Tests of Mean Vectors in High-Dimension, Low-Sample-Size Context

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Abstract: A common feature of high-dimensional data is that the data dimension is high, however, the sample size is relatively low. We call such data HDLSS data. In this paper, we consider a new one-sample test and two-sample test for high-dimensional data under the strongly spiked eigenvalue (SSE) model. We focus on the asymptotic properties of the first principal component to provide new test procedures. We consider HDLSS asymptotic theories as the dimension grows for both the cases when the sample size is fixed and the sample size goes to infinity. We introduce the noise-reduction (NR) methodology and provide asymptotic properties of the largest-eigenvalue estimation. We apply the NR method to the one-sample test and two-sample test. Finally, we give simulation studies and discuss the performance of the new one-sample test procedure.

Keywords: HDLSS; Large p, small n; Noise-reduction methodology; One-sample test; Two-sample test.

1 Introduction

In this paper, we consider the one-sample test and the two-sample test for high-dimensional data. The problem of testing mean vectors has been studied by a lot of papers, however, it is still necessary to study these problems under more suitable conditions for actual high-dimensional data.

Suppose we have two independent $d \times n_i$ data matrices, $X_i = [x_{ij}, ..., x_{in_i}]$, i = 1, 2, where x_{ij} , $j = 1, ..., n_i$, are independent and identically distributed (i.i.d.) as a d-dimensional distribution with a mean vector μ_i and covariance matrix $\Sigma_i (\geq O)$. We assume $n_i \geq 3$, i = 1, 2. The eigen-decomposition of Σ_i is given by $\Sigma_i = H_i \Lambda_i H_i^T$, where $\Lambda_i = \text{diag}(\lambda_{1(i)}, ..., \lambda_{d(i)})$ having $\lambda_{1(i)} \geq \cdots \geq \lambda_{d(i)} (\geq 0)$ and $H_i = [h_{1(i)}, ..., h_{d(i)}]$ is an orthogonal matrix of the corresponding eigenvectors. Let $X_i - [\mu_i, ..., \mu_i] = H_i \Lambda_i^{1/2} Z_i$ for i = 1, 2. Then, Z_i is a $d \times n_i$ sphered data matrix from a distribution with the zero mean and identity covariance matrix. Let $Z_i = [z_{1(i)}, ..., z_{d(i)}]^T$ and $z_{j(i)} = (z_{j1(i)}, ..., z_{jn_i(i)})^T$, j = 1, ..., d, for i = 1, 2. Note that $E(z_{jk(i)}z_{j'k(i)}) = 0$ $(j \neq j')$ and $\operatorname{Var}(z_{j(i)}) = I_{n_i}$, where I_{n_i} is the n_i -dimensional identity matrix. Let $z_{oj(i)} = z_{j(i)} - (\overline{z}_{j(i)}, ..., \overline{z}_{j(i)})^T$, j = 1, ..., d; i = 1, 2, where $\overline{z}_{j(i)} = n_i^{-1} \sum_{k=1}^{n_i} z_{jk(i)}$. Also, note that if X_i is Gaussian, $z_{jk(i)}$ s are i.i.d. as the standard normal distribution, N(0, 1). We assume that $\limsup_{d\to\infty} E(z_{jk(i)}^4) < \infty$ for all i, j, k, and $P(\lim_{d\to\infty} ||z_{o1(i)}|| \neq 0) = 1$ for i = 1, 2. As necessary, we consider the following assumption for $z_{1k(i)}, k = 1, ..., n_i$:

(A-i) $z_{1k(i)}, k = 1, ..., n_i$, are i.i.d. as N(0, 1) for i = 1, 2.

We define $\overline{x}_{in_i} = \sum_{j=1}^{n_i} x_{ij}/n_i$ and $S_{in_i} = \sum_{j=1}^{n_i} (x_{ij} - \overline{x}_{in_i})(x_{ij} - \overline{x}_{in_i})^T/(n_i - 1)$ for i = 1, 2. Let us write the eigen-decomposition of S_{in_i} as $S_{in_i} = \sum_{j=1}^d \hat{\lambda}_{j(i)} \hat{h}_{j(i)} \hat{h}_{j(i)}^T$, where $\hat{h}_{j(i)}$ denotes a unit eigenvector corresponding to $\hat{\lambda}_{j(i)}$. A famous method to test for mean vectors is Hotelling's T^2 test, however, one cannot use the test statistic in the HDLSS context such as $n_i/d \rightarrow 0$, i = 1, 2. In order to overcome such situations, Dempster [7, 8] and Srivastava [12] considered the two-sample test when the populations π_1 and π_2 are Gaussian. When π_1 and π_2 are non-Gaussian, Bai and Saranadasa [4] and Cai et al. [5] considered the test under the homoscedasticity, $\Sigma_1 = \Sigma_2$, and Chen and Qin [6] and Aoshima and Yata [1,2] considered the test under the heteroscedasticity, $\Sigma_1 \neq \Sigma_2$. We note that those two-sample tests were constructed under the eigenvalue condition as follows:

$$\frac{\lambda_{1(i)}^2}{\operatorname{tr}(\boldsymbol{\Sigma}_i^2)} \to 0 \text{ as } d \to \infty \text{ for } i = 1, 2.$$
(1.1)

Aoshima and Yata [3] called (1.1) the "non-strongly spiked eigenvalue (NSSE) model". On the other hand, Aoshima and Yata [3] considered the "strongly spiked eigenvalue (SSE) model" as follows:

$$\liminf_{d \to \infty} \left\{ \frac{\lambda_{1(i)}^2}{\operatorname{tr}(\boldsymbol{\Sigma}_i^2)} \right\} > 0 \text{ for } i = 1 \text{ or } 2.$$
(1.2)

For the SSE model, Katayama et al. [10] considered a one-sample test when x_{ij} s are Gaussian. Ishii et al. [9] considered the one-sample test for non-Gaussian cases. Ma et al. [11] considered a two-sample test for the factor model. Aoshima and Yata [3] gave two-sample tests by considering eigenstructures when $d \to \infty$ and $n_i \to \infty$, i = 1, 2. In this paper, we disscuss a one-sample test and a two-sample test for the SSE model when $d \to \infty$ while n_i s are fixed.

In Section 2, we introduce the noise-reduction (NR) methodology and provide asymptotic distribution of the largest-eigenvalue estimation in the HDLSS context. Then, we apply the NR method to the one-sample test for the SSE model in Section 3. In Section4, we consider the two-sample test for the SSE model and give a new test procedure in the HDLSS context. In Section 5, we give simulation studies and discuss the performance of the new test procedure.

2 Asymptotic Properties of the Largest Eigenvalue

In this section, we provide asymptotic properties of the largest eigenvalue. We introduce a method for eigenvalue estimation called the *noise-reduction (NR) methodology* that was proposed by Yata and Aoshima [14]. See Sections 2 and 3 in Yata and Aoshima [14] for the details. When we apply the NR methodology, the NR estimator of $\lambda_{i(i)}$ is given by

$$ilde{\lambda}_{j(i)} = \hat{\lambda}_{j(i)} - rac{\operatorname{tr}(oldsymbol{S}_{in_i}) - \sum_{k=1}^j \hat{\lambda}_{k(i)}}{n_i - 1 - j} \quad (j = 1, ..., n_i - 2).$$

Note that $\lambda_{j(i)} \geq 0$ for $j = 1, ..., n_i - 2$. Yata and Aoshima [14, 15] showed that $\lambda_{j(i)}$ has several consistency properties when $d \to \infty$ and $n_i \to \infty$. In this paper, we focus on the largest eigenvalue, $\lambda_{1(i)}$, that has the most important information in data analyses. We assume the following conditions for the largest eigenvalue:

$$\begin{array}{ll} \textbf{(A-ii)} & \frac{\mathrm{tr}(\boldsymbol{\Sigma}_{i}^{2}) - \lambda_{1(i)}^{2}}{\lambda_{1(i)}^{2}} = \frac{\sum_{j=2}^{d} \lambda_{j(i)}^{2}}{\lambda_{1(i)}^{2}} = o(1) \text{ as } d \to \infty \text{ for } i = 1,2; \\ \\ \textbf{(A-iii)} & \frac{\sum_{r,s \geq 2}^{d} \lambda_{r(i)} \lambda_{s(i)} E\{(z_{rk(i)}^{2} - 1)(z_{sk(i)}^{2} - 1)\}}{\lambda_{1(i)}^{2}} = o(1) \text{ as } d \to \infty \text{ for } i = 1,2; \end{array}$$

Note that (A-ii) is one of the SSE model (1.2). We also note that (A-ii) implies the condition that $\lambda_{2(i)}/\lambda_{1(i)} \to 0$ as $d \to \infty$. Note that (A-iii) is naturally satisfied when X_i is Gaussian and (A-ii) is met.

Remark 2.1. For a spiked model such as

$$\lambda_{j(i)} = a_{ij} d^{\alpha_{ij}} \ (j = 1, ..., m_i)$$
 and $\lambda_{j(i)} = c_{ij} \ (j = m_i + 1, ..., d)$

with positive and fixed constants, $a_{ij}s$, $c_{ij}s$ and $\alpha_{ij}s$, and a positive and fixed integer m_i , (A-ii) holds under the conditions that $\alpha_{i1} > 1/2$ and $\alpha_{i1} > \alpha_{i2}$. See Yata and Aoshima [14] for the details.

Remark 2.2. For several statistical inferences of high-dimensional data, Bai and Saranadasa [4], Chen and Qin [6] and Aoshima and Yata [2] assumed a general factor model as follows:

$$x_{ij} = \Gamma_i w_{ij} + \mu_i$$

for $j = 1, ..., n_i$, where Γ_i is a $d \times r_i$ matrix for some $r_i > 0$ such that $\Gamma_i \Gamma_i^T = \Sigma_i$, and w_{ij} , $j = 1, ..., n_i$, are i.i.d. random vectors having $E(w_{ij}) = 0$ and $Var(w_{ij}) = I_{r_i}$. As for $w_{ij} = (w_{1j(i)}, ..., w_{rj(i)})^T$, assume that $E(w_{2j(i)}^2 w_{sj(i)}^2) = 1$ and $E(w_{qj(i)} w_{sj(i)} w_{tj(i)} w_{uj(i)}) = 0$ for all $q \neq s, t, u$. From Lemma 1 in Yata and Aoshima [15], one can claim that (A-iii) holds under (A-ii) in the factor model. Also, we note that the factor model naturally holds when X_i is Gaussian.

Then, Ishii et al. [9] gave the following theorem.

Theorem 2.1 ([9]). Under (A-ii) and (A-iii), it holds that as $d \to \infty$

$$\frac{\tilde{\lambda}_{1(i)}}{\lambda_{1(i)}} = \begin{cases} ||\boldsymbol{z}_{o1(i)}||^2/(n_i-1) + o_p(1) & \text{when } n_i \text{ is fixed}, \\ 1 + o_p(1) & \text{when } n_i \to \infty \end{cases}$$

for i = 1, 2. Under (A-i) to (A-iii), it holds that as $d \to \infty$ when n_i is fixed

$$(n_i-1)\frac{\lambda_{1(i)}}{\lambda_{1(i)}} \Rightarrow \chi^2_{n_i-1} \quad for \ i=1,2.$$

3 One-Sample Test for SSE Model

In this section, we consider the one-sample test in the high-dimensional context. We consider the following test:

$$H_0: \boldsymbol{\mu}_i = \boldsymbol{0} \quad \text{vs.} \quad H_1: \boldsymbol{\mu}_i \neq \boldsymbol{0}, \tag{3.1}$$

Bai and Saranadasa [4] proposed a test statistic:

$$T_{BS} = n_i ||\overline{\boldsymbol{x}}_{in_i}||^2 - \operatorname{tr}(\boldsymbol{S}_{in_i}). \tag{3.2}$$

Srivastava and Du [13] proposed a test statistic:

$$T_S = n_i \overline{\boldsymbol{x}}_{in_i}^T \boldsymbol{D}_i^{-1} \overline{\boldsymbol{x}}_{in_i}, \qquad (3.3)$$

where $D_i = \text{diag}(s_{11(i)}, ..., s_{dd(i)})$ and $s_{jj(i)}, j = 1, ..., d$ are the diagonal elements of S_{in_i} . They gave the asymptotic normality of T_{BS} or T_S under H_0 in (3.1) for the NSSE model (1.1). On the other hand, Katayama et al. [10] gave the asymptotic distribution of T_{BS} and T_S for the SSE model (1.2) when X_i is Gaussian.

Now, we consider a new one-sample test for the SSE model by using the asymptotic properties of the largest eigenvalue. By considering T_{BS} in (3.2) under (A-ii), we have the following result.

Lemma 3.1. Under (A-ii), it holds as $d \to \infty$ that

$$\frac{||\overline{x}_{in_i} - \mu_i||^2 - tr(S_{in_i})/n_i}{\lambda_{1(i)}} = \frac{\overline{z_{1(i)}^2 - ||z_{o1(i)}/\sqrt{n_i - 1}||^2}}{n_i} + o_p(n_i^{-1}),$$

either when n_i is fixed or $n_i \to \infty$.

By using the NR method, we consider the following test statistic:

$$F_1 = \frac{|n_i||\overline{x}_{in_i}||^2 - \operatorname{tr}(S_{in_i})}{\tilde{\lambda}_{1(i)}} + 1.$$

Note that $E(\tilde{\lambda}_{1(i)}(F_1-1)/n_i) = ||\mu_i||^2$. Then, by combining Theorem 2.1 and Lemma 3.1, Ishii et al. [9] gave the following result.

Theorem 3.1 ([9]). Under (A-i) to (A-iii), it holds as $d \to \infty$ that

$$F_1 \Rightarrow egin{cases} F_{1,n_i-1} & \textit{when } n_i \textit{ is fixed}, \ \chi_1^2 & \textit{when } n_i o \infty, \end{cases}$$

under H_0 in (3.1), where F_{ν_1,ν_2} denotes a random variable distributed as F distribution with degrees of freedom, ν_1 and ν_2 ; and χ^2_{ν} denotes a random variable distributed as χ^2 distribution with ν degrees of freedom.

For a given $\alpha \in (0, 1/2)$ we test (3.1) by

rejecting
$$H_0 \iff F_1 > F_{1,n_i-1}(\alpha),$$
 (3.4)

where $F_{\nu_1,\nu_2}(\alpha)$ denotes the upper α point of F distribution with degrees of freedom, ν_1 and ν_2 . Note that $F_{1,n_i-1}(\alpha) \to \chi_1^2(\alpha)$ as $n_i \to \infty$, where $\chi_{\nu}^2(\alpha)$ denotes the upper α point of χ^2 distribution with ν degrees of freedom. Then, under (A-i) to (A-iii), it holds as $d \to \infty$ that

size =
$$\alpha + o(1)$$

either when n_i is fixed or $n_i \to \infty$.

4 Two-Sample Test for SSE Model

In this section, we consider the two-sample test in the high-dimensional context. Now, we consider the following test:

$$H_0: \mu_1 = \mu_2 \quad \text{vs.} \quad H_1: \mu_1 \neq \mu_2.$$
 (4.1)

We assume the following assumption:

(A-iv)
$$\frac{\lambda_{1(1)}}{\lambda_{1(2)}} = 1 + o(1) \text{ and } \boldsymbol{h}_{1(1)}^T \boldsymbol{h}_{1(2)} = 1 + o(1) \text{ as } d \to \infty$$

Remark 4.1. Note that (A-iv) is not a general condition for high-dimensional data, so that it is necessary to check. See Lemma 4.1 in Ishii et al. [9] for checking the condition in actual data analyses.

Let

$$T_n = ||\overline{\boldsymbol{x}}_{1n_1} - \overline{\boldsymbol{x}}_{2n_2}||^2 - \sum_{i=1}^2 \operatorname{tr}(\boldsymbol{S}_{in_i})/n_i.$$

Note that $E(T_n) = ||\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2||^2$ and

$$\operatorname{Var}(T_n) = \sum_{i=1}^{2} \frac{\operatorname{tr}(\Sigma_i^2)}{n_i(n_i-1)} + 4 \frac{\operatorname{tr}(\Sigma_1 \Sigma_2)}{n_1 n_2} + 4 \sum_{i=1}^{2} \frac{(\mu_1 - \mu_2)^T \Sigma_i(\mu_1 - \mu_2)}{n_i}$$

By using Theorem 1 in Chen and Qin [6] or Theorem 4 in Aoshima and Yata [2], we can claim that as $d \to \infty$ and $n_i \to \infty$, i = 1, 2

$$\frac{T_n}{\operatorname{Var}(T_n)^{1/2}} \Rightarrow N(0,1)$$

under H_0 in (4.1), (1.1) and some regularity conditions.

We consider an asymptotic distribution of T_n under the SSE models. We have the following results.

Lemma 4.1. Under (A-ii) and (A-iv), it holds that

$$\frac{T_n}{\lambda_{1(1)}} = (\bar{z}_{1(1)} - \bar{z}_{1(2)})^2 - \sum_{i=1}^2 \frac{||\boldsymbol{z}_{o1(i)}/\sqrt{n_i - 1}||^2}{n_i} + o_p(1) \quad \textit{under } H_0 \textit{ in (4.1)}$$

as $d \to \infty$ either when n_i s are fixed or $n_i \to \infty$.

Let $\nu = n_1 + n_2 - 2$. From Theorem 2.1, we have the following result.

Lemma 4.2. Under (A-i) to (A-iv), it holds as $d \to \infty$ when n_i s are fixed that

$$rac{\sum_{i=1}^2 (n_i-1) ilde{\lambda}_{1(i)}}{\lambda_{1(1)}} \Rightarrow \chi^2_
u.$$

Under (A-ii) to (A-iv), it holds as $d \to \infty$ and $\nu \to \infty$ that

$$\frac{\sum_{i=1}^{2} (n_i - 1) \bar{\lambda}_{1(i)}}{\nu \lambda_{1(1)}} = 1 + o_p(1).$$

Let

$$F_{2} = u_{n} \frac{T_{n} + \sum_{i=1}^{2} \tilde{\lambda}_{1(i)}/n_{i}}{\sum_{i=1}^{2} (n_{i} - 1) \tilde{\lambda}_{1(i)}},$$

where $u_n = \nu (1/n_1 + 1/n_2)^{-1}$. Then, by combining Lemmas 4.1 with 4.2, we have the following theorem.

Theorem 4.1. Under (A-i) to (A-iv), it holds as $d \to \infty$ that

$$F_2 \Rightarrow egin{cases} F_{1,
u} & ext{when }
u ext{ is fixed,} \ \chi_1^2 & ext{when }
u o \infty \end{cases}$$

under H_0 in (4.1).

For a given $\alpha \in (0, 1/2)$ we test (4.1) by

rejecting
$$H_0 \iff F_2 > F_{1,\nu}(\alpha),$$
 (4.2)

Then, under (A-i) to (A-iv), it holds that

size =
$$\alpha + o(1)$$

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

5 Simulation Studies

In order to compare the performances of the one-sample test procedures, we used computer simulations. We consider the test (3.1). In this simulation, we compared the test procedure (3.4) to T_{BS} in (3.2) and the test procedures given by Katayama et al. [10]. We set $\alpha = 0.05$ and $\Sigma_i = (I_d + d^{-1}\mathbf{1}_d\mathbf{1}_d^T)/2$, where $\mathbf{1}_d = (1, ..., 1)^T$. For such a situation, Katayama et al. [10] gave the following test procedures:

rejecting
$$H_0 \iff \frac{T_{BS}}{\sqrt{\widehat{\operatorname{tr}(\Sigma^2)}}} + 1 > \chi_1^2(\alpha),$$
 (5.1)

rejecting
$$H_0 \iff \frac{T_S - d(n_i - 1)/(n_i - 3)}{\sqrt{\widehat{\operatorname{tr}(R_i^2)}}} + 1 > \chi_1^2(\alpha),$$
 (5.2)

where $\operatorname{tr}(\Sigma_i^2)$ and $\operatorname{tr}(R_i^2)$ are the consistent estimators of $\operatorname{tr}(\Sigma_i^2)$ and $\operatorname{tr}(R_i^2)$, R_i is the population correlation matrix, given in Katyama et al. [10]. We considered the case X_i is Gaussian. Note that (A-i) to (A-iii) hold. We considered two cases (I) $d = 2^k (k = 3, ...11)$ and $n_i = 10$; and (II) $d = 2^k (k = 4, ...11)$ and $n_i = \lceil d^{1/2} \rceil$, where $\lceil x \rceil$ denotes the smallest integer $\geq x$. In order to check the size, we set (a) $\mu_i = 0$ for each case. As for the power, we set (b) $\mu_i = (1, ..., 1, 0, ..., 0)$ whose first d/2 elements are 1 for (I); and first $\lceil 3.8d/n_i \rceil$ elements are 1 for (II).

The findings were obtained by averaging the outcomes from 2000 (= R, say) replications. We defined $P_r = 1$ (or 0) when H_0 in (3.1) was falsely rejected (or not) for r = 1, ..., 2000 in (a) and defined $\overline{\alpha} = \sum_{r=1}^{R} P_r/R$ to estimate the size. We also defined $P_r = 1$ (or 0) when H_1 in (3.1) was falsely rejected (or not) for r = 1, ..., 2000 in (b) and defined $1 - \overline{\beta} = 1 - \sum_{r=1}^{R} P_r/R$ to estimate the power. Note that their standard deviations are less than 0.011. In Fig. 1, we plotted $\overline{\alpha}$ in the left panels and $1 - \overline{\beta}$ in the right panels for (I) and (II).

Throughout, the original test procedure T_{BS} in (3.2) does not give a good performance in terms of the size. It is probably because T_{BS} does not hold the asymptotic normality when (1.1) is not met. On the other hand, the tests (5.1) and (5.2) do not give good performances in terms of the size when n_i is small. We observed that the power of (3.2), (5.1) and (5.2) gave better performances compared to that of (3.4) in (I). This is because (3.2), (5.1) and (5.2) cannot control the size. In the case of (II), the size of (5.1) and (5.2) become close to α slowly as both the d and n_i are large. Contrary to that, (3.4) showed a quite good performance in terms of the size even when n_i is small. It should be noted that high-dimensional data often have SSE model and the sample size is quite small. Thus, we conclude that if one can assume (A-ii), we recommend to use the new test procedure (3.4).



Figure 1. We compared the test procedure (3.4) to (3.2), (5.1) and (5.2). We set $\alpha = 0.05$ and X_i is Gaussian. The values of $\overline{\alpha}$ are denoted by the dashed lines in the left panels and $1 - \overline{\beta}$ are denoted by the dashed lines in the right panels.

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