}^T\mathbf{Y})} \le (1 + \epsilon) \frac{c_1}{c_2}.$$

This yields  $\Pr(\hat{r} = r) \to 1$  for r > 0. The case of r = 0 can be similarly proved by noting that

$$\{\hat{r} = r\} \supseteq \{\frac{\lambda_1(\mathbf{Y}^T\mathbf{Y})}{\lambda_{n-k}(\mathbf{Y}^T\mathbf{Y})} \le \gamma_n\}.$$

Proof of Proposition 2. Since  $\hat{r}$  is a consistent estimator of r, we only need to prove

$$\frac{1}{n-k} \sum_{i=r+1}^{n-k} \lambda_i(\mathbf{Y}^T \mathbf{Y}) = \operatorname{tr}(\mathbf{\Lambda}_2) + O_P(\sqrt{p}).$$

Note that

$$\mathbf{Y}^T\mathbf{Y} = \mathbf{G}_1^T \mathbf{\Lambda} \mathbf{G}_1 = \mathbf{G}_{1A}^T \mathbf{\Lambda}_1 \mathbf{G}_{1A} + \mathbf{G}_{1B}^T \mathbf{\Lambda}_2 \mathbf{G}_{1B}.$$

By Weyl's inequality, for i = r + 1, ..., n - k, we have

$$\lambda_i(\mathbf{G}_{1B}^T \mathbf{\Lambda}_2 \mathbf{G}_{1B}) \le \lambda_i(\mathbf{Y}^T \mathbf{Y}) \le \lambda_{i-r}(\mathbf{G}_{1B}^T \mathbf{\Lambda}_2 \mathbf{G}_{1B}).$$

It follows that

$$\sum_{i=r+1}^{n-k} \lambda_i(\mathbf{G}_{1B}^T \mathbf{\Lambda}_2 \mathbf{G}_{1B}) \leq \sum_{i=r+1}^{n-k} \lambda_i(\mathbf{Y}^T \mathbf{Y}) \leq \sum_{i=1}^{n-k-r} \lambda_i(\mathbf{G}_{1B}^T \mathbf{\Lambda}_2 \mathbf{G}_{1B}).$$

Hence

$$\left|\sum_{i=r+1}^{n-k} \lambda_i(\mathbf{Y}^T \mathbf{Y}) - \operatorname{tr}(\mathbf{G}_{1B}^T \mathbf{\Lambda}_2 \mathbf{G}_{1B})\right| \le r \lambda_1(\mathbf{G}_{1B}^T \mathbf{\Lambda}_2 \mathbf{G}_{1B}) = O_P(rp).$$

But central limit theorem implies that

$$\operatorname{tr}(\mathbf{G}_{1B}^T \mathbf{\Lambda}_2 \mathbf{G}_{1B}) - (n-k) \operatorname{tr}(\mathbf{\Lambda}_2) = O_P(\sqrt{np}).$$

Thus

$$\frac{1}{n-k} \sum_{i=r+1}^{n-k} \lambda_i(\mathbf{Y}^T \mathbf{Y}) = \operatorname{tr}(\mathbf{\Lambda}_2) + \frac{1}{n-k} \Big| \sum_{i=r+1}^{n-k} \lambda_i(\mathbf{Y}^T \mathbf{Y}) - (n-k) \operatorname{tr}(\mathbf{\Lambda}_2) \Big|$$

$$=\operatorname{tr}(\mathbf{\Lambda}_2) + O_P(\frac{rp}{n}) = \operatorname{tr}(\mathbf{\Lambda}_2) + O_P(\sqrt{p}),$$

where the last equality follows form Assumption 1.

Proof of Proposition 3. Let  $\mathbf{U}_{\mathbf{Y},1;(i,j)}$  be the first r columns of  $\mathbf{U}_{\mathbf{Y};(i,j)}$ . Let  $\mathbf{U}_{\mathbf{Y},2;(i,j)}$  be a  $p \times (p-r)$  orthogonal matrix satisfying  $\mathbf{U}_{\mathbf{Y},2;(i,j)}\mathbf{U}_{\mathbf{Y},2;(i,j)}^T = \mathbf{I}_p - \mathbf{U}_{\mathbf{Y},1;(i,j)}\mathbf{U}_{\mathbf{Y},1;(i,j)}^T$ . Then by Lemma 3, we have

$$\lambda_1(\mathbf{U}_1^T\mathbf{U}_{\mathbf{Y},2;(i,j)}\mathbf{U}_{\mathbf{Y},2;(i,j)}^T\mathbf{U}_1) = \lambda_1(\mathbf{I}_r - \mathbf{U}_1^T\mathbf{U}_{\mathbf{Y},1;(i,j)}\mathbf{U}_{\mathbf{Y},1;(i,j)}^T\mathbf{U}_1) = O_P(\frac{p}{\boldsymbol{\lambda}_r n}).$$

First, we prove that  $w_{ij}^2$  is an approximation of  $Y_i^T \mathbf{U}_2 \mathbf{U}_2^T Y_j$ . For  $1 \le i < j \le n - k$ , define  $\epsilon_{ij} = w_{ij} - Y_i^T \mathbf{U}_2 \mathbf{U}_2^T Y_j$ , then we have

$$\begin{split} \epsilon_{ij} &= Y_i^T (\tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^T - \mathbf{U}_2 \mathbf{U}_2^T) Y_j \\ &= Y_i^T (\mathbf{U}_1 \mathbf{U}_1^T + \mathbf{U}_2 \mathbf{U}_2^T) (\tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^T - \mathbf{U}_2 \mathbf{U}_2^T) (\mathbf{U}_1 \mathbf{U}_1^T + \mathbf{U}_2 \mathbf{U}_2^T) Y_j \\ &= Y_i^T \mathbf{U}_2 \mathbf{U}_2^T (\tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^T - \mathbf{U}_2 \mathbf{U}_2^T) \mathbf{U}_2 \mathbf{U}_2^T Y_j \\ &+ Y_i^T \mathbf{U}_1 \mathbf{U}_1^T \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^T \mathbf{U}_2 \mathbf{U}_2^T Y_j \\ &+ Y_i^T \mathbf{U}_2 \mathbf{U}_2^T \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^T \mathbf{U}_1 \mathbf{U}_1^T Y_j \\ &+ Y_i^T \mathbf{U}_1 \mathbf{U}_1^T \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^T \mathbf{U}_1 \mathbf{U}_1^T Y_j \\ &= Y_i^T \mathbf{U}_2 \mathbf{U}_2^T (\tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^T - \mathbf{U}_{\mathbf{Y},2;(i,j)} \mathbf{U}_{\mathbf{Y},2;(i,j)}^T) \mathbf{U}_2 \mathbf{U}_2^T Y_j \\ &+ Y_i^T \mathbf{U}_2 \mathbf{U}_2^T (\mathbf{U}_{\mathbf{Y},2;(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^T \mathbf{U}_2 \mathbf{U}_2^T Y_j \\ &+ Y_i^T \mathbf{U}_1 \mathbf{U}_1^T \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^T \mathbf{U}_1 \mathbf{U}_1^T Y_j \\ &+ Y_i^T \mathbf{U}_1 \mathbf{U}_1^T \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^T \mathbf{U}_1 \mathbf{U}_1^T Y_j \\ &+ Y_i^T \mathbf{U}_1 \mathbf{U}_1^T \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^T \mathbf{U}_1 \mathbf{U}_1^T Y_j \\ &+ Y_i^T \mathbf{U}_1 \mathbf{U}_1^T \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^T \mathbf{U}_1 \mathbf{U}_1^T Y_j \\ &+ Y_i^T \mathbf{U}_1 \mathbf{U}_1^T \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^T \mathbf{U}_1 \mathbf{U}_1^T Y_j \\ &= \epsilon_{ij}^{(1)} + \epsilon_{ij}^{(2)} + \epsilon_{ij}^{(3)} + \epsilon_{ij}^{(4)} + \epsilon_{ij}^{(5)}. \end{split}$$

(5.26)

We deal with the five terms separately. First we deal with  $\epsilon_{ij}^{(1)}$ . It can be seen that  $Y_i$ ,  $Y_j$  and  $\tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}$  are mutually independent and  $\tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}\tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^T - \mathbf{U}_{\mathbf{Y},2;(i,j)}\mathbf{U}_{\mathbf{Y},2;(i,j)}^T$  is a projection matrix whose rank is not larger than n-k-2-r. Then

$$\begin{split} & & \mathrm{E}(\epsilon_{ij}^{(1)})^2 \\ & = \mathrm{E}\,\mathrm{tr}(\boldsymbol{\Lambda}_2^{1/2}\mathbf{U}_2^T(\tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}\tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^T - \mathbf{U}_{\mathbf{Y},2;(i,j)}\mathbf{U}_{\mathbf{Y},2;(i,j)}^T)\mathbf{U}_2\boldsymbol{\Lambda}_2^{1/2})^2 \\ & \leq & c_1^2(n-k-2-r) = o(p). \end{split}$$

Next we deal with  $\epsilon_{ij}^{(2)}$  we have

$$E(\epsilon_{ij}^{(2)})^{2}$$

$$= E \operatorname{tr}(\boldsymbol{\Lambda}_{2}^{1/2} \mathbf{U}_{2}^{T}(\mathbf{U}_{\mathbf{Y},2;(i,j)} \mathbf{U}_{\mathbf{Y},2;(i,j)}^{T} - \mathbf{U}_{2} \mathbf{U}_{2}^{T}) \mathbf{U}_{2} \boldsymbol{\Lambda}_{2}^{1/2})^{2}$$

$$\leq c_{1}^{2} E \operatorname{tr}(\mathbf{U}_{2}^{T}(\mathbf{U}_{\mathbf{Y},2;(i,j)} \mathbf{U}_{\mathbf{Y},2;(i,j)}^{T} - \mathbf{U}_{2} \mathbf{U}_{2}^{T}) \mathbf{U}_{2})^{2}$$

$$= c_{1}^{2} E \operatorname{tr}(\mathbf{I}_{p-r} - \mathbf{U}_{2}^{T} \mathbf{U}_{\mathbf{Y},2;(i,j)} \mathbf{U}_{\mathbf{Y},2;(i,j)}^{T} \mathbf{U}_{2})^{2}$$

$$= c_{1}^{2} E \operatorname{tr}(\mathbf{I}_{r} - \mathbf{U}_{1}^{T} \mathbf{U}_{\mathbf{Y},1;(i,j)} \mathbf{U}_{\mathbf{Y},1;(i,j)}^{T} \mathbf{U}_{1})^{2}$$

$$\leq c_{1}^{2} r E \lambda_{1}^{2} (\mathbf{I}_{r} - \mathbf{U}_{1}^{T} \mathbf{U}_{\mathbf{Y},1;(i,j)} \mathbf{U}_{\mathbf{Y},1;(i,j)}^{T} \mathbf{U}_{1})$$

$$= O(r(\frac{p}{\boldsymbol{\lambda}_{r}n})^{2}) = o(p).$$

Note that  $\epsilon_{i,j}^{(3)}$  and  $\epsilon_{i,j}^{(4)}$  have the same distribution, we have

$$E(\epsilon_{ij}^{(3)})^{2} = E(\epsilon_{ij}^{(4)})^{2}$$

$$= E \operatorname{tr}(\boldsymbol{\Lambda}_{1}^{1/2} \mathbf{U}_{1}^{T} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^{T} \mathbf{U}_{2} \boldsymbol{\Lambda}_{2} \mathbf{U}_{2}^{T} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^{T} \mathbf{U}_{1} \boldsymbol{\Lambda}_{1}^{1/2})$$

$$\leq c_{1} \boldsymbol{\lambda}_{1} E \operatorname{tr}(\mathbf{U}_{1}^{T} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^{T} \mathbf{U}_{2} \mathbf{U}_{2}^{T} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^{T} \mathbf{U}_{1})$$

$$\leq c_{1} \boldsymbol{\lambda}_{1} E \operatorname{tr}(\mathbf{U}_{1}^{T} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^{T} \mathbf{U}_{1})$$

$$\leq c_{1} \boldsymbol{\lambda}_{1} E \operatorname{tr}(\mathbf{U}_{1}^{T} \mathbf{U}_{\mathbf{Y},2;(i,j)} \mathbf{U}_{\mathbf{Y},2;(i,j)}^{T} \mathbf{U}_{1})$$

$$\leq c_{1} \boldsymbol{\lambda}_{1} r \frac{p}{\boldsymbol{\lambda}_{1} r} = o(p).$$

As for  $\epsilon_{i,j}^{(5)}$ , we have

$$E(\epsilon_{ij}^{(5)})^{2}$$

$$= E \operatorname{tr}(\boldsymbol{\Lambda}_{1}^{1/2} \mathbf{U}_{1}^{T} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^{T} \mathbf{U}_{1} \boldsymbol{\Lambda}_{1}^{1/2})^{2}$$

$$\leq \boldsymbol{\lambda}_{1}^{2} E \operatorname{tr}(\mathbf{U}_{1}^{T} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)} \tilde{\mathbf{U}}_{\mathbf{Y};(i,j)}^{T} \mathbf{U}_{1})^{2}$$

$$\leq \boldsymbol{\lambda}_{1}^{2} E \operatorname{tr}(\mathbf{U}_{1}^{T} \mathbf{U}_{\mathbf{Y},2;(i,j)} \mathbf{U}_{\mathbf{Y},2;(i,j)}^{T} \mathbf{U}_{1})^{2}$$

$$\leq \boldsymbol{\lambda}_{1}^{2} r(\frac{p}{\boldsymbol{\lambda}_{1} p})^{2} = o(p).$$

Note that

$$\begin{split} \widehat{\operatorname{tr}(\boldsymbol{\Lambda}_{2}^{2})} &= \frac{2}{(n-k)(n-k-1)} \sum_{1 \leq i < j \leq n-k} (Y_{i}^{T} \mathbf{U}_{2} \mathbf{U}_{2}^{T} Y_{j})^{2} \\ &+ \frac{2}{(n-k)(n-k-1)} \sum_{1 \leq i < j \leq n-k} \left( (\sum_{l=1}^{5} \epsilon_{ij}^{(l)}) (Y_{i}^{T} \mathbf{U}_{2} \mathbf{U}_{2}^{T} Y_{j}) + (\sum_{l=1}^{5} \epsilon_{ij}^{(l)})^{2} \right). \end{split}$$

We have

$$E \left| \frac{2}{(n-k)(n-k-1)} \sum_{1 \leq i < j \leq n-k} \left( \left( \sum_{l=1}^{5} \epsilon_{ij}^{(l)} \right) (Y_i^T \mathbf{U}_2 \mathbf{U}_2^T Y_j) + \left( \sum_{l=1}^{5} \epsilon_{ij}^{(l)} \right)^2 \right) \right| \\
\leq E \left| \left( \sum_{l=1}^{5} \epsilon_{12}^{(l)} \right) (Y_1^T \mathbf{U}_2 \mathbf{U}_2^T Y_2) + \left( \sum_{l=1}^{5} \epsilon_{12}^{(l)} \right)^2 \right| \\
\leq \sqrt{E \left( \sum_{l=1}^{5} \epsilon_{12}^{(l)} \right)^2 E \left( Y_1^T \mathbf{U}_2 \mathbf{U}_2^T Y_2 \right)^2 + E \left( \sum_{l=1}^{5} \epsilon_{12}^{(l)} \right)^2 = o(p)}.$$

It follows that

$$\widehat{\operatorname{tr}(\boldsymbol{\Lambda}_2^2)} = \frac{2}{(n-k)(n-k-1)} \sum_{1 \le i \le j \le n-k} (Y_i^T \mathbf{U}_2 \mathbf{U}_2^T Y_j)^2 + o_P(p).$$

Now we only need to prove that

$$\frac{2}{(n-k)(n-k-1)} \sum_{1 \le i \le j \le n-k} (Y_i^T \mathbf{U}_2 \mathbf{U}_2^T Y_j)^2$$

is ratio consistent. Since  $\mathrm{E}(Y_i^T\mathbf{U}_2\mathbf{U}_2^TY_j)^2 = \mathrm{tr}(\mathbf{\Lambda}_2^2)$  for i < j, we have

$$E \frac{2}{(n-k)(n-k-1)} \sum_{1 \le i < j \le n-k} (Y_i^T \mathbf{U}_2 \mathbf{U}_2^T Y_j)^2 = \operatorname{tr}(\boldsymbol{\Lambda}_2^2).$$

To prove the proposition, we only need to show that

$$\operatorname{Var}\left(\frac{2}{(n-k)(n-k-1)}\sum_{1 \le i \le j \le n-k} (Y_i^T \mathbf{U}_2 \mathbf{U}_2^T Y_j)^2\right) = o(\operatorname{tr}^2(\mathbf{\Lambda}_2^2)).$$

Note that

$$\begin{split} & \operatorname{E}\left(\frac{2}{(n-k)(n-k-1)} \sum_{1 \leq i < j \leq n-k} (Y_i^T \mathbf{U}_2 \mathbf{U}_2^T Y_j)^2\right)^2 \\ = & \frac{4}{(n-k)^2 (n-k-1)^2} \bigg(\sum_{1 \leq i < j \leq n-k} (Y_i^T \mathbf{U}_2 \mathbf{U}_2^T Y_j)^2\bigg)^2 \\ = & \frac{4}{(n-k)^2 (n-k-1)^2} \operatorname{E}\left(\sum_{i < j} (Y_i^T \mathbf{U}_2 \mathbf{U}_2^T Y_j)^4 \right. \\ & + \sum_{i < j, k < l: \{i, j\} \{k, l\} = \emptyset} (Y_i^T \mathbf{U}_2 \mathbf{U}_2^T Y_j)^2 (Y_k^T \mathbf{U}_2 \mathbf{U}_2^T Y_l)^2 \\ & + 2 \sum_{i < j < k} \left( (Y_i^T \mathbf{U}_2 \mathbf{U}_2^T Y_j)^2 (Y_i \mathbf{U}_2 \mathbf{U}_2^T Y_k)^2 \right. \\ & + (Y_i^T \mathbf{U}_2 \mathbf{U}_2^T Y_j)^2 (Y_j \mathbf{U}_2 \mathbf{U}_2^T Y_k)^2 + (Y_i^T \mathbf{U}_2 \mathbf{U}_2^T Y_k)^2 (Y_j \mathbf{U}_2 \mathbf{U}_2^T Y_k)^2 \bigg) \bigg) \\ = & \frac{4}{(n-k)^2 (n-k-1)^2} \bigg( \frac{(n-k)(n-k-1)}{2} \Big( 6 \operatorname{tr}(\boldsymbol{\Lambda}_2^4) + 3 \operatorname{tr}^2(\boldsymbol{\Lambda}_2^2) \Big) \\ & + \frac{(n-k)(n-k-1)(n-k-2)(n-k-3)}{4} \operatorname{tr}^2(\boldsymbol{\Lambda}_2^2) \bigg) \\ & + (n-k)(n-k-1)(n-k-2) \Big( 2 \operatorname{tr}(\boldsymbol{\Lambda}_2^4) + \operatorname{tr}^2(\boldsymbol{\Lambda}_2^2) \Big) \bigg) \\ = & \operatorname{tr}^2(\boldsymbol{\Lambda}_2^2) (1+o(1)). \end{split}$$

It follows that

$$\operatorname{Var}\left(\frac{2}{(n-k)(n-k-1)}\sum_{1 \le i \le j \le n-k} (Y_i^T \mathbf{U}_2 \mathbf{U}_2^T Y_j)^2\right) = o(\operatorname{tr}^2(\mathbf{\Lambda}_2^2)).$$

This completes the proof.

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