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On estimation of the noise variance in high-dimensional probabilistic principal component analysis

Damien PASSEMIER

Department of Electronic and Computer Engineering
Hong Kong University of Science and Technology

Zhaoyuan LI

Department of Statistics and Actuarial Science
The University of Hong Kong

Jianfeng YAO

Department of Statistics and Actuarial Science
The University of Hong Kong

Abstract

In this paper, we develop new statistical theory for probabilistic principal component analysis models in high dimensions. The focus is the estimation of the noise variance, which is an important and unresolved issue when the number of variables is large in comparison with the sample size. We first unveil the reasons of a widely observed downward bias of the maximum likelihood estimator of the variance when the data dimension is high. We then propose a bias-corrected estimator using random matrix theory and establish its asymptotic normality. The superiority of the new (bias-corrected) estimator over existing alternatives is first checked by Monte-Carlo experiments with various combinations of (p, n) (dimension and sample size). In order to demonstrate further potential benefits from the results of the paper to

general probability PCA analysis, we provide evidence of net improvements in two popular procedures (Ulfarsson and Solo, 2008; Bai and Ng, 2002) for determining the number of principal components when the respective variance estimator proposed by these authors is replaced by the bias-corrected estimator. The new estimator is also used to derive new asymptotics for the related goodness-of-fit statistic under the high-dimensional scheme.

Keywords. Probabilistic principal component analysis, high-dimensional data, noise variance estimator, random matrix theory, goodness-of-fit.

1 Introduction

Principal component analysis (PCA) is a very popular technique in multivariate analysis for dimensionality reduction and feature extraction. Due to dramatic development in data-collection technology, high-dimensional data are nowadays common in many fields. Natural high-dimensional data, such as images, signal processing, documents and biological data often reside in a low-dimensional subspace or low-dimensional manifold (Ding et al., 2011). In financial econometrics, it is commonly believed that the variations in a large number of economic variables can be modeled by a small number of reference variables (Stock and Watson, 1989; Forni et al., 2000; Bai and Ng, 2002; Bai, 2003). Consequently, PCA is a recommended tool for analysis of such high-dimensional data.

There is an underlying probabilistic model behind PCA, called probabilistic principal component analysis (PPCA), defined as follows. The observation vectors

$\{\mathbf{x}_i\}_{1 \leq i \leq n}$ are p -dimensional and satisfy the equation

$$\mathbf{x}_i = \mathbf{\Lambda} \mathbf{f}_i + \mathbf{e}_i + \boldsymbol{\mu}, \quad i = 1, \dots, n. \quad (1)$$

Here, \mathbf{f}_i is a m -dimensional *principal components* with $m \ll p$, $\mathbf{\Lambda}$ is a $p \times m$ matrix of *loadings*, and $\boldsymbol{\mu}$ represents the general mean and (\mathbf{e}_i) are a sequence of independent Gaussian errors with covariance matrix $\boldsymbol{\Psi} = \sigma^2 \mathbf{I}_p$. The parameter σ^2 is the noise variance we are interested in. The components (\mathbf{f}_i) are also Gaussian and unobserved.

To ensure the identification of the model, constraints have to be introduced on the parameters. There are several possibilities for the choice of such constraints, see e.g. Table 1 in Bai and Li (2012). A traditional choice is the following (Anderson, 2003, Chapter 14):

- $\mathbb{E} \mathbf{f}_i = \mathbf{0}$ and $\mathbb{E} \mathbf{f}_i \mathbf{f}_i' = \mathbf{I}$;
- The matrix $\boldsymbol{\Gamma} := \mathbf{\Lambda}' \mathbf{\Lambda}$ is diagonal with distinct diagonal elements.

Therefore, the population covariance matrix (PCM) of $\{\mathbf{x}_i\}$ is

$$\boldsymbol{\Sigma} = \mathbf{\Lambda} \mathbf{\Lambda}' + \sigma^2 \mathbf{I}. \quad (2)$$

Finding a reliable estimator of σ^2 is a nontrivial issue for high-dimensional data which we now pursue.

The PPCA model (1) can be viewed as a special instance of the approximate factor model (Chamberlain and Rothschild, 1983) when the noise covariance $\boldsymbol{\Psi}$ is a general diagonal matrix. (The model is also called a strict factor model in

statistical literature, see Anderson (2003)). For related recent papers on inference of large approximate (or dynamic) factor models, we refer to Bai (2003), Forni et al. (2000) and Doz et al. (2012).

Let $\bar{\mathbf{x}}$ be the sample mean and define the sample covariance matrix

$$\mathbf{S}_n = \frac{1}{n-1} \sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})'. \quad (3)$$

Let $\lambda_{n,1} \geq \lambda_{n,2} \geq \dots \geq \lambda_{n,p}$ be the eigenvalues of \mathbf{S}_n . The maximum likelihood estimator of the noise variance is

$$\hat{\sigma}^2 = \frac{1}{p-m} \sum_{i=m+1}^p \lambda_{n,i}. \quad (4)$$

In the classic setting where the dimension p is relatively small compared to the sample size n (low-dimensional setting), the consistency of $\hat{\sigma}^2$ is established in Anderson and Rubin (1956). Moreover, it is asymptotically normal with the standard \sqrt{n} -convergence rate, as $n \rightarrow \infty$,

$$\sqrt{n}(\hat{\sigma}^2 - \sigma^2) \xrightarrow{\mathcal{D}} \mathcal{N}(0, s^2), \quad s^2 = \frac{2\sigma^4}{p-m}. \quad (5)$$

Actually, Anderson and Amemiya (1988) provides a general CLT for m.l.e. in an approximate factor model that encompasses the present PPCA model. For the reader's convenience, we provide in Subsection 6.5 a detailed derivation of (5) from this general CLT.

The situation is, however radically different when p is large compared to the sample size n . Recent advances in high-dimensional statistics indicate that in such high-dimensional situation, the above asymptotic result is no more valid and

indeed, it has been widely observed in the literature that $\hat{\sigma}^2$ seriously underestimates the true noise variance σ^2 . Basically, when p becomes large, the sample principal eigenvalues and principal components are no longer consistent estimates of their population counterparts (Baik and Silverstein, 2006b; Johnstone and Lu, 2009; Kritchman and Nadler, 2008b). Many estimation methods developed in low-dimensional setting have been shown to perform poorly even for moderately large p and n (Cragg and Donald, 1997).

As all meaningful inference procedures in the model will unavoidably use some estimator of the noise variance σ^2 , such a severe bias needs to be corrected for high-dimensional data. There are several estimators proposed to deal with the high-dimensional situation. Kritchman and Nadler (2008a) proposes an estimator by solving a system of implicit equations; Ulfarsson and Solo (2008) introduces an estimator using the median of the sample eigenvalues $\{\lambda_{n,k}\}$; and Johnstone and Lu (2009) uses the median of the sample variances. However, these estimators are assessed by Monte-Carlo experiments only and their theoretical properties have not been investigated.

The main aim of this paper is to provide a new estimator of the noise variance for which a rigorous asymptotic theory can be established in the high-dimensional setting. First, by using recent advances in random matrix theory, we found a CLT for the m.l.e. $\hat{\sigma}^2$ in the high-dimensional setting (Theorem 1 in Section 2). Next, using this identification and random matrix theory, we propose a new estimator $\hat{\sigma}_*^2$ for the noise variance by correcting this bias. The asymptotic normality of the new estimator is thus established with explicit asymptotic mean and variance.

Although the asymptotic Gaussian distribution of the bias-corrected estima-

tor $\hat{\sigma}_*^2$ is established under the high-dimensional setting $p \rightarrow \infty$, $n \rightarrow \infty$ and $p/n \rightarrow c > 0$, if we set $c = 0$, i.e. the dimension p is infinitely smaller than n , this Gaussian limit coincides with the classical low-dimensional limit given in (5). In this sense, the new asymptotic theory extends in a continuous manner the classical low-dimensional result to the high-dimensional situation. Finite sample properties of the bias-corrected estimator $\hat{\sigma}_*^2$ have been checked via Monte-Carlo experiments in comparison with the above-mentioned three existing estimators. In terms of mean squared errors and in all the tested scenarios, $\hat{\sigma}_*^2$ outperforms very significantly two of them, and is slightly preferable than the third one, see Table 3.

In order to demonstrate further potential benefits achievable by the implementation of the bias-corrected estimator $\hat{\sigma}_*^2$, we develop three applications. Two of these applications concern an important inference problem in PPCA, namely, the determination of the number of principal components (PCs). This problem involves the noise variance estimation and many methods for choosing PCs have been proposed in the literature. We consider two benchmark procedures from different fields. The first one is proposed in Ulfarsson and Solo (2008) that employs PPCA to signal processing and proposes the Stein's unbiased risk estimator (SURE) to find the number of PCs. The second one is from Bai and Ng (2002) which develops six criteria with penalty on both p and n to identify the number of factors in the approximate factor model. The approximate factor model allows the errors (\mathbf{e}_i) be correlated. PPCA can be considered as a simplified instance of this model and indeed, Bai and Ng (2002) applies also their criteria to PPCA. Notice that the determination criteria in Bai and Ng (2002) are popular and widely cited in the literature. Furthermore, both the procedures in Ulfarsson and Solo (2008)

and Bai and Ng (2002) implement a specific estimator of the noise variance σ^2 . By substituting the bias-corrected estimator $\hat{\sigma}_*^2$ for their estimators, we demonstrate by extensive simulation that these procedures are uniformly and significantly improved.

The third application of the bias-corrected estimator $\hat{\sigma}_*^2$ concerns the goodness-of-fit test for the PPCA model. The LR test statistic as well as their classical (low-dimensional) chi-squared asymptotics are well-known since the work of Amemiya and Anderson (1990). These results are again challenged by high-dimensional data and the classical chi-squared limit is no more valid. Following an approach devised in Bai et al. (2009), we propose a correction to this goodness-of-fit test statistic involving our new estimator $\hat{\sigma}_*^2$ of noise variance to cope with the high-dimensional effects and establish its asymptotic normality.

The remaining sections are organized as follows. In Section 2, we present the main results of the paper. In Section 3, our new estimator $\hat{\sigma}_*^2$ is substituted for an estimator from the authors of the SURE criterion and it is shown that this substitution improves greatly the SURE criterion. Similarly, in Section 4, the estimator $\hat{\sigma}_*^2$ is applied to the criteria proposed by Bai and Ng (2002) to determine the number of PCs and again an improvement of these criteria is obtained. In Section 5, we develop the corrected likelihood ratio test for the goodness-of-fit of a PPCA model in the high-dimensional framework using the new estimator $\hat{\sigma}_*^2$. Technical proofs are gathered together in Section 6. Section 7 concludes.

2 Main results

The PPCA model (1) is a spiked population model (Johnstone, 2001) since the eigenvalues of PCM Σ are

$$\begin{aligned} \text{spec}(\Sigma) &= \underbrace{(\alpha_1, \dots, \alpha_1)}_{n_1}, \dots, \underbrace{(\alpha_K, \dots, \alpha_K)}_{n_K}, \underbrace{(0, \dots, 0)}_{p-m} + \sigma^2 \underbrace{(1, \dots, 1)}_p \\ &= \sigma^2 \underbrace{(\alpha_1^*, \dots, \alpha_1^*)}_{n_1}, \dots, \underbrace{(\alpha_K^*, \dots, \alpha_K^*)}_{n_K}, \underbrace{(1, \dots, 1)}_{p-m}, \end{aligned} \quad (6)$$

where (α_i) are non-null eigenvalues of $\Lambda \Lambda'$ with multiplicity numbers (n_i) satisfying $n_1 + \dots + n_K = m$ and the notation $\alpha_i^* = \alpha_i / \sigma^2 + 1$ is used. To develop a meaningful asymptotic theory in the high-dimensional context, we assume that p and n are related so that when $n \rightarrow \infty$, $c_n = p / (n - 1) \rightarrow c > 0$, that is, p can be large compared to the sample size n and for the asymptotic theory, p and n tend to infinity proportionally. Define the function

$$\phi(\alpha) = \alpha + \frac{c\alpha}{\alpha - 1}, \quad \alpha \neq 1,$$

and set $s_0 = 0$ and $s_i = n_1 + \dots + n_i$ for $1 \leq i \leq K$. The set $J_i = \{s_{i-1} + 1, \dots, s_i\}$ is then the indexes among $\{1, \dots, p\}$ associated to α_i counting the multiplicities. Following Baik and Silverstein (2006a), assumed that $\alpha_1^* \geq \dots \geq \alpha_m^* > 1 + \sqrt{c}$, i.e all the eigenvalues α_i are greater than $\sigma^2 \sqrt{c}$. It is then known that, for the spiked sample eigenvalues $\lambda_{n,k}$ of \mathbf{S}_n , $1 \leq k \leq m$, almost surely if $k \in J_i$,

$$\lambda_{n,k} \longrightarrow \sigma^2 \phi(\alpha_i^*) = \alpha_i + \sigma^2 + \sigma^2 c \left(1 + \frac{\sigma^2}{\alpha_i} \right). \quad (7)$$

Moreover, the remaining sample eigenvalues $\{\lambda_{n,k}\}_{m < k \leq p}$, called *noise eigenvalues*, will converge to a continuous distribution with support interval $[a(c), b(c)]$ where $a(c) = \sigma^2(1 - \sqrt{c})^2$ and $b(c) = \sigma^2(1 + \sqrt{c})^2$. In particular, for all $1 \leq i \leq L$ with a

prefixed range L and almost surely, $\lambda_{n,m+i} \rightarrow b(c)$. It is worth noticing that in (7), if we let $c \rightarrow 0$, we recover the low-dimensional limits $\lambda_{n,k} \rightarrow \alpha_i + \sigma^2$ (population spike eigenvalues) and $\lambda_{n,k} \rightarrow \sigma^2$ (population noise eigenvalues) discussed earlier.

In a further step, CLT for the spiked eigenvalues is established in Bai and Yao (2008) (see also Paul (2007)): the n_i -dimensional vector

$$\{\sqrt{n}(\lambda_{n,k} - \sigma^2 \phi(\alpha_k^*)), k \in J_i\} \quad (8)$$

converges to a well-determined n_i -dimensional limiting distribution. Moreover, this limiting distribution is Gaussian if and only if the corresponding population spike eigenvalue α_i is simple, i.e. $n_i = 1$.

As explained in the Introduction, when the dimension p is large compared to the sample size n , the m.l.e. $\hat{\sigma}^2$ in (4) has a negative bias. In order to identify this bias, we first establish a central limit theorem for $\hat{\sigma}^2$ under the high-dimensional scheme.

Theorem 1. *Consider the PPCA model (1) with population covariance matrix $\Sigma = \Lambda\Lambda' + \sigma^2\mathbf{I}_p$ where both the principal components and the noise are Gaussian. Assume that $p \rightarrow \infty$, $n \rightarrow \infty$ and $c_n = p/(n-1) \rightarrow c > 0$. Then, we have*

$$\frac{(p-m)}{\sigma^2\sqrt{2c}}(\hat{\sigma}^2 - \sigma^2) + b(\sigma^2) \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1),$$

where $b(\sigma^2) = \sqrt{\frac{c}{2}} \left(m + \sigma^2 \sum_{i=1}^m \frac{1}{\alpha_i} \right)$.

Therefore, for high-dimensional data, the m.l.e. $\hat{\sigma}^2$ has an asymptotic bias $-b(\sigma^2)$ (after normalization). This bias is a complex function of the noise variance and the m non-null eigenvalues of the loading matrix $\Lambda\Lambda'$. Notice that the above

CLT is still valid if $\tilde{c}_n = (p - m)/n$ is substituted for c . Now if indeed $p \ll n$, i.e. the dimension p is infinitely smaller than the sample size n , so that $\tilde{c}_n \simeq 0$ and $b(\sigma^2) \simeq 0$, and hence

$$\frac{(p - m)}{\sigma^2 \sqrt{2c}} (\hat{\sigma}^2 - \sigma^2) + b(\sigma^2) \simeq \frac{\sqrt{p - m}}{\sigma^2 \sqrt{2}} \sqrt{n} (\hat{\sigma}^2 - \sigma^2) \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1) .$$

This is nothing but the CLT (5) for $\hat{\sigma}^2$ known under the classical low-dimensional scheme. In a sense, Theorem 1 constitutes a natural and continuous extension of the classical CLT to the high-dimensional context.

The previous theory recommends to correct the negative bias of $\hat{\sigma}^2$. However, the bias $b(\sigma^2)$ depends on the number m and the values α_i of the spikes. These parameters are likely unknown in real-data applications and they need to be estimated. In the literature, consistent estimators of m have been proposed, e.g. in Bai and Ng (2002), Kritchman and Nadler (2008a), Onatski (2009) and Passemier and Yao (2012). For the values of the spikes α_i , it is easy to see that it can be estimated by inverting the function ϕ in (7) at the corresponding eigenvalues $\lambda_{n,j}$. Moreover, by applying the delta-method to (8), we can obtain the asymptotic distribution of this estimator, see Bai and Ding (2012).

As the bias depends on σ^2 which we want to estimate, a natural correction is to use the plug-in estimator

$$\hat{\sigma}_*^2 = \hat{\sigma}^2 + \frac{b(\hat{\sigma}^2)}{p - m} \hat{\sigma}^2 \sqrt{2c_n} . \quad (9)$$

This estimator will be hereafter referred as the *bias-corrected estimator*. Notice that here the number of factors m can be replaced by any consistent estimate as discussed above without affecting the limiting distribution of the estimator. The following CLT is an easy consequence of Theorem 1.

Theorem 2. *We assume the same conditions as in Theorem 1. Then, we have*

$$\frac{p-m}{\sigma^2 \sqrt{2c_n}} (\hat{\sigma}_*^2 - \sigma^2) \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1) .$$

Compared to the m.l.e. $\hat{\sigma}^2$ in Theorem 1, the bias-corrected estimator $\hat{\sigma}_*^2$ has no more a bias after normalization by $\frac{p-m}{\sigma^2 \sqrt{2c_n}}$, and it should be a much better estimator than $\hat{\sigma}^2$.

2.1 Monte-Carlo experiments

We first check by simulation the effect of bias-correction obtained in $\hat{\sigma}_*^2$ and its asymptotic normality. Independent Gaussian samples of size n are considered in three different settings:

- Model 1: $\text{spec}(\mathbf{\Sigma}) = (25, 16, 9, 0, \dots, 0) + \sigma^2(1, \dots, 1)$, $\sigma^2 = 4$, $c = 1$;
- Model 2: $\text{spec}(\mathbf{\Sigma}) = (4, 3, 0, \dots, 0) + \sigma^2(1, \dots, 1)$, $\sigma^2 = 2$, $c = 0.2$;
- Model 3: $\text{spec}(\mathbf{\Sigma}) = (12, 10, 8, 8, 0, \dots, 0) + \sigma^2(1, \dots, 1)$, $\sigma^2 = 3$, $c = 1.5$.

In Table 1, we compare the empirical bias of $\hat{\sigma}^2$ (i.e. the empirical mean of $\hat{\sigma}^2 - \sigma^2 = \frac{1}{p-m} \sum_{i=m+1}^p \lambda_{n,i} - \sigma^2$) over 1000 replications with the theoretical one $-\sigma^2 \sqrt{2cb(\sigma^2)}/(p-m)$ in different settings. In all the three models, the empirical and theoretical bias are close each other. As expected, their difference vanishes when p and n increase. The table also shows that this bias is quite significant even for large dimension and sample size such as $(p, n) = (1500, 1000)$.

Table 1: Comparison between the empirical and the theoretical bias in various settings.

Settings		Empirical bias	Theoretical bias	Difference
Model 1	$p = 100$ $n = 100$	-0.1556	-0.1589	0.0023
	$p = 400$ $n = 400$	-0.0379	-0.0388	0.0009
	$p = 800$ $n = 800$	-0.0189	-0.0193	0.0004
Model 2	$p = 20$ $n = 100$	-0.0654	-0.0704	0.0050
	$p = 80$ $n = 400$	-0.0150	-0.0162	0.0012
	$p = 200$ $n = 1000$	-0.0064	-0.0063	0.0001
Model 3	$p = 150$ $n = 100$	-0.0801	-0.0795	0.0006
	$p = 600$ $n = 400$	-0.0400	-0.0397	0.0003
	$p = 1500$ $n = 1000$	-0.0157	-0.0159	0.0002

Figure 1 presents the histograms from 1000 replications of

$$\frac{(p - m)}{\sigma^2 \sqrt{2c_n}} (\hat{\sigma}^2 - \sigma^2) + b(\sigma^2)$$

of the three models above, with sample size $n = 100$ and dimensions $p = c \times n$, compared to the density of the standard Gaussian distribution. The sampling distribution is almost normal.

To assess the quality of the bias-corrected estimator $\hat{\sigma}_*^2$, we conduct some simulation experiments using the same settings. Table 2 compares the empirical means, mean absolute deviations (MAD) and the mean squared errors (MSE) of $\hat{\sigma}^2$ and $\hat{\sigma}_*^2$ over 1000 replications. The improvement of $\hat{\sigma}_*^2$ over $\hat{\sigma}^2$ is very significant in term of MAD in all the tested cases (the difference in term of MSE is less remarkable because the squares become quite small numbers).

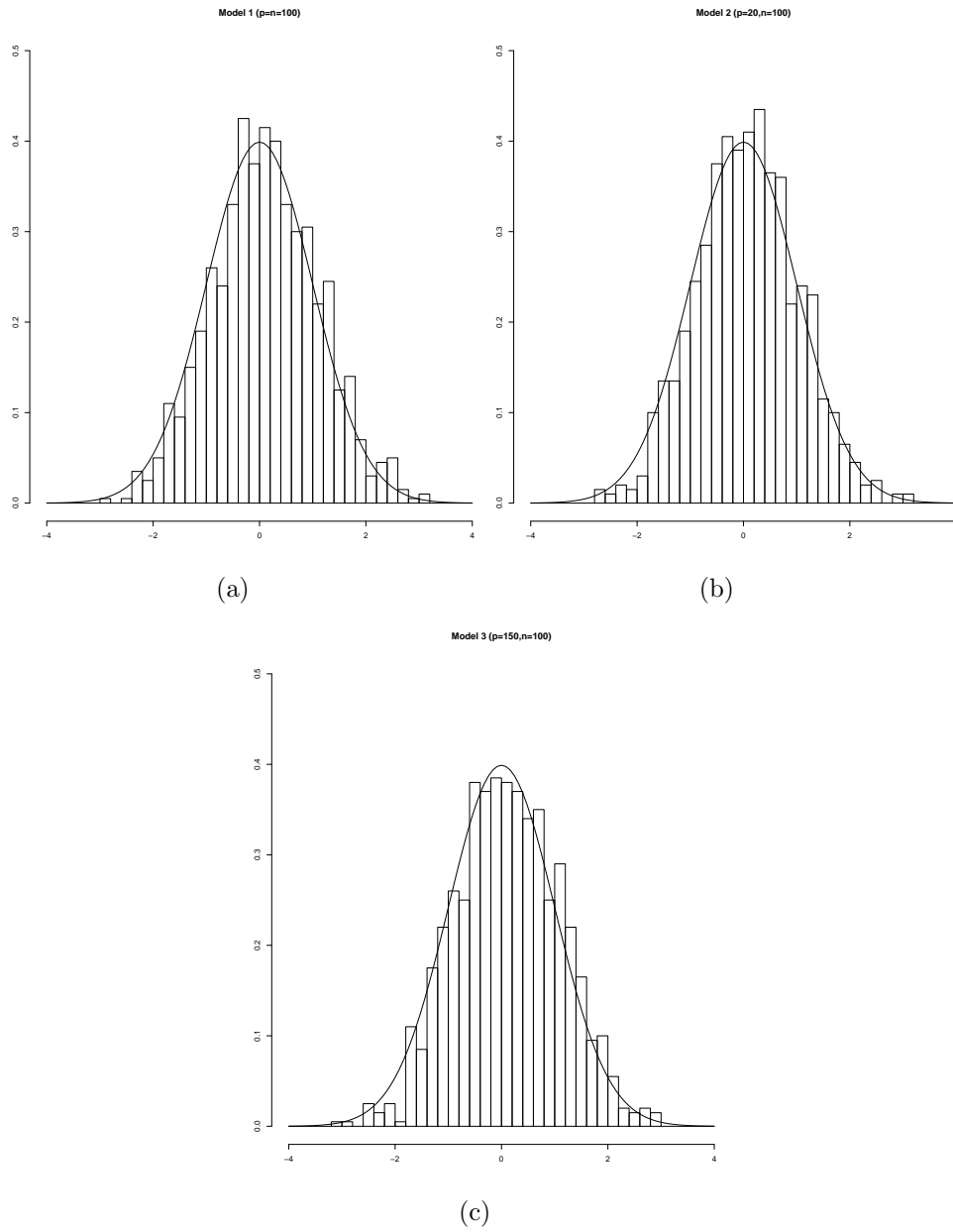


Figure 1: Histogram of $\frac{(p-m)}{\sigma^2\sqrt{2c}}(\hat{\sigma}^2 - \sigma^2) + b(\sigma^2)$ compared with the density of a standard Gaussian distribution.

Next, we compare our bias-corrected estimator to three existing estimators in the literature. For the reader's convenience, we recall their definitions:

1. The estimator $\hat{\sigma}_{\text{KN}}^2$ of Kritchman and Nadler (2008a): it is defined as the solution of the following non-linear system of $m + 1$ equations involving the $m + 1$ unknowns $\hat{\rho}_1, \dots, \hat{\rho}_m$ and $\hat{\sigma}_{\text{KN}}^2$:

$$\begin{aligned} \hat{\sigma}_{\text{KN}}^2 - \frac{1}{p-m} \left[\sum_{j=m+1}^p \lambda_{n,j} + \sum_{j=1}^m (\lambda_{n,j} - \hat{\rho}_j) \right] &= 0, \quad \text{and} \\ \hat{\rho}_j - \hat{\rho}_j \left(\lambda_{n,j} + \hat{\sigma}_{\text{KN}}^2 - \hat{\sigma}_{\text{KN}}^2 \frac{p-m}{n} \right) + \lambda_{n,j} \hat{\sigma}_{\text{KN}}^2 &= 0, \quad j = 1, \dots, m. \end{aligned}$$

We use the computing code available on the authors' web-page to carry out the simulation.

2. The estimator $\hat{\sigma}_{\text{US}}^2$ of Ulfarsson and Solo (2008): it is defined as the ratio

$$\hat{\sigma}_{\text{US}}^2 = \frac{\text{median}(\lambda_{n,m+1}, \dots, \lambda_{n,p})}{m_{p/n,1}},$$

where $m_{\alpha,1}$ is the median of the Marčenko-Pastur distribution $F_{\alpha,1}$ (more details on this distribution is given in Subsection 6.1).

3. The estimator $\hat{\sigma}_{\text{median}}^2$ of Johnstone and Lu (2009): it is defined as the median of the p sample variances

$$\hat{\sigma}_{\text{median}}^2 = \text{median} \left(\frac{1}{n} \sum_{i=1}^n x_{ij}^2, \quad 1 \leq j \leq p \right).$$

Clearly for this estimator, the data $\{x_{ij}\}$ are assumed centered.

Table 3 gives the ratios of the empirical MSEs of these estimators over the empirical MSE of the bias-corrected estimator $\hat{\sigma}_*^2$. The performances of $\hat{\sigma}_*^2$ and

Table 2: Empirical mean, MAD and MSE of $\hat{\sigma}^2$ and $\hat{\sigma}_*^2$ in various settings.

Mod.	Settings			$\hat{\sigma}^2$	MAD	MSE	$\hat{\sigma}_*^2$	MAD	MSE
	p	n	σ^2						
1	100	100		3.8464	0.1536	0.0032	3.9979	0.0021	0.0035
	400	400	4	3.9616	0.0384	0.0002	4.0000	$< 10^{-5}$	0.0002
	800	800		3.9809	0.0191	0.0001	4.0002	0.0002	0.0001
2	20	100		1.9340	0.0660	0.0043	2.0012	0.0012	0.0047
	80	400	2	1.9841	0.0159	0.0003	2.0001	0.0001	0.0003
	200	1000		1.9939	0.0061	$< 10^{-5}$	2.0002	0.0002	$< 10^{-5}$
3	150	100		2.8400	0.1600	0.0011	2.9926	0.0074	0.0013
	600	400	3	2.9605	0.0395	0.0001	2.9999	0.0001	0.0001
	1500	1000		2.9839	0.0161	$< 10^{-5}$	2.9998	0.0002	$< 10^{-5}$

$\hat{\sigma}_{\text{KN}}^2$ are similar and $\hat{\sigma}_*^2$ being slightly better. The estimator $\hat{\sigma}_{\text{US}}^2$ shows slightly better than the m.l.e. $\hat{\sigma}^2$. The estimator $\hat{\sigma}_{\text{median}}^2$ is better than $\hat{\sigma}_{\text{US}}^2$ and the m.l.e. $\hat{\sigma}^2$. But $\hat{\sigma}_{\text{median}}^2$ and $\hat{\sigma}_{\text{US}}^2$ performs poorly compared to $\hat{\sigma}_*^2$ and $\hat{\sigma}_{\text{KN}}^2$. The reader is, however reminded that the theoretic properties of $\hat{\sigma}_{\text{KN}}^2$, $\hat{\sigma}_{\text{US}}^2$ and $\hat{\sigma}_{\text{median}}^2$ are unknown and so far there have been checked via simulations only.

3 Application to the SURE criterion

Ulfarsson and Solo (2008) proposes to use Stein's unbiased risk estimator, SURE, to choose the number of PCs. This criterion uses the noise variance estimator $\hat{\sigma}_{\text{US}}^2$ defined in Section 2. It aims at minimizing the Euclidean distance between the underlying estimator of the population mean $\boldsymbol{\mu}$ and its true value. The proposed

Table 3: Comparison between three existing estimators and the proposed one in terms of ratios of MSE: $\frac{\text{MSE}(\hat{\sigma}_{KN}^2)}{\text{MSE}(\hat{\sigma}_*^2)}$, $\frac{\text{MSE}(\hat{\sigma}_{US}^2)}{\text{MSE}(\hat{\sigma}_*^2)}$ and $\frac{\text{MSE}(\hat{\sigma}_{\text{median}}^2)}{\text{MSE}(\hat{\sigma}_*^2)}$.

Mod.	Settings			$\hat{\sigma}_{KN}^2$	$\hat{\sigma}_{US}^2$	$\hat{\sigma}_{\text{median}}^2$
	p	n	σ^2			
1	100	100		1.01	4.40	1.47
	400	400	4	1.00	6.50	1.59
	800	800		1.00	4.00	1.62
2	20	100		1.04	1.85	1.67
	80	400	2	1.00	2.67	1.52
	200	1000		1.00	10.10	1.53
3	150	100		1.07	7.08	1.26
	600	400	3	1.00	7.00	1.52
	1500	1000		0.96	10.10	1.60

SURE criterion for m number of PCs (to be minimized) is

$$\begin{aligned}
R_m &= (p-m)\hat{\sigma}_{US}^2 + \hat{\sigma}_{US}^4 \sum_{j=1}^m \frac{1}{\lambda_j} + 2\hat{\sigma}_{US}^2(1-1/n)m \\
&\quad - 2\hat{\sigma}_{US}^4(1-1/n) \sum_{j=1}^m \frac{1}{\lambda_j} + \frac{4(1-1/n)\hat{\sigma}_{US}^4}{n} \sum_{j=1}^m \frac{1}{\lambda_j} + C_m, \quad (10)
\end{aligned}$$

where

$$\begin{aligned}
C_m &= \frac{4(1-1/n)\hat{\sigma}_{US}^2}{n} \sum_{j=1}^m \sum_{i=m+1}^p \frac{\lambda_j - \hat{\sigma}_{US}^2}{\lambda_j - \lambda_i} + \frac{2(1-1/n)\hat{\sigma}_{US}^2}{n} m(m-1) \\
&\quad - \frac{2(1-1/n)\hat{\sigma}_{US}^2}{n} (p-1) \sum_{j=1}^m \left(1 - \frac{\hat{\sigma}_{US}^2}{\lambda_j}\right).
\end{aligned}$$

Recall that $\hat{\sigma}_{US}^2$ is also related to m . From Section 2, we have known that $\hat{\sigma}_{US}^2$ is not as good as our bias-corrected estimator. To examine further this difference, we replace $\hat{\sigma}_{US}^2$ with $\hat{\sigma}_*^2$ in (10), referred then as SURE*, to see whether the performance of SURE can be improved.

Then simulation experiments are conducted to compare SURE with SURE*. The setup follows the paper Ulfarsson and Solo (2008) and the data are simulated according to (1) with the parameters $p = 64, p/n = [2/3, 1/2, 2/5], m = [5, 10, 15, 20]$ and $\sigma^2 = 1$. The loading matrix is set to $\mathbf{\Lambda} = \mathbf{F}\mathbf{D}^{1/2}$, where \mathbf{F} is constructed by generating a $p \times m$ matrix of Gaussian random variables and then orthogonalizing the resulting matrix, and

$$\begin{aligned}
\mathbf{D} &= \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_{m-1}, \lambda_m) \\
&= \text{diag}((m+1)^2, m^2, \dots, 3^2, \lambda_m), \quad \lambda_m = 1.5.
\end{aligned}$$

All simulations were repeated 1500 times. Table 4 shows the percentage of correct selection of PCs for SURE and SURE*. It can be seen that SURE* largely

Table 4: Comparison between SURE and SURE* in terms of percentage of correct selection of PCs.

m		$p/n = 2/3$	$p/n = 1/2$	$p/n = 2/5$
5	SURE*	1.000	1.000	1.000
	SURE	0.408	0.621	0.807
10	SURE*	0.990	1.000	0.998
	SURE	0.512	0.739	0.858
15	SURE*	0.904	0.978	0.989
	SURE	0.598	0.783	0.911
20	SURE*	0.908	0.966	0.990
	SURE	0.617	0.810	0.899

outperforms SURE in all of the tested cases, most of times by a wide margin. All the percentages of correct selection of SURE* are larger than 90% and in 4 out of 12 cases, the detection rate is 100%. Therefore, by implementing our bias-corrected estimator of the noise variance instead of the one provided by its authors, the criterion SURE has a much better performance.

4 Application to determination criteria of Bai and Ng (2002)

In econometrics, the assumption of additive white noise is reasonable for asset returns with low frequencies (e.g., monthly returns of stocks) (Ma, 2013). Bai and Ng (2002) proposes six criteria to estimate the number of PCs (or factors) under

the framework of large cross-sections (N) and large time dimensions (T). These criteria penalize both dimensions N and T and outperform the usual AIC and BIC, which are functions of N or T alone, under the assumption that both N and T grow to infinity. Notice that the dimension-sample-size pair is denoted here as (N, T) instead of (p, n) . These six criteria are as follows:

$$\begin{aligned}
PC_{p1}(m) &= V(m, \hat{F}^m) + m\hat{\sigma}_{\text{BN}}^2 \left(\frac{N+T}{NT} \right) \ln \left(\frac{NT}{N+T} \right); \\
PC_{p2}(m) &= V(m, \hat{F}^m) + m\hat{\sigma}_{\text{BN}}^2 \left(\frac{N+T}{NT} \right) \ln C_{NT}^2; \\
PC_{p3}(m) &= V(m, \hat{F}^m) + m\hat{\sigma}_{\text{BN}}^2 \left(\frac{\ln C_{NT}^2}{C_{NT}^2} \right); \\
IC_{p1}(m) &= \ln \left(V(m, \hat{F}^m) \right) + m \left(\frac{N+T}{NT} \right) \ln \left(\frac{NT}{N+T} \right); \\
IC_{p2}(m) &= \ln \left(V(m, \hat{F}^m) \right) + m \left(\frac{N+T}{NT} \right) \ln C_{NT}^2; \\
IC_{p3}(m) &= \ln \left(V(m, \hat{F}^m) \right) + m \left(\frac{\ln C_{NT}^2}{C_{NT}^2} \right), \tag{11}
\end{aligned}$$

where $\hat{\sigma}_{\text{BN}}^2$ is a consistent estimate of $(NT)^{-1} \sum_{i=1}^N \sum_{j=1}^T E(e_{ij})^2$, $V(m, \hat{F}^m) = (NT)^{-1} \sum_{i=1}^N \hat{\mathbf{e}}_i' \hat{\mathbf{e}}_i$, and $C_{NT}^2 = \min\{N, T\}$. Notice that the difference between the PC_p and the IC_p criteria is that the first family uses the V function while the second family uses its logarithm. In applications, $\hat{\sigma}_{\text{BN}}^2$ is replaced by $V(m_0, \hat{F}^{m_0})$, where m_0 is a predetermined maximum value of m . We can see that the calculations of $\hat{\sigma}_{\text{BN}}^2$ and $V(m, \hat{F}^m)$ have no explicit formula and are based on the estimation of the residuals ($\hat{\mathbf{e}}_i$). It is worth mentioning that $\hat{\sigma}_{\text{BN}}^2$ is indeed the estimator of the noise variance if the underlying model is the PPCA model. Now we substitute the proposed bias-corrected estimator $\hat{\sigma}_*^2$ for empirical $\hat{\sigma}_{\text{BN}}^2$ and update in accordance the statistic $V(m, \hat{F}^m)$. The modified criteria using $\hat{\sigma}_*^2$ are denoted as PC_{p1}^* , PC_{p2}^* , PC_{p3}^* , IC_{p1}^* , IC_{p2}^* and IC_{p3}^* .

Simulation experiments are conducted to check whether the performance of the three PC_p criteria is improved by the bias-corrected estimator. The results of three IC_p criteria are not presented here since they are very similar in our context to the results of the PC_p criteria. As in Bai and Ng (2002), the data are generated from the model:

$$X_{it} = \sum_{j=1}^m \lambda_{ij} F_{tj} + \sqrt{\theta} e_{it}, \quad (12)$$

where the PCs, the loadings and the errors (e_{it}) are $N(0, 1)$ variates, the common component of X_{it} has variance m and the idiosyncratic component has variance θ . Notice that the noise variance here is $\sigma^2 = \theta$ and $\mathbf{\Lambda} = (\lambda_{ij})$. Typically, a PC corresponding to α_j is detectable when $\alpha_j \geq \left(1 + \sqrt{\frac{N}{T}}\right) \theta$, see (7). We conduct extensive simulation by reproducing all the configuration of N and T used in Bai and Ng (2002). In particular, the last five rows of each table below correspond to small dimensions (either N or T is small).

Tables 5-8 report the empirical means of the estimator of the number of PCs over 1000 replications, for $m = 1, 3$ and 5 respectively, with standard errors in parentheses. When a standard error is actually zero, no standard error is thus indicated. For all cases, the predetermined maximum number m_0 of PCs is set to 8. When the true number of PCs is 1 (Table 5), the criteria PC_p^* can correctly detect the number almost surely and the corresponding standard errors are all zeros. In comparison, there are 11 cases where the criteria PC_p lose efficiency in finding the true number of PCs with a non-zero standard error. In the small dimensions situation (last five rows), all PC_p^* and PC_p fail when the value of N is 10: they all report the maximum value m_0 . But the criteria PC_p^* outperform PC_p in the last three cases in terms of mean and standard error. In Table 6, although

the criteria PC_p^* have some determination errors in a few cases, these errors are much smaller than the corresponding ones from the initial criteria PC_p . For the last three cases of small dimensions, the results of criteria PC_p^* are also much better than that of PC_p . In Table 7, the common component and idiosyncratic component have the same variance 5 which is large and it can be verified that in this setting, some of the 5 PC eigenvalues α_j do not satisfy the detection condition $\alpha_j \geq \left(1 + \sqrt{\frac{N}{T}}\right)\theta$. Consequently, the criteria PC_p^* are no longer uniformly better than PC_p . In Table 8, when the variance of idiosyncratic component is smaller than that of the common component, the criteria PC_p^* have again an overall better performance than the criteria PC_p . In conclusion, except some cases in Table 7, these criteria proposed in Bai and Ng (2002) can have a better performance using the bias-corrected estimator proposed in this paper for PPCA models.

5 Application to the goodness-of-fit test of a PPCA model

As a third application of the bias-corrected estimator $\hat{\sigma}_*^2$, we consider the following goodness-of-fit test for the PPCA model (1). The null hypothesis is then

$$\mathcal{H}_0 : \Sigma = \Lambda\Lambda' + \sigma^2\mathbf{I}_p,$$

where the number of PCs m is specified. Following Anderson and Rubin (1956), the likelihood ratio test (LRT) statistic is

$$T_n = -nL^*,$$

Table 5: Comparison between PC_{p1}^* , PC_{p2}^* , PC_{p3}^* and PC_{p1} , PC_{p2} , PC_{p3} in terms of the mean estimation numbers of PCs for $m = 1, \theta = 1$.

N	T	PC_{p1}^*	PC_{p2}^*	PC_{p3}^*	PC_{p1}	PC_{p2}	PC_{p3}
100	40	1.00	1.00	1.00	1.17(0.37)	1.01(0.10)	3.78(0.75)
100	60	1.00	1.00	1.00	1.00	1.00	3.63(0.76)
200	60	1.00	1.00	1.00	1.00	1.00	1.00
500	60	1.00	1.00	1.00	1.00	1.00	1.00
1000	60	1.00	1.00	1.00	1.00	1.00	1.00
2000	60	1.00	1.00	1.00	1.00	1.00	1.00
100	100	1.00	1.00	1.00	1.00	1.00	5.36(0.80)
200	100	1.00	1.00	1.00	1.00	1.00	1.00
500	100	1.00	1.00	1.00	1.00	1.00	1.00
1000	100	1.00	1.00	1.00	1.00	1.00	1.00
2000	100	1.00	1.00	1.00	1.00	1.00	1.00
40	100	1.00	1.00	1.00	1.79(0.72)	1.19(0.40)	4.91(0.90)
60	100	1.00	1.00	1.00	1.01(0.08)	1.00	4.30(0.85)
60	200	1.00	1.00	1.00	1.00	1.00	1.02(0.16)
60	500	1.00	1.00	1.00	1.00	1.00	1.00
60	1000	1.00	1.00	1.00	1.00	1.00	1.00
60	2000	1.00	1.00	1.00	1.00	1.00	1.00
4000	60	1.00	1.00	1.00	1.00	1.00	1.00
4000	100	1.00	1.00	1.00	1.00	1.00	1.00
8000	60	1.00	1.00	1.00	1.00	1.00	1.00
8000	100	1.00	1.00	1.00	1.00	1.00	1.00
60	4000	1.00	1.00	1.00	1.00	1.00	1.00
100	4000	1.00	1.00	1.00	1.00	1.00	1.00
60	8000	1.00	1.00	1.00	1.00	1.00	1.00
100	8000	1.00	1.00	1.00	1.00	1.00	1.00
10	50	8.00	8.00	8.00	8.00	8.00	8.00
10	100	8.00	8.00	8.00	8.00	8.00	8.00
20	100	1.01(0.15)	1.01(0.12)	1.08(0.53)	6.96(0.88)	6.35(0.98)	7.84(0.40)
100	10	1.08(0.73)	1.03(0.50)	1.15(1.01)	8.00	8.00	8.00
100	20	1.00(0.03)	1.00(0.03)	1.00(0.03)	5.88(0.76)	5.12(0.77)	7.35(0.63)

Table 6: Comparison between PC_{p1}^* , PC_{p2}^* , PC_{p3}^* and PC_{p1} , PC_{p2} , PC_{p3} in terms of the mean estimation numbers of PCs for $m = 3, \theta = 3$.

N	T	PC_{p1}^*	PC_{p2}^*	PC_{p3}^*	PC_{p1}	PC_{p2}	PC_{p3}
100	40	2.98(0.15)	2.95(0.22)	3.00(0.06)	3.00	3.00	3.90
100	60	3.00(0.03)	3.00(0.04)	3.00	3.01(0.08)	3.00	4.37(0.64)
200	60	3.00	3.00	3.00	3.00	3.00	4.18(0.63)
500	60	3.00	3.00	3.00	3.00	3.00	3.00
1000	60	3.00	3.00	3.00	3.00	3.00	3.00
2000	60	3.00	3.00	3.00	3.00	3.00	3.00
100	100	3.00	3.00	3.00	3.00	3.00	5.62(0.72)
200	100	3.00	3.00	3.00	3.00	3.00	3.00
500	100	3.00	3.00	3.00	3.00	3.00	3.00
1000	100	3.00	3.00	3.00	3.00	3.00	3.00
2000	60	3.00	3.00	3.00	3.00	3.00	3.00
40	100	2.99(0.10)	2.98(0.14)	3.00	3.07(0.26)	3.01(0.07)	5.04(0.72)
60	100	3.00	3.00(0.03)	3.00	3.00	3.00	4.65(0.69)
60	200	3.00	3.00	3.00	3.00	3.00	3.00
60	500	3.00	3.00	3.00	3.00	3.00	3.00
60	1000	3.00	3.00	3.00	3.00	3.00	3.00
60	2000	3.00	3.00	3.00	3.00	3.00	3.00
4000	60	3.00	3.00	3.00	3.00	3.00	3.00
4000	100	3.00	3.00	3.00	3.00	3.00	3.00
8000	60	3.00	3.00	3.00	3.00	3.00	3.00
8000	100	3.00	3.00	3.00	3.00	3.00	3.00
60	4000	3.00	3.00	3.00	3.00	3.00	3.00
100	4000	3.00	3.00	3.00	3.00	3.00	3.00
60	8000	3.00	3.00	3.00	3.00	3.00	3.00
100	8000	3.00	3.00	3.00	3.00	3.00	3.00
10	50	8.00	8.00	8.00	8.00	8.00	8.00
10	100	8.00	8.00	8.00	8.00	8.00	8.00
20	100	2.89(0.32)	2.85(0.37)	2.95(0.27)	6.55(0.74)	5.96(0.77)	7.62(0.55)
100	10	2.57(1.35)	2.43(1.19)	2.77(1.54)	8.00	8.00	8.00
100	20	2.46(0.63)	2.37(0.65)	2.65(0.52)	6.15(0.69)	5.46(0.68)	7.49(0.59)

Table 7: Comparison between PC_{p1}^* , PC_{p2}^* , PC_{p3}^* and PC_{p1} , PC_{p2} , PC_{p3} in terms of the mean estimation numbers of PCs for $m = 5, \theta = 5$.

N	T	PC_{p1}^*	PC_{p2}^*	PC_{p3}^*	PC_{p1}	PC_{p2}	PC_{p3}
100	40	3.83(0.77)	3.49(0.77)	4.51(0.58)	5.00(0.07)	4.98(0.15)	5.36(0.51)
100	60	4.66(0.50)	4.36(0.61)	4.98(0.13)	5.00(0.03)	5.00(0.06)	5.27(0.45)
200	60	4.95(0.22)	4.90(0.30)	4.99(0.08)	5.00	5.00	5.00
500	60	5.00(0.04)	5.00(0.07)	5.00(0.03)	5.00	5.00	5.00
1000	60	5.00(0.04)	5.00(0.04)	5.00	5.00	5.00	5.00
2000	60	5.00(0.03)	5.00(0.03)	5.00(0.03)	5.00	5.00	5.00
100	100	4.(0.12)	4.90(0.30)	5.00	5.00	5.00	6.18(0.63)
200	100	5.00	5.00	5.00	5.00	5.00	5.00
500	100	5.00	5.00	5.00	5.00	5.00	5.00
1000	100	5.00	5.00	5.00	5.00	5.00	5.00
2000	60	5.00	5.00	5.00	5.00	5.00	5.00
40	100	4.25(0.68)	3.92(0.75)	4.77(0.44)	4.98(0.04)	5.66(0.14)	5.66(0.57)
60	100	4.76(0.44)	4.47(0.60)	4.76(0.10)	5.00(0.03)	4.99(0.08)	5.46(0.56)
60	200	4.97(0.17)	4.94(0.24)	5.00	5.00	5.00	5.00
60	500	5.00(0.05)	5.00(0.06)	5.00(0.04)	5.00	5.00	5.00
60	1000	5.00(0.03)	5.00(0.03)	5.00	5.00	5.00	5.00
60	2000	5.00	5.00	5.00	5.00	5.00	5.00
4000	60	5.00	5.00	5.00	5.00	5.00	5.00
4000	100	5.00	5.00	5.00	5.00	5.00	5.00
8000	60	5.00	5.00	5.00	5.00	5.00	5.00
8000	100	5.00	5.00	5.00	5.00	5.00	5.00
60	4000	5.00	5.00	5.00	5.00	5.00	5.000
100	4000	5.00	5.00	5.00	5.00	5.00	5.00
60	8000	5.00	5.00	5.00	5.00	5.00	5.00
100	8000	5.00	5.00	5.00	5.00	5.00	5.00
10	50	8.00	8.00	8.00	8.00	8.00	8.00
10	100	8.00	8.00	8.00	8.00	8.00	8.00
20	100	3.64(0.91)	3.38(0.94)	4.08(0.79)	6.65(0.64)	6.12(0.64)	7.63(0.51)
100	10	3.10(2.01)	2.83(1.86)	3.53(2.27)	8.00	8.00	8.00
100	20	2.18(0.92)	1.93(0.92)	2.65(0.0.90)	6.56(0.62)	5.97(0.62)	7.66(0.50)

Table 8: Comparison between PC_{p1}^* , PC_{p2}^* , PC_{p3}^* and PC_{p1} , PC_{p2} , PC_{p3} in terms of the mean estimation numbers of PCs for $m = 5, \theta = 3$.

N	T	PC_{p1}^*	PC_{p2}^*	PC_{p3}^*	PC_{p1}	PC_{p2}	PC_{p3}
100	40	4.91(0.30)	4.81(0.41)	4.99(0.11)	5.00(0.03)	5.00	5.59(0.57)
100	60	5.00(0.04)	4.99(0.11)	5.00	5.00	5.00	5.58(0.57)
200	60	5.00	5.00	5.00	5.00	5.00	5.00
500	60	5.00	5.00	5.00	5.00	5.00	5.00
1000	60	5.00	5.00	5.00	5.00	5.00	5.00
2000	60	5.00	5.00	5.00	5.00	5.00	5.00
100	100	5.00	5.00	5.00	5.00	5.00	6.84(0.65)
200	100	5.00	5.00	5.00	5.00	5.00	5.00
500	100	5.00	5.00	5.00	5.00	5.00	5.00
1000	100	5.00	5.00	5.00	5.00	5.00	5.00
2000	100	5.00	5.00	5.00	5.00	5.00	5.00
40	100	4.97(0.17)	4.92(0.27)	5.00(0.04)	5.02(0.12)	5.00	6.22(0.66)
60	100	5.00(0.04)	4.99(0.08)	5.00	5.00	5.00	6.03(0.64)
60	200	5.00	5.00	5.00	5.00	5.00	6.03(0.03)
60	500	5.00	5.00	5.00	5.00	5.00	5.00
60	1000	5.00	5.00	5.00	5.00	5.00	5.00
60	2000	5.00	5.00	5.00	5.00	5.00	5.00
4000	60	5.00	5.00	5.00	5.00	5.00	5.00
4000	100	5.00	5.00	5.00	5.00	5.00	5.00
8000	60	5.00	5.00	5.00	5.00	5.00	5.00
8000	100	5.00	5.00	5.00	5.00	5.00	5.00
60	4000	5.00	5.00	5.00	5.00	5.00	5.00
100	4000	5.00	5.00	5.00	5.00	5.00	5.00
60	8000	5.00	5.00	5.00	5.00	5.00	5.00
100	8000	5.00	5.00	5.00	5.00	5.00	5.00
10	50	8.00	8.00	8.00	8.00	8.00	8.00
10	100	8.00	8.00	8.00	8.00	8.00	8.00
20	100	4.74(0.51)	4.62(0.57)	4.92(0.45)	7.11(0.63)	6.65(0.64)	7.85(0.37)
100	10	4.59(1.99)	4.35(1.91)	4.88(2.09)	8.00	8.00	8.00
100	20	3.86(0.79)	3.69(0.81)	4.13(0.73)	6.74(0.63)	6.19(0.62)	7.77(0.43)

where

$$L^* = \sum_{j=m+1}^p \log \frac{\lambda_{n,j}}{\widehat{\sigma}^2},$$

and $\widehat{\sigma}^2$ is the m.l.e.(4) of the variance. Keeping p fixed while letting $n \rightarrow \infty$, the classical low-dimensional theory states that T_n converges to χ_q^2 , where $q = p(p+1)/2 + m(m-1)/2 - pm - 1$, see Anderson and Rubin (1956). However, this classical approximation is again useless in the large-dimensional setting. Indeed, it will be shown below that this criterion leads to a high false-positive rate. In particular, the test becomes biased since the size will be much higher than the nominal level (see Table 9).

In a way similar to Section 2, we now construct a corrected version of T_n using Proposition 1 and calculus done in Bai et al. (2009) and Zheng (2012). As we consider the logarithm of the eigenvalues of the sample covariance matrix, we will assume in the sequel that $p < n$ and $c < 1$ to avoid null eigenvalues.

Theorem 3. *Assume the same conditions as in Theorem 1 and in addition $c < 1$. Then, we have*

$$v(c)^{-\frac{1}{2}} \{L^* - m(c) - ph(c_n) - \eta + (p - m) \log(\beta)\} \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1),$$

where

$$\begin{aligned} m(c) &= \frac{\log(1-c)}{2}, & h(c_n) &= \frac{c_n - 1}{c_n} \log(1 - c_n) - 1, \\ \eta &= \sum_{i=1}^m \log(1 + c\sigma^2\alpha_i^{-1}), & \beta &= 1 - \frac{c}{p-m} (m + \sigma^2 \sum_{i=1}^m \alpha_i^{-1}), \\ v(c) &= -2 \log(1-c) + \frac{2c}{\beta} \left(\frac{1}{\beta} - 2 \right). \end{aligned}$$

Note that the above statistic depends on the unknown variance σ^2 and the spike eigenvalues (α_i) . First of all, as explained in Section 2, consistent estimates of (α_i) are available. By using these estimates and substituting bias-corrected estimate $\widehat{\sigma}_*^2$ for σ^2 , we obtain consistent estimates $\widehat{v}(c_n)$, $\widehat{\eta}$ and $\widehat{\beta}$ of $v(c)$, η and β , respectively. Therefore, to test \mathcal{H}_0 , it is natural to use the statistic

$$\Delta_n := \widehat{v}(c_n)^{-\frac{1}{2}}(L^* - m(c_n) - ph(c_n) - \widehat{\eta} + (p - m) \log(\widehat{\beta})) .$$

Since Δ_n is asymptotically standard normal, the critical region $\{\Delta_n > q_\alpha\}$ where q_α is the α th upper quantile of the standard normal, will have an asymptotic size α . This test will be hereafter referred as the corrected likelihood ratio test (CLRT in short).

5.1 Monte-Carlo experiments

We consider again Models 1 and 2 described in Section 2, and a new one (Model 4):

- Model 1: $\text{spec}(\Sigma) = (25, 16, 9, 0, \dots, 0) + \sigma^2(1, \dots, 1)$, $\sigma^2 = 4$, $c = 0.9$;
- Model 2: $\text{spec}(\Sigma) = (4, 3, 0, \dots, 0) + \sigma^2(1, \dots, 1)$, $\sigma^2 = 2$, $c = 0.2$;
- Model 4: $\text{spec}(\Sigma) = (8, 7, 0, \dots, 0) + \sigma^2(1, \dots, 1)$, $\sigma^2 = 1$, varying c .

Table 9 gives the empirical sizes of the classical likelihood ratio test (LRT) and the new corrected likelihood ratio test (CLRT) above. For the LRT, we use the correction proposed by Bartlett (1950), that is replacing $T_n = -nL^*$ by $\widetilde{T}_n = -(n - (2p + 11)/6 - 2m/3)L^*$. The computations are done under 10000 independent replications and the nominal test level is 0.05.

Table 9: Comparison of the empirical size of the classical likelihood ratio test (LRT) and the corrected likelihood ratio test (CLRT) in various settings.

Settings		Empirical size of CLRT	Empirical size of LRT
Model 1	$p = 90$ $n = 100$	0.0497	0.9995
	$p = 180$ $n = 200$	0.0491	1
	$p = 720$ $n = 800$	0.0496	1
Model 2	$p = 20$ $n = 100$	0.0324	0.0294
	$p = 80$ $n = 400$	0.0507	0.0390
	$p = 200$ $n = 1000$	0.0541	0.0552
Model 4	$p = 5$ $n = 500$	0.0108	0.0483
	$p = 10$ $n = 500$	0.0190	0.0465
	$p = 50$ $n = 500$	0.0424	0.0445
	$p = 100$ $n = 500$	0.0459	0.0461
	$p = 200$ $n = 500$	0.0491	0.2212
	$p = 250$ $n = 500$	0.0492	0.7395
	$p = 300$ $n = 500$	0.0509	0.9994

The empirical sizes of the new CLRT are very close to the nominal one, except when the ratio p/n is very small (less than 0.1). On the contrary, the empirical sizes of the classical LRT are much higher than the nominal level especially when c is not too small, and the test will always reject the null hypothesis when p becomes large. In particular when $p/n \geq \frac{1}{2}$, the LRT test tends to reject automatically the null.

6 Proofs

Before giving the proofs, we first recall some important results from the random matrix theory which laid the foundation for the proofs of the main results of the paper.

6.1 Useful results from random matrix theory

Random matrix theory has become a powerful tool to address new inference problems in high-dimensional data. For general background and references, we refer to review papers Johnstone (2007) and Johnstone and Titterton (2009).

Let H be a probability measure on \mathbb{R}^+ and $c > 0$ a constant. We define the map

$$g(s) = g_{c,H}(s) = \frac{1}{s} + c \int \frac{t}{1+ts} dH(t) \quad (13)$$

in the set $\mathbb{C}^+ = \{z \in \mathbb{C} : \Im z > 0\}$. The map g is a one-to-one mapping from \mathbb{C}^+ onto itself (see Bai and Silverstein (2010), Chapter 6), and the inverse map $m = g^{-1}$ satisfies all the requirements of the Stieltjes transform of a probability measure on $[0, \infty)$. We call this measure $\underline{F}_{c,H}$. Next, a companion measure $F_{c,H}$ is introduced by the equation $cF_{c,H} = (c-1)\delta_0 + \underline{F}_{c,H}$ (note that in this equation, measures can be signed). The measure $F_{c,H}$ is referred as the generalized Marčenko-Pastur distribution with index (c, H) .

Let $F_n = \frac{1}{p} \sum_{i=1}^p \delta_{\lambda_{n,i}}$ be the empirical spectral distribution (ESD) of the sample covariance matrix \mathbf{S}_n defined in (3) with the $\{\lambda_{n,i}\}$ denoting its eigenvalues.

Then, it is well-known that under suitable moment conditions, F_n converges to the Marčenko-Pastur distribution of index (c, δ_{σ^2}) , simply denoted as F_{c, σ^2} , with the following density function

$$p_{c, \sigma^2}(x) = \begin{cases} \frac{1}{2\pi x c \sigma^2} \sqrt{\{b(c) - x\}\{x - a(c)\}}, & a(c) \leq x \leq b(c), \\ 0, & \text{otherwise.} \end{cases}$$

The distribution has an additional mass $(1 - 1/c)$ at the origin if $c > 1$.

The ESD H_n of Σ is

$$H_n = \frac{p - m}{p} \delta_{\sigma^2} + \frac{1}{p} \sum_{i=1}^m \delta_{\alpha_i + \sigma^2},$$

and $H_n \rightarrow \delta_{\sigma^2}$. Define the normalized empirical process

$$G_n(f) = p \int_{\mathbb{R}} f(x) [F_n - F_{c_n, H_n}](dx), \quad f \in \mathcal{A},$$

where \mathcal{A} is the set of analytic functions $f : \mathcal{U} \rightarrow \mathbb{C}$, with \mathcal{U} an open set of \mathbb{C} such that $[\mathbf{1}_{(0,1)}(c)a(c), b(c)] \subset \mathcal{U}$. We will need the following CLT which is a combination of Theorem 1.1 of Bai and Silverstein (2004) and a recent addition proposed in Zheng et al. (2014).

Proposition 1. *We assume the same conditions as in Theorem 1. Then, for any functions $f_1, \dots, f_k \in \mathcal{A}$, the random vector $(G_n(f_1), \dots, G_n(f_k))$ converges to a k -dimensional Gaussian vector with mean vector*

$$m(f_j) = \frac{f_j(a(c)) + f_j(b(c))}{4} - \frac{1}{2\pi} \int_{a(c)}^{b(c)} \frac{f_j(x)}{\sqrt{4c\sigma^4 - (x - \sigma^2 - c\sigma^2)^2}} dx, \quad j = 1, \dots, k,$$

and covariance function

$$v(f_j, f_l) = -\frac{1}{2\pi^2} \oint_{C_1} \oint_{C_2} \frac{f_j(z_1) f_l(z_2)}{(\underline{m}(z_1) - \underline{m}(z_2))^2} d\underline{m}(z_1) d\underline{m}(z_2), \quad j, l = 1, \dots, k, \quad (14)$$

where $\underline{m}(z)$ is the Stieltjes transform of $F_{c,\sigma^2} = (1-c)\delta_0 + cF_{c,\sigma^2}$. The contours \mathcal{C}_1 and \mathcal{C}_2 are non overlapping and both contain the support of F_{c,σ^2} .

An important and subtle point here is that the centering term in $G_n(f)$ in the above CLT is defined with respect to the Marcčenko-Pastur distribution F_{c_n, H_n} with “current” index (c_n, H_n) instead of the limiting distribution F_{c,σ^2} with index (c, σ^2) . In contrast, the limiting mean function $m(f_j)$ and covariance function $v(f_j, f_l)$ depend on the limiting distribution F_{c,σ^2} only.

6.2 Proof of Theorem 1

We have

$$(p-m)\widehat{\sigma}^2 = \sum_{i=1}^p \lambda_{n,i} - \sum_{i=1}^m \lambda_{n,i}.$$

By (7),

$$\sum_{i=1}^m \lambda_{n,i} \longrightarrow \sum_{i=1}^m \left(\alpha_i + \frac{c\sigma^4}{\alpha_i} \right) + \sigma^2 m(1+c) \text{ a.s.} \quad (15)$$

For the first term, we have

$$\begin{aligned} \sum_{i=1}^p \lambda_i &= p \int x dF_n(x) \\ &= p \int x d(F_n - F_{c_n, H_n})(x) + p \int x dF_{c_n, H_n}(x) \\ &= G_n(x) + p \int x dF_{c_n, H_n}(x). \end{aligned}$$

By Proposition 1, the first term is asymptotically normal

$$G_n(x) = \sum_{i=1}^p \lambda_{n,i} - p \int x dF_{c_n, H_n}(x) \xrightarrow{\mathcal{D}} \mathcal{N}(m(x), v(x)),$$

with asymptotic mean

$$m(x) = 0, \quad (16)$$

and asymptotic variance

$$v(x) = 2c\sigma^4. \quad (17)$$

The derivation of these two formula are given in the Section 6. Furthermore, by Lemma 1 of Bai et al. (2010),

$$\int x dF_{c_n, H_n}(x) = \int t dH_n(t) = \sigma^2 + \frac{1}{p} \sum_{i=1}^m \alpha_i.$$

So we have

$$\sum_{i=1}^p \lambda_{n,i} - p\sigma^2 - \sum_{i=1}^m \alpha_i \xrightarrow{\mathcal{D}} \mathcal{N}(0, 2c\sigma^4). \quad (18)$$

By (15) and (18) and using Slutsky's lemma, we obtain

$$(p-m)(\hat{\sigma}^2 - \sigma^2) + c\sigma^2 \left(m + \sigma^2 \sum_{i=1}^m \frac{1}{\alpha_i} \right) \xrightarrow{\mathcal{D}} \mathcal{N}(0, 2c\sigma^4).$$

6.3 Proof of Theorem 2

We have

$$\begin{aligned} \frac{p-m}{\sigma^2 \sqrt{2c_n}} (\hat{\sigma}_*^2 - \sigma^2) &= \frac{p-m}{\sigma^2 \sqrt{2c_n}} (\hat{\sigma}^2 - \sigma^2) + b(\hat{\sigma}^2) \frac{\hat{\sigma}^2}{\sigma^2} \\ &= \left\{ \frac{p-m}{\sigma^2 \sqrt{2c_n}} (\hat{\sigma}^2 - \sigma^2) + b(\sigma^2) \right\} + \frac{1}{\sigma^2} \{ b(\hat{\sigma}^2) \hat{\sigma}^2 - b(\sigma^2) \sigma^2 \}. \end{aligned}$$

Since $\hat{\sigma}^2 \xrightarrow{\mathcal{P}} \sigma^2$, by continuity, the second expression tends to 0 in probability and the conclusion follows from Theorem 1.

6.4 Proof of Theorem 3

We have

$$\begin{aligned}
L^* &= \sum_{i=m+1}^p \log \frac{\lambda_{n,i}}{\widehat{\sigma}^2} \\
&= \sum_{i=m+1}^p \log \frac{\lambda_{n,i}}{\sigma^2} - \sum_{i=m+1}^p \log \frac{\widehat{\sigma}^2}{\sigma^2} \\
&= \sum_{i=m+1}^p \log \frac{\lambda_{n,i}}{\sigma^2} - (p-m) \log \left(\frac{1}{p-m} \sum_{i=m+1}^p \frac{\lambda_{n,i}}{\sigma^2} \right) \\
&= L_1 - (p-m) \log \left(\frac{L_2}{p-m} \right),
\end{aligned}$$

where we have defined a two-dimensional vector $(L_1, L_2) = (\sum_{i=m+1}^p \log \frac{\lambda_{n,i}}{\sigma^2}, \sum_{i=m+1}^p \frac{\lambda_{n,i}}{\sigma^2})$.

CLT when $\sigma^2 = 1$. To start with, we consider the case $\sigma^2 = 1$. We have

$$\begin{aligned}
L_1 &= p \int \log(x) dF_n(x) - \sum_{i=1}^m \log \lambda_{n,i} \\
&= p \int \log(x) d(F_n - F_{c_n, H_n})(x) + p \int \log(x) dF_{c_n, H_n}(x) - \sum_{i=1}^m \log \lambda_{n,i}.
\end{aligned}$$

Similarly, we have

$$L_2 = p \int x d(F_n - F_{c_n, H_n})(x) + p \int x dF_{c_n, H_n}(x) - \sum_{i=1}^m \lambda_{n,i}.$$

By Proposition 1, we find that

$$p \begin{pmatrix} \int \log(x) d(F_n - F_{c_n, H_n})(x) \\ \int x d(F_n - F_{c_n, H_n})(x) \end{pmatrix} \xrightarrow{\mathcal{D}} \mathcal{N} \left(\begin{pmatrix} m_1(c) \\ m_2(c) \end{pmatrix}, \begin{pmatrix} v_1(c) & v_{1,2}(c) \\ v_{1,2}(c) & v_2(c) \end{pmatrix} \right) \quad (19)$$

with $m_2(c) = 0$ and $v_2(c) = 2c$ and

$$m_1(c) = \frac{\log(1-c)}{2}, \quad (20)$$

$$v_1(c) = -2 \log(1 - c), \quad (21)$$

$$v_{1,2}(c) = 2c. \quad (22)$$

Formulae of m_2 and v_2 have been established in the proof of Theorem 1 and the others are derived in next subsection.

In Theorem 1, with $\sigma^2 = 1$, we found that

$$\int x dF_{c_n, H_n}(x) = 1 + \frac{1}{p} \sum_{i=1}^m \alpha_i,$$

and

$$\sum_{i=1}^m \lambda_{n,i} \xrightarrow{\text{a.s.}} \sum_{i=1}^m \left(\alpha_i + \frac{c}{\alpha_i} \right) + m(1 + c).$$

For the last term of L_1 , by (7), we have

$$\log \lambda_{n,i} \longrightarrow \log(\phi(\alpha_i + 1)) = \log((\alpha_i + 1)(1 + c\alpha_i^{-1})) \text{ a.s.}$$

Furthermore, by Wang et al. (2013), we have

$$\int \log(x) dF_{c_n, H_n}(x) = \frac{1}{p} \sum_{i=1}^m \log(\alpha_i + 1) + h(c_n) + o\left(\frac{1}{p}\right),$$

where

$$h(c_n) = \int \log(x) dF_{c_n, \delta_1}(x) = \frac{c_n - 1}{c_n} \log(1 - c_n) - 1. \quad (23)$$

can be calculated using the density of the Marčenko-Pastur law (see 6.4). Summarising, we have obtained that

$$L_1 - m_1(c) - ph(c_n) + \eta(c, \alpha) \xrightarrow{\mathcal{D}} \mathcal{N}(0, v_1(c)),$$

where $h(c_n) = \frac{c_n-1}{c_n} \log(1 - c_n) - 1$ and $\eta(c, \alpha) = \sum_{i=1}^m \log(1 + c\sigma^2\alpha_i^{-1})$. Similarly, we have

$$L_2 - (p - m) + \rho(c, \alpha) \xrightarrow{\mathcal{D}} \mathcal{N}(0, v_2(c)),$$

where $\rho(c, \alpha) = c(m + \sum_{i=1}^m \alpha_i^{-1})$.

Using (19) and Slutsky's lemma,

$$\begin{pmatrix} L_1 \\ L_2 \end{pmatrix} \xrightarrow{\mathcal{D}} \mathcal{N} \left(\begin{pmatrix} m_1(c) + ph(c_n) - \eta(c, \alpha) \\ p - m - \rho(c, \alpha) \end{pmatrix}, \begin{pmatrix} v_1(c) & v_{1,2}(c) \\ v_{1,2}(c_n) & v_2(c_n) \end{pmatrix} \right),$$

with $h(c_n) = \frac{c_n-1}{c_n} \log(1 - c_n) - 1$, $\eta(c, \alpha) = \sum_{i=1}^m \log(1 + c\sigma^2\alpha_i^{-1})$ and $\rho(c, \alpha) = c(m + \sum_{i=1}^m \alpha_i^{-1})$.

CLT with general σ^2 . When $\sigma^2 = 1$,

$$\text{spec}(\mathbf{\Sigma}) = (\alpha_1 + 1, \dots, \alpha_m + 1, 1, \dots, 1),$$

whereas in the general case

$$\begin{aligned} \text{spec}(\mathbf{\Sigma}) &= (\alpha_1 + \sigma^2, \dots, \alpha_m + \sigma^2, \sigma^2, \dots, \sigma^2) \\ &= \sigma^2 \left(\frac{\alpha_1}{\sigma^2} + 1, \dots, \frac{\alpha_m}{\sigma^2} + 1, \dots, 1 \right). \end{aligned}$$

Thus, if we consider λ_i/σ^2 , we will find the same CLT by replacing the $(\alpha_i)_{1 \leq i \leq m}$ by α_i/σ^2 . Furthermore, we divide L_2 by $p - m$ to find

$$\begin{pmatrix} L_1 \\ \frac{L_2}{p-m} \end{pmatrix} \xrightarrow{\mathcal{D}} \mathcal{N} \left(\begin{pmatrix} m_1(c) + ph(c_n) - \eta(c, \alpha/\sigma^2) \\ 1 - \frac{\rho(c, \alpha/\sigma^2)}{p-m} \end{pmatrix}, \begin{pmatrix} \frac{2c}{(p-m)^2} & \frac{2c}{p-m} \\ \frac{2c}{p-m} & -2 \log(1 - c) \end{pmatrix} \right),$$

with $\eta(c, \alpha/\sigma^2) = \sum_{i=1}^m \log(1 + c\sigma^2\alpha_i^{-1})$, $\rho(c, \alpha/\sigma^2) = c(m + \sigma^2 \sum_{i=1}^m \alpha_i^{-1})$ and $h(c_n) = \frac{c_n-1}{c_n} \log(1 - c_n) - 1$.

Asymptotic distribution of L^* . We have $L^* = g(L_1, L_2/(p-m))$, with $g(x, y) = x - (p-m) \log(y)$. We will apply the multivariate delta-method on (24) with the function g . We have $\nabla g(x, y) = \left(1, -\frac{p-m}{y}\right)$ and

$$L^* \xrightarrow{\mathcal{D}} \mathcal{N}(\beta_1 - (p-m) \log(\beta_2), \nabla g(\beta_1, \beta_2) \text{cov}(L_1, L_2/(p-m)) \nabla g(\beta_1, \beta_2)'),$$

with $\beta_1 = m_1(c) + ph(c_n) - \eta(c, \alpha/\sigma^2)$ and $\beta_2 = 1 - \frac{\rho(c, \alpha/\sigma^2)}{p-m}$. After some standard calculation, we finally find

$$L^* \xrightarrow{\mathcal{D}} \mathcal{N}\left(m_1(c) + ph(c_n) - \eta\left(c, \frac{\alpha}{\sigma^2}\right) - (p-m) \log(\beta_2), -2 \log(1-c) + \frac{2c}{\beta_2} \left(\frac{1}{\beta_2} - 2\right)\right).$$

6.5 Complementary proofs

Proof of (5)

The general theory of the m.l.e. for the PPCA model (1) in the classical setting has been developed in Anderson and Amemiya (1988) with in particular the following result.

Proposition 2. *Let $\Theta = (\theta_{ij})_{1 \leq i, j \leq p} = \Psi - \Lambda(\Lambda' \Psi^{-1} \Lambda)^{-1} \Lambda'$. If $(\theta_{ij}^2)_{1 \leq i, j \leq p}$ is nonsingular, if Λ and Ψ are identified by the condition that $\Lambda' \Psi \Lambda$ is diagonal and the diagonal elements are different and ordered, if $\mathbf{S}_n \rightarrow \Lambda \Lambda' + \Psi$ in probability and if $\sqrt{n}(\mathbf{S}_n - \Sigma)$ has a limiting distribution, then $\sqrt{n}(\widehat{\Lambda} - \Lambda)$ and $\sqrt{n}(\widehat{\Psi} - \Psi)$ have a limiting distribution. The covariance of $\sqrt{n}(\widehat{\Psi}_{ii} - \Psi_{ii})$ and $\sqrt{n}(\widehat{\Psi}_{jj} - \Psi_{jj})$ in the limiting distribution is $2\Psi_{ii}^2 \Psi_{jj}^2 \xi^{ij}$ ($1 \leq i, j \leq p$), where $(\xi^{ij}) = (\theta_{ij}^2)^{-1}$.*

To prove the CLT (5), by Proposition 2, we know that the inverse of the Fisher information matrix is $\mathcal{I}^{-1}(\psi_{11}, \dots, \psi_{pp}) = (2\psi_{ii}^2 \psi_{jj}^2 \xi^{ij})_{ij}$. We have to change

the parametrization: in our case, we have $\psi_{11} = \dots = \psi_{pp}$. Let $g : \mathbb{R} \rightarrow \mathbb{R}^p$, $a \mapsto (a, \dots, a)$. The information matrix in this new parametrization becomes

$$\mathcal{I}(\sigma^2) = J' \mathcal{I}(g(\sigma^2)) J,$$

where J is the Jacobian matrix of g . As

$$\mathcal{I}(g(\sigma^2)) = \frac{1}{2\sigma^8} (\theta_{ij}^2)_{ij},$$

we have

$$\mathcal{I}(\sigma^2) = \frac{1}{2\sigma^8} \sum_{i,j=1}^p \theta_{ij}^2,$$

and

$$\begin{aligned} \Theta = (\theta_{ij})_{ij} &= \mathbf{\Psi} - \mathbf{\Lambda}(\mathbf{\Lambda}'\mathbf{\Psi}^{-1}\mathbf{\Lambda})^{-1}\mathbf{\Lambda}' \\ &= \sigma^2(\mathbf{I}_p - \mathbf{\Lambda}(\mathbf{\Lambda}'\mathbf{\Lambda})^{-1}\mathbf{\Lambda}'). \end{aligned}$$

By hypothesis, we have $\mathbf{\Lambda}'\mathbf{\Lambda} = \text{diag}(d_1^2, \dots, d_m^2)$. Consider the Singular Value Decomposition of $\mathbf{\Lambda}$, $\mathbf{\Lambda} = \mathbf{U}\mathbf{D}\mathbf{V}$, where \mathbf{U} is a $p \times p$ matrix such that $\mathbf{U}\mathbf{U}' = \mathbf{I}_p$, \mathbf{V} is a $m \times m$ matrix such that $\mathbf{V}'\mathbf{V} = \mathbf{I}_m$, and \mathbf{D} is a $p \times m$ diagonal matrix with d_1, \dots, d_m as diagonal elements. As $\mathbf{\Lambda}'\mathbf{\Lambda}$ is diagonal, $\mathbf{V} = \mathbf{I}_m$, so $\mathbf{\Lambda} = \mathbf{U}\mathbf{D}$. By elementary calculus, one can find that

$$\mathbf{\Lambda}(\mathbf{\Lambda}'\mathbf{\Lambda})^{-1}\mathbf{\Lambda}' = \text{diag}(\underbrace{1, \dots, 1}_m, \underbrace{0, \dots, 0}_{p-m}),$$

so

$$\Theta = \sigma^2 \text{diag}(\underbrace{0, \dots, 0}_m, \underbrace{1, \dots, 1}_{p-m}).$$

Finally,

$$\mathcal{I}(\sigma^2) = \frac{1}{2\sigma^8} (p-m)\sigma^4 = \frac{p-m}{2\sigma^4},$$

and the asymptotic variance of $\widehat{\sigma}^2$ is

$$s^2 = \mathcal{I}^{-1}(\sigma^2) = \frac{2\sigma^4}{p-m}.$$

Proof of (16)

By Proposition 1, for $g(x) = x$, by using the variable change $x = \sigma^2(1 + c - 2\sqrt{c}\cos\theta)$, $0 \leq \theta \leq \pi$, we have

$$\begin{aligned} m(g) &= \frac{g(a(c)) + g(b(c))}{4} - \frac{1}{2\pi} \int_{a(c)}^{b(c)} \frac{x}{\sqrt{4c\sigma^4 - (x - \sigma^2 - c\sigma^2)^2}} dx, \quad j = 1, \dots, k \\ &= \frac{\sigma^2(1+c)}{2} - \frac{\sigma^2}{2\pi} \int_0^\pi (1+c - 2\sqrt{c}\cos\theta) d\theta \\ &= 0. \end{aligned}$$

Proof of (17)

Let $\underline{s}(z)$ be the Stieltjes transform of $(1-c)\mathbf{1}_{[0,\infty)} + cF_{c,\delta_1}$. One can show that

$$\underline{m}(z) = \frac{1}{\sigma^2} \underline{s}\left(\frac{z}{\sigma^2}\right).$$

Then, in Proposition 1, we have

$$v(f_j, f_l) = -\frac{1}{2\pi^2} \oint \oint \frac{f_j(\sigma^2 z_1) f_l(\sigma^2 z_2)}{(\underline{s}(z_1) - \underline{s}(z_2))^2} d\underline{s}(z_1) d\underline{s}(z_2), \quad j, l = 1, \dots, k. \quad (24)$$

For $g(x) = x$, we have

$$\begin{aligned} v(g) &= -\frac{1}{2\pi^2} \oint \oint \frac{g(\sigma^2 z_1) g(\sigma^2 z_2)}{(\underline{s}(z_1) - \underline{s}(z_2))^2} d\underline{s}(z_1) d\underline{s}(z_2) \\ &= -\frac{\sigma^4}{2\pi^2} \oint \oint \frac{z_1 z_2}{(\underline{s}(z_1) - \underline{s}(z_2))^2} d\underline{s}(z_1) d\underline{s}(z_2) \\ &= 2c\sigma^4, \end{aligned}$$

where $-\frac{1}{2\pi^2} \oint \oint \frac{z_1 z_2}{(\underline{s}(z_1) - \underline{s}(z_2))^2} d\underline{s}(z_1) d\underline{s}(z_2) = 2c$ is calculated in Bai et al. (2009) (it corresponds to $v(z_1, z_2)$, Section 5, proof of (3.4)).

Proof of (20)

By Proposition 1, for $\sigma^2 = 1$ and $g(x) = \log(x)$, by using the variable change $x = 1 + c - 2\sqrt{c} \cos \theta$, $0 \leq \theta \leq \pi$, we have

$$\begin{aligned} m(g) &= \frac{g(a(c)) + g(b(c))}{4} - \frac{1}{2\pi} \int_{a(c)}^{b(c)} \frac{x}{\sqrt{4c - (x - 1 - c)^2}} dx, \quad j = 1, \dots, k \\ &= \frac{\log(1 - c)}{2} - \frac{1}{2\pi} \int_0^\pi \log(1 + c - 2\sqrt{c} \cos \theta) d\theta \\ &= \frac{\log(1 - c)}{2} - \frac{1}{4\pi} \int_0^{2\pi} \log |1 - \sqrt{c} e^{i\theta}|^2 d\theta \\ &= \frac{\log(1 - c)}{2}, \end{aligned}$$

where $\int_0^{2\pi} \log |1 - \sqrt{c} e^{i\theta}|^2 d\theta = 0$ is calculated in Bai and Silverstein (2010).

Proof of (21)

By Proposition 1 and (24), for $\sigma^2 = 1$ and $g(x) = x$, we have

$$\begin{aligned} v(g) &= -\frac{1}{2\pi^2} \oint \oint \frac{g(z_1)g(z_2)}{(\underline{s}(z_1) - \underline{s}(z_2))^2} d\underline{s}(z_1) d\underline{s}(z_2) \\ &= -\frac{1}{2\pi^2} \oint \oint \frac{\log(z_1) \log(z_2)}{(\underline{s}(z_1) - \underline{s}(z_2))^2} d\underline{s}(z_1) d\underline{s}(z_2) \\ &= -2 \log(1 - c_n), \end{aligned}$$

where the last integral is calculated in Bai and Silverstein (2010).

Proof of (23)

F_{c_n, δ_1} is the Marčenko-Pastur distribution of index c_n . By using the variable change $x = 1 + c_n - 2\sqrt{c_n} \cos \theta$, $0 \leq \theta \leq \pi$, we have

$$\begin{aligned}
\int \log(x) dF_{c_n, \delta_1}(x) &= \int_{a(c_n)}^{b(c_n)} \frac{\log x}{2\pi x c_n} \sqrt{(b(c_n) - x)(x - a(c_n))} dx \\
&= \frac{1}{2\pi c_n} \int_0^\pi \frac{\log(1 + c_n - 2\sqrt{c_n} \cos \theta)}{1 + c_n - 2\sqrt{c_n} \cos \theta} 4c_n \sin^2 \theta d\theta \\
&= \frac{1}{2\pi} \int_0^{2\pi} \frac{2 \sin^2 \theta}{1 + c_n - 2\sqrt{c_n} \cos \theta} \log |1 - \sqrt{c_n} e^{i\theta}|^2 d\theta \\
&= \frac{c_n - 1}{c_n} \log(1 - c_n) - 1,
\end{aligned}$$

where the last integral is calculated in Bai and Silverstein (2010).

Proof of (22)

In the normal case with $\sigma^2 = 1$, Zheng (2012) gives the following equivalent expression of (14):

$$v(f_j, f_l) = - \lim_{r \rightarrow 1^+} \frac{\kappa}{4\pi^2} \oint \oint_{|\xi_1|=|\xi_2|=1} f_j(|1 + h\xi_1|^2) f_l(|1 + h\xi_2|^2) \frac{1}{(\xi_1 - r\xi_2)^2} d\xi_1 d\xi_2,$$

where $\kappa = 2$ in the real case and $h = \sqrt{c}$ in our case. We take $f_j(x) = \log(x)$ and $f_l(x) = x$, so we need to calculate

$$v(\log(x), x) = - \lim_{r \rightarrow 1^+} \frac{1}{2\pi^2} \oint \oint_{|\xi_1|=|\xi_2|=1} |1 + \sqrt{c}\xi_2|^2 \frac{\log(|1 + \sqrt{c}\xi_1|^2)}{(\xi_1 - r\xi_2)^2} d\xi_1 d\xi_2.$$

We follow the calculations done in Zheng (2012): when $|\xi| = 1$, $|1 + \sqrt{c}\xi|^2 = (1 + \sqrt{c}\xi)(1 + \sqrt{c}\xi^{-1})$, so $\log(|1 + \sqrt{c}\xi|^2) = \frac{1}{2} (\log(1 + \sqrt{c}\xi)^2 + \log(1 + \sqrt{c}\xi^{-1})^2)$.

Consequently,

$$\begin{aligned}
\oint_{|\xi_1|=1} \frac{\log(|1 + \sqrt{c}\xi_1|^2)}{(\xi_1 - r\xi_2)^2} d\xi_1 &= \frac{1}{2} \oint_{|\xi_1|=1} \frac{\log(1 + \sqrt{c}\xi_1)^2}{(\xi_1 - r\xi_2)^2} d\xi_1 + \frac{1}{2} \oint_{|\xi_1|=1} \frac{\log(1 + \sqrt{c}\xi_1^{-1})^2}{(\xi_1 - r\xi_2)^2} d\xi_1 \\
&= \frac{1}{2} \oint_{|\xi_1|=1} \log(1 + \sqrt{c}\xi_1)^2 \left(\frac{1}{(\xi_1 - r\xi_2)^2} + \frac{1}{(1 - r\xi_1\xi_2)^2} \right) d\xi_1 \\
&= 0 + i\pi \left(\frac{1}{(r\xi_2)^2} \frac{2\sqrt{c}}{1 + \frac{\sqrt{c}}{r\xi_2}} \right) \\
&= 2i\pi \frac{\sqrt{c}}{r\xi_2(r\xi_2 + \sqrt{c})}.
\end{aligned}$$

Thus,

$$\begin{aligned}
v(\log(x), x) &= \frac{1}{i\pi} \oint_{|\xi_2|=1} |1 + \sqrt{c}\xi_2|^2 \frac{\sqrt{c}}{\xi_2(\xi_2 + \sqrt{c})} d\xi_2 \\
&= \frac{1}{i\pi} \oint_{|\xi|=1} (1 + c + c(\xi + \xi^{-1})) \frac{\sqrt{c}}{\xi(\xi + \sqrt{c})} d\xi \\
&= \frac{1}{i\pi} \oint_{|\xi|=1} \left(\frac{\sqrt{c}(1+c)}{\xi(\xi + \sqrt{c})} + \frac{c}{\xi + \sqrt{c}} + \frac{c}{\xi^2(\xi + \sqrt{c})} \right) d\xi \\
&= 2(1 + c - (1 + c) + c + 1 - 1) \\
&= 2c.
\end{aligned}$$

7 Conclusions

In this paper, we propose a bias-corrected estimator of the noise variance for PPCA models in the high-dimensional framework. The main appeal of our estimator is that it is developed under the assumption that $p/n \rightarrow c > 0$ as $p, n \rightarrow \infty$ and is thus appropriate for a wide range of large-dimensional datasets. Extensive Monte-Carlo experiments demonstrated the superiority of the proposed estimator over several existing estimators (notice however no theoretical justification has

been proposed in the literature for these estimators). Moreover, by implementing the proposed estimator of the noise variance within two well-known determination algorithms for the number of principal components, we demonstrate that significant improvement can be obtained. In an additional application and using this new estimator, we construct the asymptotic theory of the goodness-of-fit test for high-dimensional PPCA models. The overall message from the paper is that in a high-dimensional PPCA model, when an estimator of the noise variance σ^2 is needed, the bias-corrected estimator $\hat{\sigma}_*^2$ from the paper should be recommended.

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