LIMITING LAWS FOR DIVERGENT SPIKED EIGENVALUES
AND LARGEST NON-SPIKED EIGENVALUE OF SAMPLE
COVARIANCE MATRICES

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Abstract. We study the asymptotic distributions of the spiked eigenvalues and
the largest nonspiked eigenvalue of the sample covariance matrix under a general
covariance matrix model with divergent spiked eigenvalues, while the other eigen-
values are bounded but otherwise arbitrary. The limiting normal distribution
for the spiked sample eigenvalues is established. It has distinct features that the
asymptotic mean relies on not only the population spikes but also the nonspikes
and that the asymptotic variance in general depends on the population eigenvec-
tors. In addition, the limiting Tracy-Widom law for the largest nonspiked sample
eigenvalue is obtained.

Estimation of the number of spikes and the convergence of the leading eigen-
vector are also considered. The results hold even when the number of the spikes
diverges. As a key technical tool, we develop a Central Limit Theorem for a
type of random quadratic forms where the random vectors and random matrices
involved are dependent. This result can be of independent interest.

KEYWORDS: Extreme eigenvalues, factor model, principal component anal-
ysis, sample covariance matrix, spiked covariance matrix model, Tracy-Widom
distribution.

1. Introduction

Covariance matrix plays a fundamental role in multivariate analysis and high-
dimensional statistics. There has been significant recent interest in studying the
properties of the leading eigenvalues and eigenvectors of the sample covariance ma-
trix, especially in the high-dimensional setting. See, for example, [2, 10, 12, 13, 21,
26–29, 31]. These problems are not only of interest in their own right they also have
close connections to important statistical problems such as principal component
analysis and testing for the covariance structure of high-dimensional data.

Principal component analysis (PCA) is a widely used technique in multivariate
analysis for a range of purposes, including dimension reduction, data visualization,
clustering, and feature extraction [1, 20]. PCA is particularly well suited for the set-
tings where the signal of interest lies in a much lower dimensional subspace and it
has been applied in a broad range of fields such as genomics, image recognition, data compression, and financial econometrics. For example, widely used factor models in financial econometrics typically assume that a small number of unknown common factors drive the asset returns [15]. In PCA, the leading eigenvalues and eigenvectors of the population covariance matrix need to be estimated from data and are conventionally estimated by their empirical counterparts. It is thus important to understand the spectral properties of the sample covariance matrix.

1.1. The Problem. To be concrete, consider the data matrix \( Y = \Gamma X \) where \( X = (x_1, \cdots, x_n) \) is a \((p + l) \times n\) random matrix whose entries are independent with zero mean and unit variance and \( \Gamma \) is a \( p \times (p + l) \) deterministic matrix with \( l/p \to 0 \). Let \( \Sigma = \Gamma \Gamma^\top \) be the population covariance matrix. The sample covariance matrix is defined as

\[
S_n = \frac{1}{n} YY^\top = \frac{1}{n} \Gamma XX^\top \Gamma^\top.
\]

(1.1)

Denote the singular value decomposition (SVD) of \( \Gamma \) by

\[
\Gamma = V \Lambda^\frac{1}{2} U,
\]

(1.2)

where \( V \) and \( U \) are \( p \times p \) and \( p \times (p + l) \) orthogonal matrices respectively (\( V V^\top = U U^\top = I \)), and \( \Lambda \) is a diagonal matrix consisting in descending order of the eigenvalues \( \mu_1 \geq \cdots \geq \mu_p \) of \( \Sigma \).

In statistical applications such as PCA, one is most interested in the setting where there is a clear separation between a few leading eigenvalues and the rest. In this case, the leading principal components account for a large proportion of the total variability of the data. We consider in the present paper the setting where there are \( K \) spiked eigenvalues that are separated from the rest. More specifically, we assume that \( \mu_1 \geq \cdots \geq \mu_K \) tend to infinity, while the other eigenvalues \( \mu_{K+1} \geq \cdots \geq \mu_p \) are bounded but otherwise arbitrary. Write

\[
\Lambda = \begin{pmatrix} \Lambda_S & 0 \\ 0 & \Lambda_P \end{pmatrix},
\]

(1.3)

where \( \Lambda_S = \text{diag}(\mu_1, \ldots, \mu_K) \) and \( \Lambda_P = \text{diag}(\mu_{K+1}, \ldots, \mu_p) \).

A typical example of (1.3) is the factor model

\[
Y = \Lambda F + T Z = (\Lambda^\top T) \begin{pmatrix} F \\ Z \end{pmatrix}
\]

(1.4)

where \( \Lambda \) is \( p \times K \)-dimensional factor loading, \( F \) is the corresponding \( K \times n \) factor, \( T \) is \( p \times p \) matrix and \( Z \) is the idiosyncratic noise matrix. A common assumption is that the singular values of the factor part \( \Lambda F \) are significantly larger than those of the noise part (otherwise the signals are overwhelmed by noise). Indeed, [30] considered the weak factor model to test the number of factors, where the leading eigenvalues contributed by the factor part are of order \( p^\theta \) for some \( \theta \in (0, 1) \). [4] and [23] assume that the leading eigenvalues of the pervasive factor model are of order \( p \). Here \( \Gamma = (\Lambda^\top T) \) is not a square matrix, and thus it is necessary to consider the setting where \( \Gamma \) is rectangular.
A second example is the covariance matrix $\Sigma$ used in the intraclass correlation model, where the covariance matrix is of the form

$$\Sigma = (1 - \rho)I + \rho ee^T.$$  

Here $I$ is the identity matrix, $e = (1, 1, \ldots, 1)^T$ and $0 < \rho < 1$. It is easy to see that the leading eigenvalue of $\Sigma$ is $p\rho + (1 - \rho)$, while the other eigenvalues are equal to $(1 - \rho)$.

We study in the present paper the asymptotic distributions of the leading eigenvalues and the largest nonspiked eigenvalue of the sample covariance matrix $S_n$, under the general spiked covariance matrix model given in (1.2) and (1.3) with divergent spiked eigenvalues $\mu_1 \geq \cdots \geq \mu_K$. In many statistical applications, determining the number of principal components is an important problem. We also consider estimation of the number of spikes as well as the convergence of the leading eigenvectors.

The model defined through (1.2) and (1.3) belongs to the class of spiked covariance matrix models. Johnstone [26] was the first to introduce a special spiked covariance matrix model, where the population covariance matrix is diagonal and is of the form

$$\Sigma = \text{diag}(\mu_1^2, \ldots, \mu_K^2, 1, \ldots, 1)$$

with $\mu_1 > \mu_2 \cdots \geq \mu_K > 1$. [26] established the limiting Tracy-Widom distribution for the maximum eigenvalue of the real Wishart matrices when $p$ and $n$ are comparable. The spiked covariance matrix model (1.5) in [26] has been extended in various directions. So far the focus has mostly been on the settings of bounded spiked eigenvalues with all the nonspiked eigenvalues being equal to 1. See more discussion in Section 1.3.

1.2. Our contributions. In this paper, we first establish the limiting normal distribution for the spiked eigenvalues of the sample covariance matrix $S_n$. The limiting distribution has a distinct feature. Unlike in the more conventional settings, the asymptotic variance in general depends on the population eigenvectors. More precisely, the variance of a spiked sample eigenvalue depends on the right singular vector matrix $U$ defined in the SVD (1.2) (but not the left singular vector matrix $V$). The limiting distribution of the spiked sample eigenvalues also precisely characterizes the dependence on the corresponding population spiked eigenvalues as well as the nonspiked ones. New technical tools are needed to establish the result. In particular, we develop a Central Limit Theorem (CLT) for a type of random quadratic forms where the random vectors and random matrices involved are dependent. This result can be of independent interest. In addition, we establish the limiting Tracy-Widom law for the largest nonspiked eigenvalue of $S_n$.

The limiting distributions for the spiked eigenvalues and the largest nonspiked eigenvalue have important applications. In particular, based on our theoretical results, we propose an algorithm for estimating the number of the spikes, which is of interest in many statistical applications. We also consider the properties of the sample eigenvectors corresponding to the spiked eigenvalues and show that they are consistent estimators of the population eigenvectors in terms of the $L_2$ norm. An important improvement of our paper over many known results in the literature is
that our results hold even when the number of the spikes diverges as \( n, p \to \infty \), and we allow the nonspiked eigenvalues to be unequal.

1.3. Background and related work. Since the seminal work of Johnstone [26], the special spiked covariance matrix model (1.5) has been studied much further and the model has been extended in various directions. See, for example [2, 3, 6, 11–13, 27, 28, 31, 33, 34]. We discuss briefly here some of these results. This review is by no means exhaustive.

Paul [31] showed that if \( p/n \to \gamma \in (0, 1) \) as \( n \to \infty \), and the largest eigenvalue \( \mu_1 \) of \( \Sigma \) satisfies \( \mu_1 \leq (1 + \sqrt{\gamma}) \), then the leading sample principal eigenvector \( \hat{v}_1 \) is asymptotically almost surely orthogonal to the leading population eigenvector \( v_1 \), i.e., \( |v_1' \hat{v}_1| \to 0 \) almost surely. Thus, in this case, \( \hat{v}_1 \) is not useful at all as an estimate of \( v_1 \). Even when \( \mu_1 > (1 + \sqrt{\gamma}) \), the angle between \( v_1 \) and \( \hat{v}_1 \) still does not converge to zero unless \( \mu_1 \to \infty \).

Baik and Silverstein [2] considered a case where the covariance matrix

\[
\Sigma = V \begin{pmatrix} \Lambda_S & 0 \\ 0 & I \end{pmatrix} V^\top
\]

(1.6)

with \( \Lambda_S \) being a diagonal matrix of fixed rank and \( V \) a unitary matrix. It is shown that the spiked eigenvalues tend to some limits in probability, assuming that the spectral norm of \( \Lambda_S \) is bounded and \( \lim_{n \to \infty} \frac{p}{n} = \gamma \in (0, \infty) \). Bai and Yao [6] further showed that the spiked eigenvalues converge in distribution to Gaussian distribution or the eigenvalues of a finite dimensional matrix with i.i.d. Gaussian entries. Baik, et al. [3] investigated the asymptotic behavior of the largest eigenvalue when the entries of \( X \) follow the standard complex Gaussian distribution and observed a phase transition phenomenon that the asymptotic distribution depends on the scale of the spiked population eigenvalues. Recently, Bloemendal et al. [11] obtained the precise large deviation of the spiked eigenvalues and non-spiked eigenvalues under a more general model than (1.6). We should note that the above results only consider the the case of bounded spiked eigenvalues with the nonspiked eigenvalues all being equal to 1.

Jung and Marron [28] and Shen et al. [33] considered the model

\[
Y = V \Lambda^{\frac{1}{2}} X,
\]

(1.7)

where the entries of \( X \) are i.i.d. standard normal random variables, and \( \Lambda = \text{diag}(\mu_1, ..., \mu_K, \mu_{K+1}, \cdots, \mu_p) \) is the diagonal matrix consisting of the population eigenvalues, and \( V \) is an orthogonal matrix. [28] and [33] showed the almost sure convergence of the spiked eigenvalues when the spiked population eigenvalues satisfy that \( p/(\mu_j n), j = 1, \cdots, K \) tend to positive constants or zero and \( \mu_{K+1}, \cdots, \mu_p \) are approximately equal to one. The almost sure convergence of the eigenvectors associated with the spikes is also investigated.

Wang and Fan [34] further developed the asymptotic distribution of the largest sample eigenvalues of the model (1.7) under a more general setting, which allows \( \mu_{K+1}, \cdots, \mu_p \) to be any bounded number and the entries of \( X \) to be i.i.d. subGaussian random variables. The asymptotic behaviors of the corresponding eigenvectors are also discussed in [34]. Here we would like to point out that [34] did not provide the
limits in probability of spikes for general $\mu_{K+1}, \ldots, \mu_p$ when $p/(\mu_j n), j = 1, \cdots, K$, tend to positive constants. To the best of our knowledge, the asymptotic behavior of the spiked eigenvalues for general $\mu_{K+1}, \ldots, \mu_p$ when $p/(\mu_j n), j = 1, \cdots, K$, converge to positive constants is still open.

Note that [28], [33] and [34] swapped the roles of the sample size $n$ and the dimension $p$ so that they essentially studied the matrix $X^T \Lambda X$. This is equivalent to assuming that the population covariance matrix is diagonal. Indeed, as will be seen later, in general the asymptotic variance of the spiked eigenvalues depends on the population eigenvectors. This phenomenon does not occur under the previously studied model.

1.4. Organization of the paper. The rest of the paper is organized as follows. Section 2 establishes the limiting normal distribution for the spiked eigenvalues and the limiting Tracy-Widom distribution for the largest nonspiked eigenvalue of the sample covariance matrix $S_n$. An algorithm for identifying the number of spikes is developed in Section 3. Section 4 considers the properties of the principal components and shows that the sample eigenvectors corresponding to the spiked eigenvalues are consistent estimators of the population eigenvectors in terms of the $L_2$ norm. Most of the results developed for $S_n$ also hold for the centralized sample covariance matrices and this is discussed in Section 5. Section 6 investigates the numerical performance through simulations and an application of a factor model. The proof of one of the main results is given in Section 7 and the proof of the other results is provided in the supplementary material [14].

2. Asymptotics for Spiked Eigenvalues and Largest Nonspiked Eigenvalue of $S_n$

We investigate in this section the limiting laws for the leading eigenvalues and the largest nonspiked eigenvalue of the sample covariance matrix $S_n$ under the general spiked covariance matrix model (1.2) and (1.3) with divergent spiked eigenvalues $\mu_1 \geq \cdots \geq \mu_K$, while the other eigenvalues are bounded but otherwise arbitrary. We begin with the notation that will be used throughout the rest of the paper.

For two sequences of positive numbers $a_n$ and $b_n$, we write $a_n \gtrless b_n$ for some absolute constant $c > 0$, and $a_n \lessgtr b_n$ when $b_n \gtrless a_n$. We write $a_n \sim b_n$ when both $a_n \gtrsim b_n$ and $a_n \lessapprox b_n$ hold. Moreover, we write $a_n \ll b_n$ when $a_n/b_n \to 0$. For a sequence of random variables $A_n$, if $A_n$ converges to $b$ in probability, then we write $A_n \xrightarrow{i.p.} b$. We say an event $A_n$ holds with high probability if $\mathbb{P}(A_n) \geq 1 - O(n^{-l})$ for some constant $l > 0$. Denote the $j$-th largest eigenvalue of a matrix $M$ by $\lambda_j(M)$ and the largest singular value by $\|M\|$. Set $\|M\|_F = \sqrt{\text{tr}(MM^T)}$. For simplicity, denote by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_K \geq \cdots \geq \lambda_p$ the ordered eigenvalues of the sample covariance matrix $S_n$, and denote by $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_K \geq \cdots \geq \mu_p$ the ordered eigenvalues of the population covariance matrix $\Sigma$. Throughout this paper $c$ and $C$ are constants that may vary from place to place.

To investigate the sample covariance matrix $S_n$ in (1.1) with the population covariance matrix $\Sigma$ specified in (1.2) and (1.3) we make the following assumptions.
Assumption 1. \( \{x_j = (x_{1j}, \cdots, x_{pj})^T, j = 1, \ldots, n\} \) are i.i.d. random vectors. \( \{x_{ij} : i = 1, \ldots, p + l, j = 1, \ldots, n\} \) are independent random variables such that 
\[
E x_{ij} = 0, \quad E| x_{ij}^2 | = 1, \quad E| x_{ij}^4 | = \gamma_{4i} \quad \text{and} \quad \sup_i \gamma_{4i} \leq C.
\]

Assumption 2. \( p \gtrsim n \) and the \( K \) largest population eigenvalues \( \mu_i \) are such that 
\[
d_i \equiv \frac{p}{n} \mu_i \to 0, \quad i = 1, 2, \ldots, K.
\]
And for \( i = K + 1, \ldots, p, \mu_i \) are bounded by \( C \). Moreover, \( \frac{K^2}{n^{1/6}} \to 0 \) and \( K^2 d_K \to 0 \).

Assumption 2'. \( \frac{p}{n} \to 0, \quad \mu_i \gg 1, \quad i = 1, \ldots, K \) and \( K \ll \min\{p, n^{1/6}\} \).

Note that we do not assume that \( p \) and \( n \) are of the same order. The following theorems hold either under Assumption 2 or Assumption 2' except Theorem 2.5. We only give the proofs under Assumption 2. The proofs under Assumption 2' are similar and thus we omit them.

Assumption 3. There exists a positive constant \( c \) not depending on \( n \) such that 
\[
\frac{\mu_i - 1}{\mu_i} \geq c > 1, \quad i = 1, 2, \ldots, K.
\]

Assumption 3 implies that the spiked eigenvalues are well-separated. It also implies that \( \lambda_1 > \lambda_2 > \ldots > \lambda_K \) with probability tending to 1 by Theorem 2.1 below.

2.1. Asymptotic behavior of the spiked sample eigenvalues. Our first result gives the limits in probability for the spiked eigenvalues of \( S_n, \lambda_1 \geq \ldots \geq \lambda_K \).

Theorem 2.1. Suppose that Assumption 1 holds. Moreover, either Assumption 2 or Assumption 2' holds. Then
\[
\frac{\lambda_i}{\mu_i} - 1 = O_p(d_i + \frac{K^4}{n} + \frac{1}{\mu_i}), \quad \text{uniformly for all } i = 1, \ldots, K.
\]

Remark 1. As mentioned in the introduction, PCA is an important statistical tool for analyzing high-dimensional data. Several recent results on high-dimensional PCA are quite relevant to Theorem 2.1. Recently \cite{7} considered AIC and BIC criteria for selecting the number of significant components in high dimensional PCA when \( p \) and \( n \) are comparable. Comparing to the paper \cite{7}, Theorem 2.1 here covers Lemma 2.2(i) of \cite{7} and we allow \( K \) to tend to infinity. Their assumption \( \mu_{K+1} = \cdots = \mu_p = 1 \) is also relaxed to bounded eigenvalues here. In addition, checking the proof of Theorems 3.3 and 3.4 of \cite{7}, we find that for general population covariance matrices, their criteria \( A_j \) and \( B_j \) for estimating the number of spikes may not work since it highly depends on the assumption \( \mu_{K+1} = \cdots = \mu_p = 1 \), as demonstrated in Table 4 given in Section 6. In addition, Theorem 2.1 also covers part of Theorem 3.1 in \cite{33} where it assumes normality for the data.

Note that \( \frac{\lambda_i}{\mu_i} \to 1 \) does not imply that \( \lambda_i \) is a good estimator of \( \mu_i \) due to the fact that \( \mu_i \) tends to infinity. Moreover, Theorem 2.1 does not precisely characterize how the nonspiked population eigenvalues affect the spiked sample eigenvalues. To see this, it is helpful to make a comparison with the conventional setting studied in \cite{2}.
Consider the model \((1.6)\) and recall the assumptions of \([2]\) that \(1 + \sqrt{\gamma} < \mu_i = O(1)\) and \(\gamma = \lim_{n \to \infty} \frac{p}{n} \in (0, \infty)\). It was shown in \([2]\) that
\[
\lambda_i \overset{a.s.}{\to} \mu_i + \frac{\gamma \mu_i}{\mu_i - 1},
\]
(2.2)
So the effect of the population eigenvalues on the corresponding sample eigenvalues can be precisely characterized in the setting considered in \([2]\). On the other hand, one cannot see the effect of the nonspiked population eigenvalues on the spiked sample eigenvalues from (2.2). Note that if there are no spikes, then all the sample eigenvalues are not bigger than \((1 + \sqrt{\gamma})^2\) with probability one. When there are sufficiently large spikes, the sample spikes are pulled outside of the boundary \((1 + \sqrt{\gamma})^2\) due to the population spikes with probability one. Moreover, (2.2) precisely quantifies the effect of the population spike. In view of this, one would ask whether there is a similar phenomenon for unbounded spikes. Indeed, it is natural to imagine that for the case \(\mu_i \to \infty\), the term \(\gamma \mu_i / (\mu_i - 1)\) will not disappear and thus one needs to subtract it from \(\lambda_i\) in order to obtain the CLT. Surprisingly, a more precise limit of \(\lambda_i\) turns out to be determined not only by \(\mu_i\) but also the nonspiked eigenvalues. This is very different from (2.2) and can be seen clearly from (2.9) below.

We now characterize how the population eigenvalues including spiked eigenvalues and non-spiked eigenvalues affect the sample spiked eigenvalues. To this end, corresponding to (1.3), partition \(U\) as \(U = \begin{pmatrix} U_1 \\ U_2 \end{pmatrix}\), where \(U_1\) is the \(K \times (p + l)\) submatrix of \(U\), and define
\[
(2.3) \quad \Sigma_1 = U_1^\top A_P U_2.
\]
For any distribution function \(H\), its Stieltjes transform is defined by
\[
m_H(z) = \int \frac{1}{\lambda - z} dH(\lambda), \quad \text{for all } z \in \mathbb{C}^+.
\]
For any \(\theta \neq 0\), let \(\tilde{m}_\theta(z)\) be the unique solution to the following equation
\[
(2.4) \quad \tilde{m}_\theta(z) = - \left( z - \frac{1}{n} \text{tr}(I + \tilde{m}_\theta(z) \Sigma_1 \Sigma_1^{-1} \Sigma_1^{-1})^{-1} \right)^{-1}, \quad z \in \mathbb{C}^+,
\]
where \(\mathbb{C}^+\) denotes the complex upper half plane and \(\Sigma_1\) is defined in (2.3). Here \(\tilde{m}_\theta(z)\) is the limit of the Stieltjes transform of the empirical distribution function of the random matrix \(\frac{1}{n\theta} X^\top \Sigma_1 X\), associated with the nonspiked population eigenvalues. Indeed, as will be seen, for \(\theta \gg \frac{p}{n}\),
\[
\tilde{m}_\theta(z) - \frac{1}{n} \text{tr}(z I - \frac{1}{n\theta} X^\top \Sigma_1 X)^{-1} \to 0
\]
for \(z \in \mathbb{C}^+\) by a slight modification of the proof of Appendix 7.2. One can also refer to (1.6) of [9] or (6.12)-(6.15) of [5] for (2.4). One may see below that \(\tilde{m}_\theta(z)\) describes the collective contribution of the nonspiked eigenvalues of \(\Sigma\) to the spiked sample eigenvalues.

By (2.4), we set \(\theta_i\) to be the solution to
\[
(2.5) \quad \tilde{m}_{\theta_i}(1) + \frac{\theta_i}{\mu_i} = 0,
\]
where $\tilde{m}_{\theta_i}(1) = \lim_{z \in \mathbb{C}^+ \to 1} \tilde{m}_{\theta_i}(z)$. It turns out that $\theta_i$ instead of $\mu_i$ is the more precise limit of the spiked sample eigenvalues $\lambda_i$. From (2.5) one can see that $\theta_i$ depends on $\mu_i$ as well as the nonspiked part $\Sigma_1$. Indeed, this point can be seen more clearly from (2.9) below. To the best of our knowledge, such a dependence of $\theta_i$ on $\mu_i$ as well as the nonspiked part $\Sigma_1$ has never been appeared in the literature before.

**Assumption 4.** Assume that the following limits exist:

$$
\sigma_i = \lim_{p \to \infty} \sqrt{\frac{p}{p+q}} \sum_{j=1}^{p+q} (\gamma_{ij} - 3) u_{ij}^2 + 2, \quad \sigma_{ij} = \lim_{p \to \infty} \sum_{s=1}^{p+q} (\gamma_{js} - 3) u_{is}^2 u_{js}^2.
$$

We are ready to state the asymptotic distribution of the spiked eigenvalues of $S_n$.

**Theorem 2.2.** Suppose that Assumptions 1, 3, and 4 hold. Moreover, either Assumption 2 or Assumption 2′ hold. Then for all $i = 1, 2, \ldots, K$,

$$
\sqrt{n} \frac{\lambda_i - \theta_i}{\theta_i} \xrightarrow{D} N(0, \sigma_i^2).
$$

Moreover, for any fixed $r \geq 2$

$$
\left( \sqrt{n} \frac{\lambda_1 - \theta_1}{\theta_1}, \ldots, \sqrt{n} \frac{\lambda_r - \theta_r}{\theta_r} \right) \xrightarrow{D} N(0, \Sigma^{(r)}),
$$

where $\Sigma^{(r)} = (\Sigma_{ij}^{(r)})$ with

$$
\Sigma_{ij}^{(r)} = \begin{cases} 
\sigma_i^2, & i = j \\
\sigma_{ij}, & i \neq j
\end{cases}
$$

It follows from (2.4) and (2.5) that $\tilde{m}_{\theta_i}(1) \to -1$. Therefore $\frac{\theta_i}{\mu_i} \to 1$. However, we can not replace $\theta_i$ by $\mu_i$ in (2.7) directly because the convergence rate of $\frac{\theta_i}{\mu_i}$ to 1 is unknown. Indeed, by (2.4), we have

$$
\theta = -\frac{\theta}{\tilde{m}_{\theta_i}(1)} + \frac{p - K}{n} \int \frac{tdF_{\Lambda P}(t)}{1 + t\tilde{m}_{\theta_i}(1)\theta^{-1}},
$$

where $F_{\Lambda_P}$ is the empirical spectral distribution of $\Lambda_P$. Here for any $n \times n$ symmetric matrix $A$ with real eigenvalues, the empirical spectral distribution (ESD) of $A$ is defined as

$$
F_A(x) = \frac{1}{n} \sum_{i=1}^{n} I_{\{\lambda_i(A) \leq x\}}.
$$

Together with (2.5), we conclude that

$$
\theta_i = \mu_i(1 + \frac{p - K}{n} \int \frac{tdF_{\Lambda P}(t)}{\mu_i - t}).
$$

By the Taylor’s expansion we have

$$
\frac{\theta_i}{\mu_i} = 1 + ff + O\left(\frac{p}{n\mu_i^2}\right),
$$
where
\[ f = \frac{1}{p-K} \sum_{j=K+1}^{p} \mu_j \quad \text{and} \quad f_i = \frac{p-K}{n\mu_i}. \]

In particular, for the special case \( \mu_{K+1} = \ldots = \mu_p = 1 \), (2.9) yields that
\[ \theta_i = \mu_i (1 + \frac{p-K}{n(\mu_i - 1)}). \]

It is interesting to note that, although here the spiked eigenvalues \( \mu_1, \ldots, \mu_K \) are divergent, this is consistent with the right hand side of (2.2), which is for the conventional setting of bounded spiked eigenvalues. It then follows from (2.10) that
\[ \sqrt{n} \left( \frac{\lambda_i}{\mu_i} - 1 - ff_i + O \left( \frac{p}{n\mu_i^2} \right) \right) \overset{D}{\to} N \left( 0, \sigma_i^2 \right). \]

**Remark 2.** We note that Assumption 4 is not needed if we consider the individual asymptotic distribution of the spiked sample eigenvalues. To see this, it suffices to normalize \((\lambda_i - \theta_i)/\theta_i\) by \(\sigma_i = \sqrt{\sum_{j=1}^{p+1} (\gamma_{ij} - 3)u_{ij}^4 + 2}\). Moreover, the joint distribution of \(\frac{\lambda_i - \theta_i}{\sigma_i \theta_i}, i = 1, \ldots, r\) tends to the normal distribution with the covariance matrix being the correlation matrix corresponding to \(\Sigma^{(r)}\).

**Remark 3.** It is helpful to compare the above theorem with Theorem 3.1 of [34]. Besides the difference between the models in (1.2) and (1.7), one of the key differences is that \(\sigma_i^2\) in (2.12) depends on the entries of the eigenvector matrix \(U\) while the variance in Theorem 3.1 of [34] does not depend on it. This is due to the fact that [34] assumes that \(U = I\). Secondly, Theorem 3.1 of [34] involves \(O_p \left( \sqrt{n\mu_i} \right) \) which reduces to \(O \left( \frac{p}{n\mu_i^2} \right) \) (essentially \(O(\frac{1}{\mu_i})\)) in (2.12) by dropping the additional \(\sqrt{n}\). Thirdly we also allow \(K\) to diverge. Fourthly [34] assumes \(x_{ij}\) to be subGaussian random variables while Theorem 2.2 holds under the bounded fourth moment assumption.

In view of (2.10) we need to estimate \(f\) and \(f_i\) in practice. A natural estimator of \(f_i\) is \(\frac{p-K}{n\lambda_i}\) by Theorem 2.1. For \(f\), one can use
\[ \hat{f} = \frac{1}{n} \text{tr} \left( \Gamma XX^\top \Gamma \right) - \sum_{i=1}^{K} \lambda_i \]
\[ \frac{p-K-pK/n}{p-K-pK/n} \]
which was proposed in [34]. When \(p \sim n\), by Proposition 1 in the next section, \(K\) can be estimated accurately.

Moreover, Theorem 2.2 can be extended to the case when the population eigenvalues \(\mu_i\) have multiplicity more than one.

**Assumption 5.** Suppose that \(K \ll n^{1/6}\), \(\alpha_{\mathcal{L}} = \mu_K = \ldots = \mu_{K-k_{\mathcal{L}}} < \alpha_{\mathcal{L}-1} = \mu_{K-k_{\mathcal{L}}+1} < \ldots < \alpha_1 = \mu_1 = \ldots = \mu_1\), and there exists a constant \(c\) such that \(\frac{\alpha_{i+1}}{\alpha_i} \geq c > 1, i = 1, 2, \ldots, \mathcal{L}\). Moreover, \(n_1, \ldots, n_{\mathcal{L}}\) are finite.
Assumption 6. Suppose that the following limits exist
\[ G(r_1, k_1, k_2, l_1, l_2) = \lim_{n \to \infty} n^2 \times \text{Cov}(u^T_{r_1+k_2} x_1 u^T_{r_1+l_1} x_1, u^T_{r_1+k_2} x_1 u^T_{r_1+l_1} x_1). \]

If either the fourth moments \( \gamma_{4s} = 3, s = 1, \ldots, p+l \) or the entries of the population eigenvectors satisfy \( \min_{r \in \{k_1, k_2, l_1, l_2\}} \max_j |u_{r_i+r,j}| = o(1) \), then
\[ g(r_i, k_1, k_2, l_1, l_2) = \begin{cases} 1 & \text{if } k_1 = k_2 \text{ and } l_1 = l_2 \text{ or } k_1 = l_2 \text{ and } l_1 = k_2 \\ 0 & \text{otherwise}. \end{cases} \]

Then we have the following result.

Theorem 2.3. Suppose that Assumptions 1, 5 and 6 hold. Moreover, either Assumption 2 or Assumption 2’ holds. Let
\[ \theta_i = \alpha_i(1 + \frac{p-K}{n} \int \frac{t dF_\lambda(t)}{\alpha_i - t}). \]

Let \( r_i = \sum_{j=0}^{i-1} n_j \), for \( i = 1, 2, \ldots, L \). Then
\[ (2.14) \quad \sqrt{n} \theta_i (\lambda_{r_i+1} - \theta_i, \lambda_{r_i+2} - \theta_i, \ldots, \lambda_{r_i+n_i} - \theta_i) \xrightarrow{D} \mathcal{R}_i, \]
where \( \mathcal{R}_i \) are the eigenvalues of \( n_i \times n_i \) Gaussian matrix \( \mathcal{S}_i \) with \( \mathbb{E} \mathcal{S}_i = 0 \) and the covariance of the \( (\mathcal{S}_i)_{k_1,l_1} \) and \( (\mathcal{S}_i)_{k_2,l_2} \) being \( G(r_i, k_1, k_2, l_1, l_2) \).

The proof of Theorem 2.2 requires new technical tools. The following CLT for a type of random quadratic forms, where the random vectors and random matrices involved are dependent, plays a key role in the proof. This result can be of independent interest.

Theorem 2.4. Suppose that Assumption 1 holds and the spectral norm of \( \Sigma_1 \) is bounded. In addition, suppose that there exist orthogonal unit vectors \( w_1 \) and \( w_2 \) such that \( w_1^T U_2 = w_2^T U_2 = 0 \) and \( w_1^T w_2 = 0 \). If \( \frac{\theta}{n} \to \infty \) and \( \theta \to \infty \), then
\[ (2.15) \quad \sqrt{n} \frac{\theta}{\sigma_1} \left( w_1^T X(nI - X^T \Sigma_1 \theta X)^{-1} X^T w_1 + \tilde{m}_\theta(1) \right) \xrightarrow{D} N(0,1) \]
and
\[ (2.16) \quad \sqrt{n} \frac{\theta}{\sigma_{12}} w_1^T X(nI - X^T \Sigma_1 \theta X)^{-1} X^T w_2 \xrightarrow{D} N(0,1) \]
where \( \tilde{\sigma}_1^2 = \sum_{j=1}^{p+l} [\gamma_{4j} - 3] w^4_{ij} + 2, \tilde{\sigma}_{12}^2 = \sum_{j=1}^{p+l} [\gamma_{4s} - 3] w^2_{1s} w^2_{2s} + 1 \) and \( w_{ij} \) is the \( j \)-th element of \( w_i \), \( i = 1, 2 \).

2.2. Tracy-Widom law for the largest nonspiked eigenvalue of \( S_n \). We now turn to the limiting distribution of the largest nonspiked eigenvalue of the sample covariance matrix \( S_n \). The limiting law is of interest in its own right and it is also important for the estimation of the number of the spikes. To this end we introduce additional assumptions.

Assumption 7. There exist constants \( c_k \) such that \( \mathbb{E}|x_{ij}|^k \leq c_k \) for all \( k \in \mathbb{N}^+ \).
Assumption 8. Recall (1.3) and (2.3). Let $m_{\Sigma_1}(z)$ be the Steiltjes transform of the limit of the spectral distribution (LSD) of $\frac{1}{n}X^\top\Sigma_1X$ and let $\gamma_+$ be the right most end point of the LSD of $X^\top\Sigma_1X$. Suppose that

$$
\limsup_n \mu_{K+1}d < 1,
$$

where $d = \lim_{z \in \mathbb{C}^+ \to \gamma_+} m_{\Sigma_1}(z)$.

Intuitively, (2.17) restricts the upper bound of $\mu_{K+1}$ to ensure $\lambda_{K+1}$ to be a nonspiked eigenvalue. Denote the $i$-th largest eigenvalue of $\frac{1}{n}X^\top\Sigma_1X$ by $\nu_i$. Note that the limiting law of $\nu_1$ is the Type-1 Tracy-Widom distribution.

Theorem 2.5. Suppose Assumptions 3, 7, and 8 hold. In addition, either Assumption 2 or 5 holds. Recalling $l$ above (1.1), $l \ll n^{1/6}$ and $p \sim n$. For any $i$ satisfying $1 \leq i - K \leq \log n$, we have, with high probability,

$$
|\lambda_i - \nu_{i-K}| \leq n^{-2/3-\epsilon},
$$

In particular, $\lambda_{K+1}$ has limiting Type-1 Tracy-Widom distribution.

Remark 4. Theorem 2.5 shows that the non-spiked sample eigenvalues $\lambda_{K+1}, \lambda_{K+2}, \ldots, \lambda_{K+r}$ share the same asymptotic distribution as $\nu_1, \nu_2, \ldots, \nu_r$ since the fluctuation of $\nu_1, \nu_2, \ldots, \nu_r$ are $n^{-2/3} \gg n^{-2/3-\epsilon}$. Here $r$ is a fixed integer. See [8] and [22] for more details.

3. Estimating The Number of Spiked Eigenvalues

Identifying the number of spikes is an important problem for a range of statistical applications. For example, a critical step in PCA is the determination of the number of the significant principal components. This issue arises in virtually all practical applications where PCA is used. Choosing the number of principal components is often subjective and based on heuristic methods. As an application of the main theorems discussed in the last section, we propose in this section a procedure to identify the number of the spiked eigenvalues.

Suppose that the conditions of Theorem 2.5 hold. Define the asymptotic variance of $\nu_1$ by (see also (3) of [18])

$$
\sigma_n^3 = \frac{1}{d^3}(1 + \frac{p-K}{n}) \int (\frac{\lambda d}{1-\lambda d})^3 dF_{\lambda P}(\lambda)),
$$

By Theorem 2.5, $\lambda_{K+1}$ has the same asymptotic distribution as $\nu_1$. Together with Theorem 1 of [18], we have

$$
n^{2/3}\frac{\lambda_{K+1} - \gamma_+}{\sigma_n} \xrightarrow{D} TW_1,
$$

where $TW_1$ is the Type-1 Tracy-Widom distribution. Onatski [30] also established such a result for the complex case, but Theorem 1 of [30] requires that the spiked eigenvalues are much bigger than $n^{2/3}$ and $p/n = o(1)$. Moreover, the statistics used in [30] does not estimate $\gamma_+$ and $\sigma_n$, while our approach estimates them.

Recall that $\gamma_+$ is the asymptotic mean of $\lambda_{K+1}$. From (3.2) one can see that the confidence interval of $\gamma_+$ is $[\lambda_{K+1} - w^*\sigma_n n^{-2/3}, \lambda_{K+1} + w^*\sigma_n n^{-2/3}]$, where $w^*$ is a
suitable critical value from the Type-1 Tracy-Widom distribution. This, together with Theorem 2.2, implies that it suffices to count the number of the eigenvalues of $S_n$ that lie beyond $(\gamma_+ + w^* \sigma_n n^{-2/3} \log n)$ to estimate the number of spikes $K$ where $\log n$ can be replaced by any number tending to infinity. However, in practice $\gamma_+$ and $\sigma_n$ are unknown and need to be estimated.

We first consider estimation of $\sigma_n$. It turns out that

$$\sigma_n = \left( - \lim_{z \to \gamma_+} \frac{\int dF_0(x)}{(x-z)^3} \right)^{1/3},$$

where $F_0(x)$ is the limit of the spectral distribution function of $\frac{1}{\sqrt{n}}X^* \Sigma_i X$ (see Section 7 in the supplementary material). Moreover, one can verify that with high probability

$$\lambda_{K+1} \leq \lambda_{n^{1/6}} + \log n \times n^{-5/9}$$

(see Section 7 in the supplementary material). In view of (3.4) we estimate $F_0(x)$ by its empirical version $\hat{\lambda}_{n^{1/6}}, \hat{\lambda}_{n^{1/6}+1}, \ldots, \hat{\lambda}_{n}$ in (3.3), i.e. we exclude the first $n^{1/6}$ eigenvalues of $S_n$. Moreover, for $\gamma_+$ in (3.3), we use $\lambda_{n^{1/6}} + n^{-4/9}$ to replace it. The reason for using $\lambda_{n^{1/6}} + n^{-4/9}$ to estimate $\gamma_+$ instead of $\lambda_{n^{1/6}}$ is to avoid singularity in $\int \frac{dF_0(x)}{(x-\gamma_+)^3}$. The estimator of $\sigma_n$ is then given by

$$\hat{\sigma}_n = \left( - \frac{1}{n^{-1/6}} \sum_{i=n^{1/6}}^{n} \frac{1}{(\lambda_i - z_0)^2} \right)^{1/3},$$

where $z_0 = \lambda_{n^{1/6}} + n^{-4/9}$.

We next consider estimation of $\gamma_+$, the asymptotic mean of $\lambda_{K+1}$. By the assumption that $K \ll n^{1/6}$, it follows from Theorems 2.2 and 2.5 that $\lambda_{n^{1/6}}$ is not a spiked eigenvalue. Based on this, an upper bound of $\lambda_{K+1}$ is given in (3.4). Hence we use the following $\hat{p}_0$ as an initial upper bound of $\lambda_{K+1}$

$$\hat{p}_0 = \lambda_{n^{1/6}} + \log n \times n^{-5/9}.$$

Although $\hat{p}_0$ is a good upper bound for $\lambda_{K+1}$ theoretically, it does not depend on $\sigma_n$ and hence in practice $\hat{p}_0$ may not work well. Based on (3.2), we propose the following iteration approach to update $\hat{p}_0$. The idea behind the iteration is that even if $\hat{p}_0$ is not larger than $\lambda_{K+1}$ in practice, $\hat{p}_0$ is still close to $\lambda_{K+1}$. Thus by (3.2), there is at least one eigenvalue in the interval $[\hat{p}_0, \hat{p}_0 + w^* \sigma_n n^{-2/3}]$, where $m_n \to \infty$.

1. Define the initial value $\hat{p}_0$ in (3.5).
2. Suppose that we have $\hat{p}_{m-1}$. If there is at least one eigenvalue of $S_n$ belonging to $[\hat{p}_{m-1}, \hat{p}_{m-1} + 2.02 (\log n) \sigma_n n^{-2/3}]$, where 2.02 is the $99\%$ quantile of Type-1 Tracy-Widom distribution, we renew $\hat{p}_m = \hat{p}_{m-1} + 2.02 \log n \sigma_n n^{-2/3}$. Here $\log n$ can be also replaced by the other number tending to infinity too. Otherwise the iteration stops.
3. After getting $\hat{p}_n$, we return to Step 2 until the iteration stops.
4. Denote the final value of the above iteration by $\hat{p}_{\text{end}}$. We define $K$ to be the number of eigenvalues larger than $\hat{p}_{\text{end}}$. 


Theorem 2.5 implies that $\hat{K}$ is a good estimator of the number of significant components $K$.

**Proposition 1.** Under the conditions of Theorem 2.5, we have $\hat{K} = K$ with high probability.

**Identifying The Number of Factors.** A closely related problem is the estimation of the number of factors under a factor model, which is widely used in financial econometrics. Consider the factor model

$$y_t = \Lambda f_t + T \varepsilon_t, \quad t = 1, 2, \ldots, n,$$

where $\Lambda$ is $p \times K$-dimensional factor loading, $f_t$ is the corresponding $K$-dimensional factor, $\{\varepsilon_{it} : i = 1, 2, \ldots, p; t = 1, 2, \ldots, n\}$ are the independent idiosyncratic components.

In many applications, the number of factors $K$ is unknown. An important step in factor analysis is to determine the value of $K$. Let $F = (f_1, \ldots, f_n)$, $Z = (\varepsilon_1, \ldots, \varepsilon_n)$ and $Y = (y_1, \ldots, y_n)$. Then (3.6) can be rewritten as

$$Y = \Lambda F + TZ = (\Lambda \ T) \begin{pmatrix} F \\ Z \end{pmatrix}.$$

Suppose that $\begin{pmatrix} F \\ Z \end{pmatrix}$ satisfies Assumptions 1 and 7 and $(\Lambda \ T)$ satisfies Assumptions 2 and 8. It is easy to conclude that the $(K + 1)$-st largest eigenvalue of $\frac{1}{n} YY^t$ follows the Type-1 Tracy-Widom distribution asymptotically. The following result is a direct consequence of Proposition 1.

**Corollary 1.** For the model (3.6), if $\begin{pmatrix} F \\ Z \end{pmatrix}$ satisfies Assumptions 1 and 7 and $(\Lambda \ T)$ satisfies Assumptions 2 and 8, $K \ll n^{1/6}$ and $p \sim n$, then we have $\hat{K} = K$ with high probability.

Comparing to the approaches in [4] and [30], here we allow the number of factors $K$ to diverge with $n$. Moreover, we only assume that the spiked population eigenvalues diverge to infinity, while [4] and [30] assume that they are much larger than $n^{2/3}$ or grow linearly with $n$.

4. Estimating the Eigenvectors

As mentioned in the introduction, the leading eigenvectors of the population covariance matrix are of significant interest in PCA and many other statistical applications. They are conventionally estimated by their empirical counterparts.

We consider in this section estimation of the population eigenvectors associated with the spiked population eigenvalues $\mu_1, \ldots, \mu_K$, involved in $\sigma_i^2$ in (2.7). To this end, we first characterize the relationship between the sample eigenvectors and the corresponding population eigenvectors. Write the population eigenvectors matrix $V$ as $V = (v_1, \cdots, v_p)$. 
Theorem 4.1. Suppose that the conditions of Theorem 2.2 hold. Let $\xi_i$ be the eigenvector of $S_n$ corresponding to the eigenvalue $\lambda_i$. Then for $1 \leq i \leq K$, we have

\begin{equation}
\mathbf{v}_i^\top \xi_i \xi_i^\top \mathbf{v}_i \xrightarrow{i.p.} 1.
\end{equation}

Theorem 4.1 also implies that for $i = 1, \ldots, K$, $j = 1, \ldots, p$, $i \neq j$, we have

\begin{equation}
\mathbf{v}_j^\top \xi_i \xi_i^\top \mathbf{v}_j \xrightarrow{i.p.} 0.
\end{equation}

One should notice that the convergence is uniformly for $j = 1, \ldots, p$ since $1 = \xi_i^\top \xi_i = \sum_{j=1}^p \mathbf{v}_j^\top \xi_i \xi_i^\top \mathbf{v}_j$.

Theorem 4.1 shows that the sample eigenvector $\xi_i$ is a good estimator of $\mathbf{v}_i$ up to a sign difference. An immediate application of Theorem 4.1 is to estimate $\sigma_j^2$ for the case when $\mathbf{V} = \mathbf{U}^\top$ and $\gamma_{41} = \ldots = \gamma_{4p} = \gamma_4$ by Corollary 2. This corollary shows that the empirical eigenvector plays an important role in statistical inference of the spiked eigenvalue.

Corollary 2. Under the conditions of Theorem 4.1, we have

\begin{equation}
\sum_{j=1}^p \mathbf{v}_{ij}^4 - \sum_{j=1}^p \xi_{ij}^4 \xrightarrow{i.p.} 0.
\end{equation}

We now consider the extension to the case when the multiplicity of the population eigenvalues $\mu_i$ is more than one. Correspondingly the following corollary holds and its proof is the same as that of Theorem 4.1.

Corollary 3. Recall the definition of $r_i$ above (2.14). Under the conditions of Theorem 2.3, the angle between $\mathbf{v}_k$, $k \in \{r_i-1 + 1, \ldots, r_i\}$ and the subspace spanned by $\{\xi_j, j = r_i-1 + 1, \ldots, r_i\}$ tends to 0 in probability. In other words, we have

\begin{equation}
\mathbf{v}_k^\top \left( \sum_{j=r_i-1+1}^{r_i} \xi_j \xi_j^\top \right) \mathbf{v}_k \xrightarrow{i.p.} 1, \; k \in \{r_i-1 + 1, \ldots, r_i\}.
\end{equation}

Corollary 3 shows that the sample eigenvectors $\{\xi_j, j = r_i-1 + 1, \ldots, r_j\}$ are close to the space spanned by $\{\mathbf{v}_j, j = r_i-1 + 1, \ldots, r_j\}$.

5. Centralized sample covariance matrices

So far we have focused on the non-centralized sample covariance matrix $S_n$. We now turn to its centralized version

\[ \tilde{S}_n = \frac{1}{n} \sum_{i=1}^n \Gamma(x_i - \bar{x})(x_i - \bar{x})^\top = \Gamma \mathbf{X}(\mathbf{I} - \frac{1}{n} \mathbf{1}\mathbf{1}^\top)\mathbf{X}^\top \Gamma, \]

where $\mathbf{1}$ is the $n \times 1$ vector with all elements being 1. Denote $(\mathbf{I} - \frac{1}{n} \mathbf{1}\mathbf{1}^\top)$ by $\Upsilon$. First we have the following Lemma.

Lemma 1. Under the conditions of Theorem 1, we have

\begin{equation}
\frac{\sqrt{n}}{\sigma_1} \left( \mathbf{w}_1^\top \mathbf{X} \Upsilon (n\mathbf{I} - \Upsilon \mathbf{X}^\top \frac{\Sigma_1}{\theta} \mathbf{X}\Upsilon)^{-1} \mathbf{X}^\top \mathbf{w}_1 + \tilde{m}_\theta(1) \right) \xrightarrow{D} N(0, 1)
\end{equation}
and

\[
\frac{\sqrt{n}}{\tilde{\sigma}_{12}} \mathbf{w}_1^\top \mathbf{X} \mathbf{Y} (n \mathbf{I} - \mathbf{Y} \mathbf{X}^\top \frac{\Sigma_1}{\theta} \mathbf{X} \mathbf{Y})^{-1} \mathbf{Y} \mathbf{X}^\top \mathbf{w}_2 \xrightarrow{D} N(0, 1)
\]

where \( \tilde{\sigma}^2_1 = \sum_{j=1}^{p+l} [(\gamma_{4j} - 3) \mathbf{w}_{1j}^4] + 2 \), \( \tilde{\sigma}^2_{12} = \sum_{s=1}^{p+l} [(\gamma_{4s} - 3) \mathbf{w}_{1s}^2 \mathbf{w}_{2s}^2] + 1 \) and \( \mathbf{w}_{ij} \) is the \( j \)-th element of \( \mathbf{w}_i \), \( i = 1, 2 \).

By Lemma 1 and checking carefully the proofs of the main results, it can be seen that all arguments remain valid if \( \mathbf{X} \) is replaced by \( \mathbf{X} \mathbf{Y} \) (note that \( \mathbf{Y}_2 = \mathbf{Y} \)). So Theorem 2.1–Corollary 3 hold for \( \frac{1}{n} \mathbf{X} \mathbf{Y} \mathbf{X}^\top \mathbf{Y}^\top \) as well.

6. Numerical Results

In this section we illustrate some of the theoretical results obtained earlier through numerical experiments. We first use simulation to confirm that the asymptotic behavior of the spiked eigenvalues is indeed affected by the population eigenvectors.

Let \( K = 2 \) and \( \Lambda_P = \text{diag}(\mu_3, ..., \mu_p) \). Suppose that \( \{\mu_i, i = 3, ..., p\} \) are i.i.d. copies of the uniform random variable \( U(1, 2) \). Define \( \mathbf{v}_1 = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})^\top \), \( \mathbf{v}_2 = (\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}})^\top \), \( \mathbf{V} = (\mathbf{v}_1, \mathbf{v}_2) \) and \( \Lambda_S = \text{diag}(800, 200) \). We now define two different population matrices

\[
\Sigma_2 = \begin{pmatrix} \Lambda_S & 0 \\ 0 & \Lambda_P \end{pmatrix}, \quad \Sigma_3 = \begin{pmatrix} \mathbf{V} \Lambda_S \mathbf{V}^\top & 0 \\ 0 & \Lambda_P \end{pmatrix}.
\]

Then the eigenvalues of \( \Sigma_2 \) and \( \Sigma_3 \) are the same but the eigenvectors corresponding to the first two largest eigenvalues are different. Consider the case \( p = n \) and \( \mathbf{X} = (x_{ij}) \) are i.i.d. \( U(-\sqrt{3}, \sqrt{3}) \). Denote by \( \lambda_1 \) and \( \lambda_1 \) respectively the largest eigenvalues of the sample covariance matrices \( \frac{1}{n} \Sigma_2^{1/2} \mathbf{X} \mathbf{X}^\top \Sigma_2^{1/2} \) and \( \frac{1}{n} \Sigma_3^{1/2} \mathbf{X} \mathbf{X}^\top \Sigma_3^{1/2} \).

Table 1 reports the sample variance of the rescaled eigenvalues \( \sqrt{n} \lambda_1 \) and \( \sqrt{n} \lambda_1 \). It can be seen that the behavior of the spiked sample eigenvalues is indeed affected by the population eigenvectors.

**Table 1.** The variances of the rescaled largest eigenvalues

| p   | 200   | 400   | 600   | 800   | 1000  |
|-----|-------|-------|-------|-------|-------|
| \( \Sigma_2 \) | 0.8111 | 0.7965 | 0.8287 | 0.7574 | 0.7874 |
| \( \Sigma_3 \) | 1.2507 | 1.4051 | 1.2800 | 1.5012 | 1.3911 |

We now consider estimating the number of factors under the factor model (3.7):

\[
\mathbf{Y} = \Lambda \mathbf{F} + \mathbf{T} \mathbf{Z}.
\]

In the simulation, the entries of \( \mathbf{F} \) and \( \mathbf{Z} \) follow the standard Gaussian distribution. Consider two choices: \( \mathbf{T} = \mathbf{T}_1 \) or \( \mathbf{T}_2 \), where \( \mathbf{T}_1 = \mathbf{I} \), \( \mathbf{T}_2 = \text{diag}(1, 1, ..., 1, \frac{1}{\sqrt{p/2}}, ..., \frac{1}{\sqrt{p/2}}) \).
Let $\Lambda$ be a $p \times K$ matrix with nonzero entries being $(\Lambda_{11}, \ldots, \Lambda_{KK}) = (\sqrt{b_1^2 - 1}, \ldots, \sqrt{b_K^2 - 1})$ where $K = 5 \lceil n^{1/7} \rceil + 1$, and $(b_1, \ldots, b_K) = (\sqrt{6}, \ldots, \sqrt{6 + K - 1}) \ast r + 1, 0 \leq r \leq 1$.

Since the estimator in [30] performs better than that in [4], we shall only consider the estimator given in [30] for our comparisons. We compare the accuracy of estimating the number of factors $K$ for three methods: our procedure proposed in Section 3, the method introduced in [30], and the approach given in [7], which are denoted by CHP, Ons, and BYK, respectively. Here we omit the simulation results of BIC used in [7] for reasons of space. The initial value of $\hat{p}_0$ in (3.5) is replaced by $\lambda_{15} \lceil n^{1/6} \rceil + \log n \times n^{-5/9}$ according to our extensive simulations in order to reduce the number of updating iteration. Here we replace $\lambda_{\lceil n^{1/6} \rceil}$ by $\lambda_{15} \lceil n^{1/6} \rceil$ and one should note that all of the conclusions in Section 3 still hold since 15 is a constant. The approach in Section 5.3 of [30] uses the ratio of the differences of the adjacent sample eigenvalues to conduct the sequential test of

$$H_0 : K = k_0 \text{ vs } H_1 : k_0 < K < k_1,$$

from $k_0 = 0$ to $k_0 = k_1 - 1$. [7] uses AIC based on sample eigenvalues to estimate $K$.

Different combinations of $n$ and $p$ are considered. The following tables report the proportion of times the number of factors is correctly identified, i.e. $\hat{K} = K$, where for each $(n, p)$ we repeat 500 times. Different choices of $r$ (ranging from 0.3 to 1) are also considered. From Tables 2 and 3, one can see that the accuracy of our approach increases as $(n, p)$ become larger. Comparing to [30], one can find that our approach works much better when the number of factors increases with $n$. This is reasonable since the estimator given in [30] is very sensitive to the predetermined non-spiked eigenvalue (i.e. $k_1$ in [30]). If $k_1$ is too large, the power may be poor. Tables 2 and 3 show that the method based on the AIC criterion and our procedure have similar performance. But as mentioned earlier in Remark 1, the model in [7] only allows that $\mu_{K+1} = \ldots = \mu_p = 1$, which is a special case of what we consider in the present paper. Indeed, Table 4 also confirms that for the non-identity matrix $T_2$, the method based on the AIC criterion performs much worse than our approach. Therefore, our procedure is preferred for the case where $\mu_{K+1}, \ldots, \mu_p$ are unknown.

7. Proofs

In this section, we prove one of the main results, Theorem 2.4. The proof of Theorem 2.2 is involved. For reasons of space, we prove Theorem 2.2 in detail in the supplement [14]. The proofs of the other results and additional technical lemmas are also provided in the supplement [14].

7.1. Proof of Theorem 2.4. The main idea of this proof is to first express $w_1^\top X(nI - X^\top \Sigma X)^{-1} X^\top w_1$ as a sum of martingale differences and then apply the central limit theorem for the martingale difference.

We below consider the case $p \succ n$ and prove (2.15) only because the case $p \succ n$ can be proved similarly. First of all, we need to do truncation and centralization on $x_{ij}$ as in the first paragraph of Section 12 in the supplement [14].
Table 2. Ratio of Identifying The Correct Number of Factors with $T_1$

| $r \backslash (n,p)$ | $(50,50)$ | $(50,100)$ | $(50,150)$ |
|---------------------|----------|-----------|------------|
|                     | CHP      | Ons       | BYK        |
| 0.3                 | 0.608    | 0.052     | 0.610      |
| 0.4                 | 0.816    | 0.064     | 0.706      |
| 0.5                 | 0.904    | 0.044     | 0.662      |
| 0.6                 | 0.892    | 0.038     | 0.612      |
| 0.7                 | 0.906    | 0.050     | 0.636      |
| 0.8                 | 0.914    | 0.060     | 0.638      |
| 0.9                 | 0.908    | 0.054     | 0.648      |
| 1.0                 | 0.914    | 0.050     | 0.616      |

Table 3. Ratio of Identifying The Correct Number of Factors with $T_1$

| $r \backslash (n,p)$ | $(100,100)$ | $(100,200)$ | $(100,300)$ |
|---------------------|-------------|-------------|-------------|
|                     | CHP         | Ons         | BYK         |
| 0.3                 | 0.954       | 0.052       | 0.974       |
| 0.4                 | 0.980       | 0.038       | 0.982       |
| 0.5                 | 0.956       | 0.056       | 0.974       |
| 0.6                 | 0.972       | 0.050       | 0.976       |
| 0.7                 | 0.970       | 0.058       | 0.974       |
| 0.8                 | 0.954       | 0.040       | 0.974       |
| 0.9                 | 0.954       | 0.050       | 0.980       |
| 1.0                 | 0.950       | 0.052       | 0.972       |

Table 4. Ratio of Identifying The Correct Number of Factors with $T_2$

| $r \backslash (n,p)$ | $(100,100)$ | $(100,200)$ | $(100,300)$ |
|---------------------|-------------|-------------|-------------|
|                     | CHP         | Ons         | BYK         |
| 0.3                 | 0.946       | 0.062       | 0.490       |
| 0.4                 | 0.928       | 0.042       | 0.454       |
| 0.5                 | 0.944       | 0.044       | 0.424       |
| 0.6                 | 0.926       | 0.052       | 0.440       |
| 0.7                 | 0.926       | 0.034       | 0.434       |
| 0.8                 | 0.918       | 0.060       | 0.450       |
| 0.9                 | 0.928       | 0.052       | 0.434       |
| 1.0                 | 0.930       | 0.048       | 0.410       |
In the sequel, we prove the central limit theorem for (7.5) with high probability. Let (7.3)

\[ \sum \]

where \( \tilde{X} \) is the truncated and centralized version of \( X \). The argument is standard and we omit the details here. Therefore, for simplicity we below assume that

\[ E x_{ij} = 0, \quad |x_{ij}| \leq \delta_n \sqrt{n p}. \]

**Calculation of The Variance.** Define the following events

\[ F_d = \{ \left\| \frac{1}{n} X^T \Sigma_1 X \right\| \leq 4 \left\| \Sigma_1 (1 + p) \right\|, \quad F_d^{(k)} = \{ \left\| \frac{1}{n} X_k^T \Sigma_1 X_k \right\| \leq 4 \left\| \Sigma_1 (1 + p) \right\|, \quad k = 1, \ldots, n, \]

where \( X_k = X - x_k e_k^T \), \( x_k \) is the \( k \)-th column of \( X \) and \( e_k = (0, \ldots, 0, 1, 0, \ldots, 0)^T \) is a \( M \)-dimensional vector with only \( k \)-th element being 1. By Theorem 2 of [16], we have

\[ I(F_d) = 1 \quad \text{and} \quad I(F_d^{(k)}) = 1, \quad k = 1, \ldots, n \]

with high probability.

We define \( \tilde{\Sigma}_d = \tilde{\Sigma}_1 \), \( A = I - \frac{1}{n} X^T \Sigma_1 X \), \( A_k = I - \frac{1}{n} X_k^T \Sigma_1 X_k \) and \( A_{(k)} = A_k - \frac{1}{n} X_k^T \Sigma_1 x_k e_k^T \). Then \( A = A_k - \frac{1}{n} (e_k x_k^T \Sigma_1 X_k + X_k^T \Sigma_1 x_k e_k^T + e_k x_k^T \Sigma_1 x_k e_k^T) \).

Therefore,

\[ x_1^T X(nI - \Sigma_1^{-1} X^T)^{-1} X^T w_1 = \frac{1}{n} x_1^T X A^{-1} X^T w_1. \]

By the definition of \( X_k \) and \( A_k \), we observe that the \( k \)-th row and \( k \)-th column of \( A_k \) are 0 except for the diagonal entry. Hence it is not hard to conclude the following important facts

\[ e_k^T A_k^{-1} e_k = 1, \]

\[ e_i^T A_k^{-1} e_k = 0, \quad i \neq k \]

and

\[ X_k A_k^{-1} e_k = X_k e_k = 0. \]

In the sequel, we prove the central limit theorem for \( \frac{1}{n} w_1^T X A^{-1} X^T w_1 I(F_d) \) instead of \( \frac{1}{n} w_1^T X A^{-1} X^T w_1 \). In fact, it follows from (7.1) that \( I(F_d) = 1 \) with high probability. Therefore \( \frac{1}{n} w_1^T X A^{-1} X^T w_1 I(F_d) \) have the same central limit theorem. Let \( E_k = E(\cdot | x_1, \ldots, x_k) \), \( E = E(\cdot) \) and write

\[ w_1^T X A^{-1} X^T w_1 I(F_d) = E w_1^T X A^{-1} X^T w_1 I(F_d) \]

\[ = \sum_{k=1}^n (E_k - E_{k-1}) w_1^T X A^{-1} X^T w_1 I(F_d) \]

\[ = \sum_{k=1}^n (E_k - E_{k-1}) (w_1^T X A^{-1} X^T w_1 I(F_d) - w_1^T X_k A_k^{-1} X_k^T w_1 I(F_d^{(k)})) \]
\[
\sum_{k=1}^{n} (E_k - E_{k-1}) (w_i^TXA^{-1}X^Tw - w_i^TX_kA_k^{-1}X_k^Tw) I(F_d) + o_p(n^{-2})
\]

where the third equality follows from (7.1), \( I_1 = (w_i^T x_k)^2 e_k^T A^{-1} e_k \), \( I_2 = \sum_{i \neq k} w_i^T x_k w_i^T e_i A^{-1} e_k \), and \( I_3 = \sum_{i,j \neq k} w_i^T x_i w_j^T e_j A^{-1} e_j \). We define

\[
a_k = 1 - \frac{1}{n} (x_k^T \Sigma_1 X_k A^{-1}_{(k)} e_k + x_k^T \Sigma_1 X_k e_k e_k^T A^{-1}_{(k)} e_k)
\]

and

\[
b_k = 1 - \frac{1}{n} e_k^T A_k^{-1} X_k^T \Sigma_1 x_k.
\]

We next simplify the formula. Noting that \( w_i^T X = w_i^T X_k + w_i^T x_k e_i^T \), by the formulas

\[
W^{-1} = Q^{-1} - \frac{Q^{-1}(W - Q)Q^{-1}}{1 + tr(Q^{-1}(W - Q))}
\]

and

\[
(Q + \sum_{j=1}^{m} ab_j^T)^{-1} a = \frac{Q^{-1} a}{1 + \sum_{j=1}^{m} b_j^T Q^{-1} a},
\]

we have

\[
A^{-1} = A^{-1}_{(k)} + \frac{A^{-1}_{(k)} (e_k x_k^T \Sigma_1 X_k + e_k x_k^T \Sigma_1 x_k e_k) A^{-1}_{(k)}}{na_k}
\]

\[
= A_k^{-1} + \frac{A_k^{-1} X_k^T \Sigma_1 x_k e_k^T A^{-1}_{(k)}}{nb_k} + \frac{A_{(k)} (e_k x_k^T \Sigma_1 X_k + e_k x_k^T \Sigma_1 x_k e_k) A^{-1}_{(k)}}{na_k}
\]

and

\[
I_1 = (w_i^T x_k)^2 e_k^T A^{-1} e_k = \frac{(w_i^T x_k)^2 e_k^T A^{-1}_{(k)} e_k}{a_k}
\]

\[
= \frac{(w_i^T x_k)^2 e_k^T A^{-1}_{(k)} e_k}{a_k (1 - \frac{1}{n} e_k^T A_k^{-1} X_k^T \Sigma_1 x_k)} = \frac{(w_i^T x_k)^2 e_k^T A^{-1}_{(k)} e_k}{a_k b_k} = \frac{(w_i^T x_k)^2}{a_k b_k}
\]

Moreover, it follows from (7.3), (7.4) and (7.9) that

\[
b_k = 1 - \frac{1}{n} e_k^T A_k^{-1} X_k^T \Sigma_1 x_k = 1
\]

and

\[
a_k = 1 - \frac{1}{n} x_k^T \Sigma_1 X_k A^{-1}_{(k)} e_k = 1 - \frac{1}{n^2} e_k^T A_k^{-1} e_k x_k^T \Sigma_1 X_k A_k^{-1} X_k^T \Sigma_1 x_k
\]

\[
= 1 - \frac{1}{n^2} x_k^T \Sigma_1 X_k A_k^{-1} X_k^T \Sigma_1 x_k.
\]
By the Cauchy interlacing property we know

\[(7.15) \quad \frac{1}{n^2} x_k^T \tilde{\Sigma}_1 x_k A_k^{-1} x_k^T \tilde{\Sigma}_1 x_k I(F_d) \leq \frac{1}{n^2} x_k^T \tilde{\Sigma}_1 x_k \| A_k^{-1} x_k^T \tilde{\Sigma}_1 x_k \| I(F_d) \leq \frac{1}{n^2} x_k^T \tilde{\Sigma}_1 x_k \| A_k^{-1} \| \| x_k^T \tilde{\Sigma}_1 x_k \| I(F_d) \leq 2 \left( \frac{p}{n\theta} \right)^2. \]

This implies that

\[(7.16) \quad a_k I(F_d) = 1 + O\left( \frac{p}{n\theta} \right)^2. \]

As for the term \(i \neq k\), by (7.4), (7.5), (7.9) and (7.10) we have

\[(7.17) \quad A^{-1} e_k = \frac{A^{-1}_k e_k}{a_k} = \frac{A_k^{-1} e_k}{a_k} + \frac{A_k^{-1} X_k^T \tilde{\Sigma}_1 x_k}{a_k E_k} = \frac{A_k^{-1} e_k}{a_k} + \frac{A_k^{-1} X_k^T \tilde{\Sigma}_1 x_k}{a_k}. \]

We then conclude that

\[(7.18) \quad I_2 = \sum_{i \neq k} w_i^T x_iw_i^T x_i e_i^T A^{-1} e_k = \frac{w_i^T X_kA_k^{-1} x_i^T \tilde{\Sigma}_1 x_k w_i}{na_k}. \]

It follows from (7.4), (7.5) and (7.11) that for \(i, j \neq k\)

\[(7.19) \quad I_3 = \sum_{i,j \neq k} w_i^T x_iw_i^T x_j e_i^T A^{-1} e_j \]

\[= \sum_{i,j \neq k} w_i^T x_iw_i^T x_j e_i^T A_k^{-1} e_j + \sum_{i,j \neq k} w_i^T x_iw_i^T x_j e_i^T A_k^{-1} (e_kx_k^T \tilde{\Sigma}_1 x_k e_j + e_kx_k^T \tilde{\Sigma}_1 x_k) A_k^{-1} e_j \]
\[= \frac{w_i^T x_kA_k^{-1} X_k^T w_i}{na_k} + \frac{w_i^T X_kA_k^{-1} (e_kx_k^T \tilde{\Sigma}_1 x_k e_j + e_kx_k^T \tilde{\Sigma}_1 x_k) A_k^{-1} X_k^T w_i}{na_k}. \]

Consider \((\mathbb{E}_k - \mathbb{E}_{k-1}) (I_3 - w_i^T X_kA_k^{-1} X_k^T w_i) I(F_d)\) next.

We claim that

\[(7.20) \quad \frac{w_i^T X_kA_k^{-1} (e_kx_k^T \tilde{\Sigma}_1 x_k e_j + e_kx_k^T \tilde{\Sigma}_1 x_k) A_k^{-1} X_k^T w_i}{na_k} \]

is negligible. Let \(B_k = \tilde{\Sigma}_1 x_kA_k^{-1} X_k^T w_i X_kA_k^{-1} X_k^T \tilde{\Sigma}_1\). Indeed, by (7.9) and (7.3)-(7.5) we have \(A_k^{-1} = A_k^{-1} + \frac{1}{n} A_k^{-1} X_k^T \tilde{\Sigma}_1 x_k e_k^T A_k^{-1}\). This, together with (7.3), (7.4) and (7.5) implies that

\[(7.20) = \frac{w_i^T X_kA_k^{-1} X_k^T \tilde{\Sigma}_1 x_k e_i^T A_k^{-1} e_kx_k^T \tilde{\Sigma}_1 x_k A_k^{-1} X_k^T w_i}{n^2a_k} = \frac{x_k^T B_k x_k}{n^2a_k}. \]

It follows from (7.19) and (7.3)-(7.5) that

\[
\sum_{k=1}^n (\mathbb{E}_k - \mathbb{E}_{k-1}) (I_3 - w_i^T X_kA_k^{-1} X_k^T w_i) I(F_d) = \sum_{k=1}^n (\mathbb{E}_k - \mathbb{E}_{k-1}) \frac{x_k^T B_k x_k}{n^2a_k} I(F_d(k)) + o_p(n^{-2}).
\]
Considering the second moment of the above equation, by Lemma 8.10 of [5] we have

\[
\sum_{k=1}^{n} \mathbb{E}[(E_k - E_{k-1}) \frac{x_k^I B_k x_k}{n^2 a_k}^2 I(F_d^{(k)})] \leq \frac{4}{n^2} \sum_{k=1}^{n} \mathbb{E}[x_k^I B_k x_k]^2 I(F_d^{(k)})
\]

\[
\leq \frac{8}{n^2} \sum_{k=1}^{n} \mathbb{E}[x_k^I B_k x_k - \text{tr} B_k]^2 I(F_d^{(k)}) + \frac{8}{n^2} \sum_{k=1}^{n} \mathbb{E}[\text{tr} B_k]^2 I(F_d^{(k)})
\]

\[
\leq \frac{C p^2}{n \theta^2} N,
\]

where we used the inequality

\[
\text{tr} B_k \leq X_k A_k^{-1} X_k^I \sum_k^2 X_k A_k^{-1} X_k^I I(F_d^{(k)}) = O\left(\frac{p^2}{\theta^2}\right).
\]

We conclude that

\[
\frac{1}{n} \sum_{k=1}^{n} (E_k - E_{k-1}) (I_3 - w_k^I X_k A_k^{-1} X_k^I w_1) I(F_d) = o_p\left(\frac{1}{\sqrt{n}}\right),
\]

which is negligible.

Next we consider \( I_1 \) and \( I_2 \). It follows from (7.12) and (7.18) that

\[
\sum_{k=1}^{n} (E_k - E_{k-1}) (I_1 + 2 I_2) I(F_d)
\]

\[
= \frac{2}{\sqrt{n}} \sum_{k=1}^{n} (E_k - E_{k-1}) \left(\frac{(w_k^I x_k)^2}{2a_k} + \frac{w_k^I X_k A_k^{-1} X_k^I \sum_k x_k x_k^I w_1}{na_k}\right) I(F_d).
\]

We claim that the second term of (7.22) is negligible. Actually, similar to (7.21), it is easy to show that

\[
\sum_{k=1}^{n} (E_k - E_{k-1}) \frac{w_k^I X_k A_k^{-1} X_k^I \sum_k x_k x_k^I w_1}{na_k} I(F_d) = o_p(\sqrt{n})
\]

Therefore, the leading term of (7.22) is

\[
\frac{1}{\sqrt{n}} \sum_{k=1}^{n} (E_k - E_{k-1}) \frac{(w_k^I x_k)^2}{a_k} I(F_d)
\]

\[
= \frac{1}{\sqrt{n}} \sum_{k=1}^{n} (E_k - E_{k-1}) \frac{(1 - a_k)(w_k^I x_k)^2}{a_k} I(F_d) + \frac{1}{\sqrt{n}} \sum_{k=1}^{n} (E_k - E_{k-1}) (w_k^I x_k)^2 I(F_d).
\]

Similar to (7.21), by (7.16) we can show that

\[
\frac{1}{\sqrt{n}} \sum_{k=1}^{n} (E_k - E_{k-1}) \frac{(1 - a_k)(w_k^I x_k)^2}{a_k} I(F_d) = o_p(1).
\]

It suffices to show CLT for

\[
\frac{1}{\sqrt{n}} \sum_{k=1}^{n} (E_k - E_{k-1}) (w_k^I x_k)^2 = \frac{1}{\sqrt{n}} \sum_{k=1}^{n} [(w_k^I x_k)^2 - 1].
\]
By the CLT for the sum of i.i.d. variables, we conclude that
\[
\frac{1}{\sqrt{n\sigma}} \sum_{k=1}^{n} (E_k - E_{k-1})(w^T_k x_k)^2 \overset{D}{\rightarrow} N(0, \sigma^2),
\]
where
\[
(7.24) \quad \sigma^2 = \frac{1}{n} E \left[ (w^T_1 x_k)^2 - 1 \right]^2 = \frac{1}{n} \sum_{i=1}^{p+l} \gamma_{4i} w^4_{1i} + 3 \sum_{i \neq j}^{p+l} \frac{w^2_{1i} w^2_{1j} - 1}{n} = \sum_{i=1}^{}\left(\gamma_{4i} - 3\right) w^4_{1i} + 2.
\]

7.2. Calculation of the Mean. This section is to calculate the expectation of \( \frac{1}{n} w^T X A^{-1} X^T w_1 I(F_d) \). The strategy is to prove that
\[
(7.25) \quad \sqrt{n} E \left[ \frac{1}{n} w^T X^0 A^{-1} (X^0)^T w_1 I(F_d) + \tilde{m}_\theta(1) \right] \to 0,
\]
and
\[
(7.26) \quad \frac{1}{\sqrt{n}} E \left[ w^T X A^{-1} X^T w_1 I(F_d) - w^T X^0 A^{-1} (X^0)^T w_1 I(F_d) \right] \to 0,
\]
where \( X^0 = (x^0_1, ..., x^0_n) \) is \((p + l) \times n \) matrix with i.i.d. standard Gaussian random variables. As before, we omit \( I(F_d) \) in the following proof.

We prove (7.26) first by the Lindeberg’s strategy. Define
\[
Z^1_k = \sum_{i=1}^{k} x_i e^T_i + \sum_{i=k+1}^{n} x^0_i e^T_i, \quad Z^0_k = \sum_{i=1}^{k-1} x_i e^T_i + \sum_{i=k}^{n} x^0_i e^T_i,
\]
\[
Z_k = \sum_{i=1}^{k-1} x_i e^T_i + \sum_{i=k+1}^{N} x^0_i e^T_i, \quad \hat{A}^1_k = I - \frac{1}{n} (Z^1_k)^T \hat{\Sigma} Z^1_k,
\]
\[
\hat{A}^0_k = I - \frac{1}{n} (Z^0_k)^T \hat{\Sigma} Z^0_k \quad \text{and} \quad \hat{A}_k = I - \frac{1}{n} Z^T_k \hat{\Sigma} Z_k.
\]

Then we have \( X = Z^1_N, X^0 = Z^0_1, Z^0_{k+1} = Z^1_k \). It follows that
\[
(7.27) \quad \frac{1}{\sqrt{n}} E \left[ w^T X A^{-1} X^T w_1 - w^T X^0 A^{-1} (X^0)^T w_1 \right]
\]
\[
= \frac{1}{\sqrt{n}} \sum_{k=1}^{n} E \left[ w^T Z^1_k (\hat{A}^1_k)^{-1} (Z^1_k)^T w_1 - w^T Z^0_k (\hat{A}^0_k)^{-1} (Z^0_k)^T w_1 \right]
\]
\[
= \frac{1}{\sqrt{n}} \sum_{k=1}^{n} E \left[ w^T Z^1_k (\hat{A}^1_k)^{-1} (Z^1_k)^T w_1 - w^T Z_k \hat{A}^{-1} Z^1_k w_1 \right]
\]
\[
+ \frac{1}{\sqrt{n}} \sum_{k=1}^{n} E \left[ w^T Z^0_k (\hat{A}^0_k)^{-1} Z^0_k w_1 - w^T Z^0_k (\hat{A}^0_k)^{-1} Z^0_k w_1 \right].
\]
For any $k$, similar to the expansions from (7.11)-(7.20), we can get

(7.28) \[ E \left[ w_1^T Z_k^1 (\hat{A}_k^1)^{-1} (Z_k^1)^T w_1 - w_1^T Z_k \hat{A}_k^{-1} Z_k^T w_1 \right] \]

\[ = E \left[ \frac{(w_1 x_k)^2}{\bar{a}_k} + \frac{2w_1^T Z_k \hat{A}_k^{-1} Z_k^T \bar{\Sigma}_1 x_k x_k^T w_1}{n \bar{a}_k} + \frac{x_k^T \hat{B}_k x_k}{n^2 \bar{a}_k^2} \right], \]

where $\hat{B}_k = \tilde{\Sigma}_1 Z_k \hat{A}_k^{-1} Z_k^T$ and $\bar{a}_k = 1 - \frac{1}{n^2} tr \hat{\Sigma}_1 Z_k \hat{A}_k^{-1} Z_k^T \tilde{\Sigma}_1 x_k x_k^T$. Let $\bar{a}_k = 1 - \frac{1}{n^2} tr \hat{\Sigma}_1 Z_k \hat{A}_k^{-1} Z_k^T \tilde{\Sigma}_1 x_k$. By Lemma 8.10 of [5], we conclude that

(7.30) \[ E|\tau_k|^2 = E \left[ \frac{(w_1 x_k)^2}{\bar{a}_k} - \frac{(w_1 x_k)^2}{\bar{a}_k^2} \right] \leq C \frac{d^2}{n^2} \| \Sigma \| \| \Sigma \|^2 = O \left( \frac{d^2}{P} \right). \]

Consider the first term at the right hand side of (7.28). It follows from (7.29), (7.30) and Holder’s inequality that

(7.31) \[ |E \left( \frac{(w_1 x_k)^2}{\bar{a}_k} - \frac{(w_1 x_k)^2}{\bar{a}_k^2} \right) | = \left| E \frac{(w_1 x_k)^2 \tau_k}{\bar{a}_k^2} \right| \leq C \sqrt{E(w_1 x_k)^4} \sqrt{E \tau_k^2} = O \left( \frac{d}{\sqrt{P}} \right). \]

Thus we conclude that

(7.32) \[ \frac{1}{\sqrt{n}} \sum_{k=1}^n E \left[ w_1^T Z_k^1 (\hat{A}_k^1)^{-1} (Z_k^1)^T w_1 - w_1^T Z_k \hat{A}_k^{-1} Z_k^T w_1 \right] \]

\[ = \frac{1}{\sqrt{n}} \sum_{k=1}^n E \left[ \frac{1}{\bar{a}_k} + \frac{2w_1^T Z_k \hat{A}_k^{-1} Z_k^T \bar{\Sigma}_1 w_1}{n \bar{a}_k} + \frac{tr \hat{B}_k}{n^2 \bar{a}_k^2} \right] + o(1). \]

By the same arguments above, we can also get

(7.33) \[ \frac{1}{\sqrt{n}} \sum_{k=1}^n E \left[ w_1^T Z_k \hat{A}_k^{-1} Z_k^T w_1 - w_1^T Z_k^0 (\hat{A}_k^0)^{-1} (Z_k^0)^T w_1 \right] \]

\[ = - \frac{1}{\sqrt{n}} \sum_{k=1}^n E \left[ \frac{1}{\bar{a}_k} + \frac{2w_1^T Z_k \hat{A}_k^{-1} Z_k^T \bar{\Sigma}_1 w_1}{n \bar{a}_k} + \frac{tr \hat{B}_k}{n^2 \bar{a}_k^2} \right] + o(1). \]

Combining (7.27), (7.32) and (7.33), the equation (7.26) holds.

We next prove (7.25). To simplify notation, we use $X$ for $X^0$ and hence assume that $X$ follows standard normal distribution. By $w_1^T U_2 = 0$, we conclude that $w_1^T X$
is independent of $A$ and hence $\frac{1}{n}\mathbb{E}\mathbf{w}_i^\top XA^{-1}X^\top \mathbf{w}_i = \frac{1}{n}\text{tr}A^{-1}$. By (6.2.4) of [5](or Lemma 3.1 of [9]), we have

$$\frac{1}{n}\text{tr}A^{-1} = \mathbb{E}\frac{1}{1 + r_1^\top \Delta_1^{-1}r_1},$$

where we denote $\Delta = \Sigma_1^{1/2}XX^\top \Sigma_1^{1/2} - I$, $r_i = \frac{1}{\sqrt{n}}\Sigma_1^{1/2}\mathbf{x}_i$ and $\Delta_j = \sum_{i\neq j}r_i^\top r_i - I$. By Lemma 8.10 of [5], we have

$$\mathbb{E}|r_1^\top \Delta^{-1}_1 r_1 - \frac{1}{\theta_n}\text{tr}\Delta^{-1}_1 | \leq \frac{C}{n^2}\text{tr}\Sigma_1 - \frac{o(1)}{\theta_n}\text{tr}\Delta_1^{-1}\Sigma_1 \leq o(M^{-1}),$$

which concludes that $\mathbb{E}\frac{1}{1 + r_1^\top \Delta^{-1}_1 r_1} = \mathbb{E}\frac{1}{1 + \frac{1}{\theta_n}\text{tr}\Delta^{-1}_1 r_1} + o(n^{-1/2}).$ Moreover,

$$\mathbb{E}\left|\frac{1}{1 + \frac{1}{\theta_n}\text{tr}\Delta^{-1}_1 r_1} - \frac{1}{1 + \frac{1}{\theta_n}\text{tr}\Delta^{-1}_1 \Sigma_1}\right|^2 \leq \frac{C}{n^2}\mathbb{E}\text{tr}\Delta^{-1}_1 \Sigma_1 - \mathbb{E}\text{tr}\Delta^{-1}_1 \Sigma_1 o(n^{-2}).$$

Hence $\mathbb{E}\frac{1}{1 + \frac{1}{\theta_n}\text{tr}\Delta^{-1}_1 \Sigma_1} = \frac{1}{1 + \frac{1}{\theta_n}\text{tr}\Delta^{-1}_1 \Sigma_1} + o(n^{-1/2})$. Define $\beta_i = \frac{1}{1 + r_1^\top \Delta^{-1}_1 r_1}$, $b_i = \frac{1}{1 + \frac{1}{\theta_n}\text{tr}\Delta^{-1}_1 \Sigma_1}$, and $\alpha_i = r_1^\top \Delta^{-1}_1 r_i - \frac{1}{\theta_n}\text{tr}\Sigma_1^{-1}$. By the equality that $A_\theta + I - b(\theta)\Sigma_1 = \sum_{i \neq 1}r_i^\top r_i - b(\theta)\Sigma_1$, we have

$$A_\theta^{-1} = -(I - b_1(\theta)\Sigma_1)^{-1} + b_1(\theta)A(\theta) + B(\theta) + C(\theta),$$

where

$$A(\theta) = \sum_{i \neq 1}(I - b_1(\theta)\Sigma_1)^{-1}(r_i^\top r_i - \frac{1}{\theta_n}\Sigma_1)\Delta^{-1}_1,$$

$$B(\theta) = \sum_{i \neq 1}(\beta_i - b_1)(I - b_1(\theta)\Sigma_1)^{-1}r_i^\top \Delta^{-1}_1,$$

$$C(\theta) = n^{-1}b_1(I - b_1(\theta)\Sigma_1)^{-1}\Sigma_1\sum_{i \neq 1}(\Delta^{-1}_1 - \Delta^{-1}_1).$$

For $A(\theta)$, similar to (7.34) we have

$$\frac{1}{n}\text{tr}A(\theta)\Sigma_1 \leq \frac{1}{n}\sum_{i \neq 2}\mathbb{E}|r_i^\top \Delta^{-1}_1 (I - b_1(\theta)\Sigma_1)^{-1}r_i - \frac{1}{\theta_n}\text{tr}(\Sigma_1^{1/2}XX^\top \Sigma_1^{1/2})| = o(M^{-1}).$$

Similar to the previous inequalities (7.34)-(7.35) or as in Chapter 9 of [5], we can also show that $B(\theta)$ and $C(\theta)$ are negligible. Hence we get

$$\frac{1}{n}\text{tr}A^{-1}_\theta \Sigma_1 = -\frac{1}{n}\text{tr}(I - b_1(\theta)\Sigma_1)^{-1}\Sigma_1 + o(n^{-1/2}),$$

which implies that

$$\frac{1}{n}\text{tr}A^{-1} = \frac{1}{1 - \frac{1}{n}\text{tr}(I - \frac{1}{n}\text{tr}A^{-1}\Sigma_1)^{-1}\Sigma_1} + o(n^{-1/2}),$$

where we denote $\Delta = \Sigma_1^{1/2}XX^\top \Sigma_1^{1/2} - I$, $r_i = \frac{1}{\sqrt{n}}\Sigma_1^{1/2}\mathbf{x}_i$ and $\Delta_j = \sum_{i\neq j}r_i^\top r_i - I$.
By the Steiltjes transform of the limit of the ESD of any sample covariance matrix, there exists only one $\tilde{m}_\theta(z)$ such that (One can also refer to (1.6) of [9] or (6.12)-(6.15) of [5])

$$ (7.40) \quad \tilde{m}_\theta(z) = -\frac{1}{z - \frac{1}{n} tr(I + \tilde{m}_\theta(z)\Sigma_1)^{-1}\Sigma_1}, \quad z \in \mathbb{C}^+. $$

Consider the difference between (7.39)-(16.4) and denote $\delta = \frac{1}{n} E tr A^{-1} + \tilde{m}_\theta(1)$. It is easy to conclude that

$$ (7.41) \quad \delta(1 + \frac{1}{n} tr \left[ (I - \frac{1}{n} (E tr A^{-1})\hat{\Sigma}_1)^{-1}\hat{\Sigma}_1 (I + \tilde{m}_\theta(1)\hat{\Sigma}_1)^{-1}\hat{\Sigma}_1 \right] (1 - \frac{1}{n} tr (I + \tilde{m}_\theta(1)\Sigma_1)^{-1}\Sigma_1) ) = o(n^{-1/2}). $$

Together with the fact that $||\hat{\Sigma}_1|| = O(\theta^{-1})$, it follows that $\delta = O(1/\sqrt{n})$. Therefore, we have shown that

$$ (7.41) \quad \sqrt{n} (\frac{1}{n} E tr A^{-1} + \tilde{m}_\theta(1)) \to 0. \quad \square $$

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Supplement to “Limiting Laws for Divergent Spiked Eigenvalues and Largest Non-spiked Eigenvalue of Sample Covariance Matrices”

This note summarizes the supplementary materials to the paper “Limiting Laws for Divergent Spiked Eigenvalues and Largest Non-spiked Eigenvalue of Sample Covariance Matrices”. We first briefly discuss the quantities $\gamma_+$ and $\sigma_n$ defined in Section 3 and then provide detailed proofs of the main theorems and some technical results given in the paper. More specifically, we prove in detail here Theorems 2.1, 2.2, 2.3, 4.1, 2.5, Lemma 1 and Corollary 2.

8. Discussion on $\gamma_+$ and $\sigma_n$

Below we discuss the unknown parameters $\gamma_+$ and $\sigma_n$. In order to find an upper bound of $\lambda_{K+1}$, by (3.2), a key step is to estimate $\sigma_n$ and $\gamma_+$. By (3) and (11) of [18], we have

$$\sigma_n = \left(\frac{1}{2} \frac{\partial^3 f(z)}{\partial z^3} \biggr|_{z \to d}\right)^{1/3},$$

where

$$f(z) = -\gamma_+ z + \log(z) - \frac{p - K}{n} \int \log(1 - z \lambda) dF_{\Lambda_0}(\lambda) + C, \; C \text{ is a constant.}$$

It is straightforward to get

$$(8.1) \quad \frac{\partial f(s)}{\partial s} = -\gamma_+ + \frac{1}{s} + \frac{p - K}{n} \int \frac{\lambda dF_{\Lambda_0}(\lambda)}{1 - \lambda s},$$

Let $t = -m_{\Sigma_1}(z)$. Then by the equality that

$$z = -\frac{1}{t} + \frac{p - K}{n} \int \frac{\lambda dF_{\Lambda_0}(\lambda)}{1 + \lambda t},$$

we have $\frac{\partial f(t)}{\partial t} = -\gamma_+ - z$. Therefore, $\frac{\partial^3 f(t)}{\partial t^3} = -\frac{\partial^2 z}{\partial t^2}$. Recall the definition of $t$,

$$t = -m_{\Sigma_1}(z) = -\int \frac{dF_0(x)}{x - z},$$

where $F_0(x)$ is the c.d.f. determined by $m_{\Sigma_1}(z)$. We have the following two equations:

$$(8.2) \quad 1 = -\frac{\partial z}{\partial t} \int \frac{dF_0(x)}{(x - z)^2}, \quad 0 = -\frac{\partial^2 z}{\partial t^2} \int \frac{dF_0(x)}{(x - z)^2} + 2\left(\frac{\partial z}{\partial t}\right)^2 \int \frac{dF_0(x)}{(x - z)^3},$$

It follows from (3.1), (8.1)-(8.2) that

$$(8.3) \quad \sigma_n = \left(- \lim_{z \to \gamma_+} \int \frac{dF_0(x)}{(x - z)^3}\right)^{1/3}$$

By the singular value inequality or interlacing inequality, we have

$$\lambda_n^{1/6} \geq \nu_n^{1/6 + K}.$$ 

By Theorem 3.14 of [24], we have

$$|\nu_n^{1/6 + K} - \gamma_n^{1/6 + K}| \leq n^{-2/3},$$
with high probability, where
\[ i_n = \int_{\gamma_i}^{\gamma_+} dF_0(x). \]
By Lemmas 2.3 and 2.5 of [8], we have
\[ \frac{dF_0(x)}{dx} \sim \sqrt{\gamma_+ - x}, \]
then
\[ \gamma_+ - \nu_{1/6+K} \sim n^{-5/9}. \]
Therefore \( \gamma_+ - \nu_{1/6+K} \leq \frac{\log n}{2} \times n^{-5/9} \) with high probability. Therefore, together with Theorem 2.5, with high probability
\[ \lambda_{K+1} = \lambda_{n1/6} + \log n \times n^{-5/9}. \] (8.4)

9. PROOF OF THEOREM 2.1

Below, we consider \( i = 1, \ldots, K \). Note that the non-zero eigenvalues of \( \Gamma XX^T \Gamma^T \) are equal to those of \( UXX^T U^T \Lambda \). By Weyl’s inequality, we have
\[ |\sigma_i(\Lambda^{1/2} UX) - \sigma_i\left( \begin{pmatrix} \Lambda S^{1/2} \\ 0 \\ 0 \end{pmatrix} UX \right)| \leq \left\| \begin{pmatrix} 0 \\ 0 \\ \Lambda^{1/2}_P \end{pmatrix} \right\| UX, \]
where \( \sigma_i(A) \) is the \( i \)-th largest singular value of \( A \). By Theorem 1 of [16], under Assumption 2(ii), with probability tending to 1, we have
\[ \left\| \frac{1}{n} U_2 XX^T U_2^T \Lambda_P \right\| \leq \left\| \frac{1}{n} U_2 XX^T U_2^T \right\| \left\| \Lambda_P \right\| \leq \left\| \frac{1}{n} XX^T \right\| \left\| \Lambda_P \right\| \leq \frac{2CP}{n}. \]
Define \( B = \left( \begin{pmatrix} \Lambda S^{1/2} \\ 0 \\ 0 \end{pmatrix} \right) \). By assumption 3, we have
\[ \lambda_i\left( \frac{1}{n} UXX^T U^T B \right) - \lambda_i\left( \frac{1}{n} UXX^T U^T \right) = O_p(d_i). \] (9.1)
Moreover, it is easy to see that the non-zero eigenvalues of \( \lambda_i\left( \frac{1}{n} UXX^T U^T B \right) \) are the same as those of the \( K \times K \) block \( C = \frac{1}{n} \Lambda_S^{1/2} U_1 XX^T U_1^T \Lambda_S^{1/2} \), where \( U_1 \) is the first \( K \) rows of \( U \). By Theorem 7.1 of [6] and Chebyshev’s inequality, we can show that \( \| \frac{1}{n} U_1 XX^T U_1^T - I_K \|_\infty = O_p\left( \frac{K^4}{\sqrt{n}} \right) \). Moreover, the determinant for calculating the eigenvalue \( \lambda_i\left( \frac{1}{n} \Lambda_S^{1/2} U_1 XX^T U_1^T \Lambda_S^{1/2} \right) \) is equivalent to
\[ \det\left( \frac{1}{n} U_1 XX^T U_1^T - \lambda_i(C) \Lambda_S^{-1} \right) = 0. \] (9.2)
By the Leibniz’s formula for the determinant, it is easy to conclude that \( \frac{\lambda_i(C)}{\mu_i} - 1 = O_p\left( \frac{K^4}{n} \right) \) uniformly for all \( i = 1, ..., K \). Combining with (9.1), we conclude that
\[ \frac{\lambda_i\left( \frac{1}{n} UXX^T U^T \right)}{\mu_i} - \mu_i = O_p\left( \frac{K^4}{n} + d_i \right) \]
uniformly for all \( i = 1, ..., K \).
10. Proof of Theorem 2.2

10.1. Outline of The Proof. If $\lambda_i$ is the spiked eigenvalue of $S_n$, then by the determinantal equation (10.7) below we conclude that $\lambda_i$ satisfies the following equation

\[(10.1) \; \det(\Lambda_{S}^{-1} - \frac{1}{n}U_1X(\lambda_iI - \frac{1}{n}X^\top U_2^\top \Lambda P U_2X)^{-1}X^\top U^\top_i) = 0.\]

We will prove that the diagonal entries of $\frac{1}{n}U_1X(\lambda_iI - \frac{1}{n}X^\top U_2^\top \Lambda P U_2X)^{-1}X^\top U^\top_i$ dominate the determinant above. Roughly speaking, by ignoring the negligible terms we can get the following equation

\[(10.2) \; \mu_i^{-1} - \frac{1}{n}u^\top_i X(\lambda_iI - \frac{1}{n}X^\top U_2^\top \Lambda P U_2X)^{-1}X^\top u_i = 0.\]

We can further get

\[
\mu_i^{-1} - \frac{1}{n}u^\top_i X(\theta_iI - \frac{1}{n}X^\top U_2^\top \Lambda P U_2X)^{-1}X^\top u_i \approx (\lambda_i - \theta_i)\frac{1}{n}u^\top_i X(\theta_iI - \frac{1}{n}X^\top U_2^\top \Lambda P U_2X)^{-2}X^\top u_i.
\]

Therefore, the CLT of $(\lambda_i - \theta_i)$ is determined by the asymptotic distribution of $\frac{1}{n}u^\top_i X(\theta_iI - \frac{1}{n}X^\top U_2^\top \Lambda P U_2X)^{-1}X^\top u_i$. From the CLT of the random quadratic forms in Theorem 2.4, similarly, the correlation of $\lambda_i$ and $\lambda_j$ are also determined by $\frac{1}{n}u^\top_i X(\theta_iI - \frac{1}{n}X^\top U_2^\top \Lambda P U_2X)^{-1}X^\top u_i$ and $\frac{1}{n}u^\top_j X(\theta_jI - \frac{1}{n}X^\top U_2^\top \Lambda P U_2X)^{-1}X^\top u_j$.

**Proof of Theorem 2.2 under Assumption 7**

This section is to prove a weaker version of Theorem 2.2 first, i.e. We assume that Assumption 7 holds instead of Assumption 1. Assumption 7 is then removed at Section 12 in the supplementary. Define $B(x) = xI - \frac{1}{n}X^\top U_2^\top \Lambda P U_2X$.

First of all, we prove CLT for a fixed $i$, $i \in \{1, ..., K\}$. By the definition of $\lambda_i$, it solves the equation

\[
\det(\Lambda_{S}^{-1} - \frac{1}{n}X^\top U_2^\top \Lambda P U_2X - \frac{1}{n}X^\top U_2^\top \Lambda S U_1X) = 0.
\]

By the simple fact that $\det(I - CD) = \det(I - DC)$, we have

\[(10.3) \; \det(\Lambda_{S}I - \frac{1}{n}X^\top U_2^\top \Lambda UX) = 0.\]

Recalling the notations above Assumption 1, (10.3) is equivalent to

\[(10.4) \; \det(\Lambda_{S}I - \frac{1}{n}X^\top U_2^\top \Lambda P U_2X - \frac{1}{n}X^\top U_2^\top \Lambda S U_1X) = 0.\]

By Theorem 2.1, $\Lambda_{S}I - \frac{1}{n}X^\top U_2^\top \Lambda P U_2X$ is invertible with probability tending to 1. Hence with probability tending to 1, (10.4) is equivalent to

\[(10.5) \; \det(I - \frac{1}{n}X^\top U_2^\top \Lambda S U_1X(\Lambda_{S}I - \frac{1}{n}X^\top U_2^\top \Lambda P U_2X)^{-1}) = 0.\]

Therefore, $\lambda_i$ satisfies the following equation

\[(10.6) \; \det(I - \frac{1}{n}\Lambda_{S}^{1/2} U_1X B^{-1}(\lambda_i)X^\top U_2^\top \Lambda_{S}^{1/2}) = 0.\]

i.e.

\[(10.7) \; \det(\Lambda_{S}^{-1} - \frac{1}{n}U_1X B^{-1}(\lambda_i)X^\top U^\top_i) = 0.\]
Recalling (2.5), we have
\[ m_{\theta_i}(1) + \frac{\theta_i}{\mu_i} = 0. \]
Since \( m_{\theta_i}(x) \) is a increasing function of \( x \) for \( x \geq 1/2 \) outside the spectrum of \( m_{\theta_i}(x) \) and \( \| \sum_k \| = O_p(d_i) \), we conclude that \( \theta_i = \mu_i(1+O(d_i)) \). We denote \( \frac{\lambda_i - \theta}{\theta} \) by \( \delta_i \). For convenience, we only prove the central limit theorem for \( \lambda_1 \) and the other eigenvalues can be handled similarly. First of all, we have
\[(10.8) \quad U_1XB^{-1}(\lambda_1)XU_1^\top = U_1XB^{-1}(\theta_1)XU_1^\top - \delta_1 U_1XB^{-1}(\lambda_1)B^{-1}(\theta_1)XU_1^\top. \]
Hence (10.7) can be rewritten as
\[(10.9) \quad \text{det}(\theta_1A_{S^{-1}} - \frac{\theta_1}{n} U_1XB^{-1}(\theta_1)XU_1^\top + \frac{\delta_1\theta_1^2}{n} U_1XB^{-1}(\lambda_1)B^{-1}(\theta_1)XU_1^\top) = 0. \]
To illustrate the main idea of our proof, we give a simple example. Suppose \( K = 2 \) and we have shown that
\[ \theta_1A_{S^{-1}} - \frac{\theta_1}{n} U_1XB^{-1}(\theta_1)XU_1^\top = \begin{pmatrix} \hat{S}_n & O_p(\frac{1}{\sqrt{n}}) \\ O_p(\frac{1}{\sqrt{n}}) & 1 + o_p(1) \end{pmatrix} \]
and
\[ \frac{\theta_1^2}{n} U_1XB^{-1}(\lambda_1)B^{-1}(\theta_1)XU_1^\top = - \left( 1 + o_p(1) \quad o_p(1) \right) \left( o_p(1) \quad 1 + o_p(1) \right), \]
where \( \sqrt{n} \hat{S}_n \overset{D}{\to} N(0,1) \). Then (10.9) becomes
\[ \text{det}\left( \begin{pmatrix} \hat{S}_n + \delta_1(1 + o_p(1)) & O_p(\frac{1}{\sqrt{n}}) + o_p(\delta_1) \\ O_p(\frac{1}{\sqrt{n}}) + o_p(\delta_1) & 1 + o_p(1) + \delta_1(1 + o_p(1)) \end{pmatrix} \right) = 0. \]
By Leibniz’s formula for the determinant of a matrix, we have
\[ \delta_1(1 + o_p(1)) + \hat{S}_n(1 + o_p(1)) + o_p(\frac{1}{\sqrt{n}}) = 0, \]
which implies that \( \sqrt{n} \delta_1 = \sqrt{n} \hat{S}_n + o_p(1) \overset{D}{\to} N(0,1) \).

By the example above, similar to the proof of Theorem 3.1 in [6], the key steps are to establish the central limit theorem for the entries of \( \sqrt{n} \theta_1 U_1XB^{-1}(\theta_1)XU_1^\top \) and the entry wise limit of \( \sqrt{n} \theta_1 U_1XB^{-2}(\theta_1)XU_1^\top \) by Leibniz’s formula for the determinant of a matrix.

Let \( u_i^\top \) be the i-th row of \( U_1 \). By Theorem 2.4, we have
\[(10.10) \quad \sqrt{n}\left(\frac{\theta_1}{n} u_i^\top XB^{-1}(\theta_1)Xu_i + \tilde{m}_{\theta_1}(1)\right) \overset{D}{\to} N(0, \sigma_i^2) \]
and
\[ \frac{1}{\sqrt{n}}\theta_1 u_i^\top XB^{-1}(\theta_1)Xu_j \overset{D}{\to} N(0, \sigma_{ij}) \quad i \neq j, \]
where \( \sigma_i \) and \( \sigma_{ij} \) are defined above (2.6). By Chebyshev’s inequality and the proof of Theorem 2.4 we have
\[ \text{P}(\max_{1 \leq i, j \leq k} \left| \frac{\theta_1}{n} u_i^\top XB^{-1}(\theta_1)Xu_j + \delta_{ij} \tilde{m}_{\theta_1}(1) \right| \geq \epsilon) \leq \frac{1}{\epsilon^2} \]
for a fixed \( \epsilon > 0 \).
$$\leq \sum_{1 \leq i,j \leq k} P(|\frac{\theta_1}{n}u_i^\top XB^{-1}(\theta_1)X^\top u_j + \delta_{ij}\hat{m}_{\theta_1}(1)| \geq \frac{\epsilon}{\sqrt{n}})$$

(10.11) $$\leq \sum_{1 \leq i,j \leq k} \frac{N^2(\theta_1)u_i^\top XB^{-1}(\theta_1)X^\top u_j + \delta_{ij}\hat{m}_{\theta_1}(1))^2}{t^2} = O\left(K^2 \epsilon^2\right),$$

which implies that $$\max_{1 \leq i,j \leq k} |\frac{\theta_1}{n}u_i^\top XB^{-1}(\theta_1)X^\top u_j + \delta_{ij}\hat{m}_{\theta_1}(1)| = O_p\left(\frac{K}{\sqrt{n}}\right).$$ It follows that

$$\theta_1A_{S^{-1}} - \frac{\theta_1}{n}U_1XB^{-1}(\theta_1)X^\top U_1^\top = \begin{bmatrix}
\hat{S}_n & O_p\left(\frac{K}{\sqrt{n}}\right) & \ldots & \ldots & O_p\left(\frac{K}{\sqrt{n}}\right) \\
O_p\left(\frac{K}{\sqrt{n}}\right) & O_p(1) & \ldots & \ldots & O_p\left(\frac{K}{\sqrt{n}}\right) \\
\ldots & \ldots & \ldots & \ldots & \ldots \\
O_p\left(\frac{K}{\sqrt{n}}\right) & \ldots & O_p(1) & O_p\left(\frac{K}{\sqrt{n}}\right) & O_p(1)
\end{bmatrix},$$

where $$\hat{S}_n = \frac{\theta_1}{n}u_1^\top XB^{-1}(\theta_1)X^\top u_1 + \hat{m}_{\theta_1}(1).$$ Moreover, we claim that there exists $$\delta_n \to 0$$ such that

$$\|\frac{\theta_1^2}{n}U_1XB^{-2}(\theta_1)X^\top U_1^\top + (1 + \delta_n)\hat{m}_{\theta_1}(1)I\|_{\infty} = O_p\left(\frac{K}{\sqrt{n}}\right),$$

whose proof is given in section 10.1.1. By Theorem 2.1 and (2.5) we have

$$\|\frac{\theta_1^2}{n}U_1XB^{-1}(\lambda_1)B^{-1}(\theta_1)X^\top U_1^\top - \frac{\theta_1^2}{n}U_1XB^{-2}(\theta_1)X^\top U_1^\top\|_{\infty}$$

(10.14) $$= \delta_1\|\frac{\theta_1^2}{n^2}U_1XB^{-1}(\lambda_1)X^\top \Sigma_{\delta_2}XB^{-2}(\theta_1)X^\top U_1^\top\|_{\infty} = O_p\left(\frac{K^4}{n} + d_1\right),$$

which, together with (10.13), implies that

$$\|\frac{\theta_1^2}{n^2}U_1XB^{-1}(\lambda_1)B^{-1}(\theta_1)X^\top U_1^\top + (1 + \delta_n)\hat{m}_{\theta_1}(1)I\|_{\infty} = O_p\left(\frac{K^4}{\sqrt{n}} + K^4 + d_1\right).$$

By Leibniz formula for determinant and a tedious calculation, one can show that

$$\delta_1(1 + O_p(K^2d_1 + \frac{K^6}{n})) + \hat{S}_n(1 + o_p(1)) + o_p\left(\frac{1}{\sqrt{n}}\right) = 0.$$ 

By (10.10) we have shown that

$$\sqrt{n}\delta_1 \xrightarrow{D} N(0, \sigma^2_1),$$

and the proof of this section is complete.

10.1.1. Proof of (10.13). The proof of (10.13) is similar to Section 7.2 and we merely give a sketch of the proof. We consider a special entry $$E(\frac{\theta_1}{n}u_i^\top XB^{-2}(\theta_1)X^\top u_1 + (1 + \delta_n)\hat{m}_{\theta_1}(1))^2$$ of (10.13) as an example. First of all, as in (7.6)-(7.24), one can
show that $E\frac{\theta^2}{n}u_1^T XB^{-2}(\theta_1)X^\top u_1 - E\frac{\theta^2}{n}u_1^T XB^{-2}(\theta_1)X^\top u_1|^2 = O\left(\frac{1}{n}\right)$. Therefore by Chebyshev’s inequality, we have

$$\frac{1}{n}\|\theta^2 U_1 XB^{-2}(\theta_1)X^\top U_1 - E\theta^2 U_1 XB^{-2}(\theta_1)X^\top U_1\|_\infty = O_p\left(\frac{K}{\sqrt{n}}\right).$$

Next, by the interpolation method introduced in Section 7.2 we can show that

$$\frac{\theta^2}{n}E u_1^T XB^{-2}(\theta_1)X^\top u_1 + (1 + \delta_n)\tilde{m}_{\theta_1}(1)$$

$$= \frac{\theta^2}{n}E u_1^T X^0 B_0^{-2}(\theta_1)(X^0)^\top u_1 + (1 + \delta_n)\tilde{m}_{\theta_1}(1) + o\left(\frac{1}{\sqrt{n}}\right),$$

where $B_0(\theta_1) = \theta I - \frac{1}{n}(X^0)^\top U_2^\top \Lambda P U_2 X^0$ and the above equation implies that

$$\|\frac{\theta^2}{n}U_1 X^0 B_0^{-2}(\theta_1)(X^0)^\top U_1 + (1 + \delta_n)\tilde{m}_{\theta_1}(1)I\|_\infty$$

$$= \|\frac{\theta^2}{n}U_1 X^0 B_0^{-2}(\theta_1)(X^0)^\top U_1 + (1 + \delta_n)\tilde{m}_{\theta_1}(1)I\|_\infty + O_p\left(\frac{K}{\sqrt{n}}\right).$$

Moreover, note that

$$E\frac{\theta^2}{n}u_1^T X^0 B_0^{-2}(\theta_1)(X^0)^\top u_1 + (1 + \delta_n)\tilde{m}_{\theta_1}(1)I = \frac{\theta^2}{n}Etr[B_0^{-2}(\theta_1)] + (1 + \delta_n)\tilde{m}_{\theta_1}(1)I.$$

Let $\tilde{\nu}_i$ be the i-th largest eigenvalue of $\theta_1 B_0^{-1}(\theta_1)$. Then we have

$$\frac{\theta^2}{n}Etr[B_0^{-2}(\theta_1)] = \frac{1}{n}E \sum_{i=1}^{n} \tilde{\nu}_i^2.$$

By (7.41) we have $\frac{1}{n}E \sum_{i=1}^{n} \tilde{\nu}_i = -\tilde{m}_{\theta_1}(1) + o\left(\frac{1}{\sqrt{n}}\right)$. Together with the simple fact that $\tilde{\nu}_1 = 1 + O(\sqrt{d_K})$ with high probability, we conclude that there exists such $\delta_n \rightarrow 0$ such that

$$\frac{1}{n}E \sum_{i=1}^{n} \tilde{\nu}_i^2 = -(1 + \delta_n)\tilde{m}_{\theta_1}(1) + o\left(\frac{1}{\sqrt{n}}\right).$$

Up to now, we have shown that

$$E\|\frac{\theta^2}{n} U_1 X^0 B_0^{-2}(\theta_1)(X^0)^\top U_1 + (1 + \delta_n)\tilde{m}_{\theta_1}(1)I\|_\infty = O\left(\frac{K}{\sqrt{n}}\right)$$

and hence

$$E\|\frac{\theta^2}{n} U_1 X B^{-2}(\theta_1)X^\top U_1 + (1 + \delta_n)\tilde{m}_{\theta_1}(1)I\|_\infty = O\left(\frac{K}{\sqrt{n}}\right).$$

10.1.2. Joint Distribution (2.7). This section aims at proving the asymptotic joint distribution of the spiked eigenvalues. i.e. (2.7). By the argument leading to (7.23), we conclude that it suffices to consider the asymptotic joint distribution of

$$\left(\frac{1}{\sqrt{n}} \sum_{k=1}^{n} ((u_1 x_k)^2 - 1), ..., \frac{1}{\sqrt{n}} \sum_{k=1}^{n} ((u_r x_k)^2 - 1)\right), \ r \geq 2.$$
The covariance of the cross term is
\[
\frac{1}{n} \sum_{k=1}^{n} \mathbb{E} \left[ \left( (u_i x_k)^2 - 1 \right) \left( (u_j x_k)^2 - 1 \right) \right] = \frac{1}{n} \left( \sum_{s=1}^{p+l} (\gamma_{4s} - 3) u_i^2 u_j^2 \right)
\]
\[
\rightarrow \lim_{n \to \infty} \sum_{s=1}^{p+l} (\gamma_{4s} - 3) u_i^2 u_j^2 = \sigma_{ij}.
\]

11. PROOF OF LEMMA 1

Proof. Recalling \( A = I - \frac{1}{n} X^T \tilde{\Sigma}_1 X \), let \( A_Y = I - \frac{1}{n} YX^T \tilde{\Sigma}_1 XY \) and \( A_{(Y)} = I - \frac{1}{n} X^T \tilde{\Sigma}_1 XY \). By Theorem 2.4, it suffices to show that
\[
\frac{1}{n} (w_i^T X A_{(Y)}^{-1} X^T w_1 - w_i^T X Y A_Y^{-1} YX^T w_1) I(F_d) = o_{L_1}(1/\sqrt{n}),
\]
\[
\frac{1}{n} (w_i^T X A_{(Y)}^{-1} X^T w_2 - w_i^T X Y A_Y^{-1} YX^T w_2) I(F_d) = o_{L_1}(1/\sqrt{n}),
\]
where \( \tilde{\Sigma}_1 = \frac{\Sigma}{\tilde{\Sigma}_1} \). We prove (11.1) and (11.2) can be shown similarly. In the following proof we also omit \( I(F_d) \) to simplify notation. First of all, we have
\[
\frac{1}{n} \left( w_i^T X A_{(Y)}^{-1} X^T w_1 \right) = \frac{1}{n} \left( w_i^T X A_Y^{-1} X^T w_1 \right)
\]
\[
- \frac{2}{n^2} w_i^T X 11^T A_Y^{-1} 11^T X^T w_1 + \frac{2}{n^2} w_i^T X 11^T A_Y^{-1} 11^T X^T w_1.
\]

Let \( \Delta = \frac{1}{n} YX^T \tilde{\Sigma}_1 XY A_Y^{-1} \). It is easy to see that
\[
\frac{1}{n} A_Y^{-1} = \frac{1}{n} I + \Delta,
\]
and \( \| \Delta \| = o(\frac{1}{n}) \). It follows that
\[
\frac{2}{n^2} w_i^T X 11^T A_Y^{-1} X^T w_1 = \frac{2}{n^2} w_i^T X 11^T X^T w_1 + \frac{2}{n^2} w_i^T X 11^T \Delta X^T w_1.
\]

A direct calculation indicates that
\[
\frac{2}{n^2} E \left[ w_i^T X 11^T X^T w_1 \right] = \frac{2}{n^2}.
\]

Holder’s inequality ensures that
\[
\frac{2}{n^2} E \left| w_i^T X 11^T \Delta X^T w_1 \right| \leq \frac{2}{n^2} \sqrt{E \left[ w_i^T X 11^T X^T w_1 \right]} \sqrt{E \left[ w_i^T X \Delta 11^T \Delta X^T w_1 \right]} = o(1/\sqrt{n}).
\]

Therefore,
\[
\frac{2}{n^2} w_i^T X 11^T A_Y^{-1} X^T w_1 = o_{L_1}(1/\sqrt{n}).
\]
Similarly, we have
\[
\frac{2}{n^3} w_1^T X 1^T \Sigma_1^{-1} 1^T X^T w_1 = o_{L_1}(1/\sqrt{n}).
\]
In view of (11.3), it remains to show that
\[
(11.6) \quad \frac{1}{n} w_1^T X A^{-1}_Y X^T w_1 - \frac{1}{n} w_1^T X A^{-1} X^T w_1 = o_{L_1}(1/\sqrt{n}).
\]
It is not hard to see that
\[
(11.7) \quad \frac{1}{n} A^{-1}_Y - \frac{1}{n} A^{-1} = \frac{1}{n^2} A^{-1} (\frac{1}{n^2} 11^T X^T \Sigma_1 X 11^T - \frac{1}{n} 11^T X^T \Sigma_1 X - X^T \Sigma_1 X \frac{1}{n} 11^T) A^{-1}.
\]
By (11.7), consider one term in the left hand side of (11.6) first, i.e.
\[
(11.8) \quad \frac{1}{n} w_1^T X A^{-1}_Y 11^T X^T \Sigma_1 X A^{-1} X^T w_1.
\]
By the property that $T 1 = 0$ and $Y^2 = Y$, we have
\[
\frac{1}{n} A^{-1}_Y = \frac{1}{n} \sum_{k=0}^{\infty} (\frac{1}{n} Y X^T \Sigma_1 X Y)^k = 1.
\]
It follows from (11.4) that
\[
\mathbb{E}(11.8) = \frac{1}{n^3} \mathbb{E}[w_1^T X 1^T X^T \Sigma_1 X A^{-1} X^T w_1] \leq \frac{1}{n^3} \sqrt{\mathbb{E}(w_1^T X 1)^2} \sqrt{\mathbb{E}(1^T X^T \Sigma_1 X A^{-1} X^T w_1)^2} = o(1/\sqrt{n}).
\]
Similar to (11.9), one can prove
\[
\frac{1}{n^3} w_1^T X A^{-1}_Y 11^T X^T \Sigma_1 X 11^T A^{-1} X^T w_1 = o_{L_1}(1/\sqrt{n}).
\]
For the remaining term of (11.7)
\[
\frac{1}{n} w_1^T X (n I - Y X^T \Sigma_1 X Y)^{-1} X^T \Sigma_1 X 11^T (n I - X^T \Sigma_1 X)^{-1} X^T w_1,
\]
Similar to (11.9), it suffices to show
\[
(11.10) \quad \frac{1}{n} w_1^T X A^{-1} = O_{L_1}(1/\sqrt{n}).
\]
Actually, applying the same strategy as in (7.6)-(7.24), we can prove that
\[
(11.11) \quad \frac{1}{n} w_1^T X A^{-1} 1 I(F_d) - \frac{1}{n} \mathbb{E} w_1^T X A^{-1} 1 I(F_d) = O_{L_1}(1/\sqrt{n}).
\]
Moreover, applying the strategy of Section 7.2, one can show that
\[
(11.12) \quad \frac{1}{n} \mathbb{E} w_1^T X A^{-1} 1 I(F_d) = O(1/\sqrt{n}).
\]
The detailed proof of (11.11) and (11.12) is omitted since it is even simpler than that of Theorem 2.4.
12. RELAX ASSUMPTION 7: TRUNCATION AND CENTRALIZATION

This section is to truncate and centralize $x_{ij}$. By assumption 1, there exists a positive sequence $\delta_n$ satisfying
\begin{equation}
\lim_{n \to \infty} \frac{1}{np\delta_n^4} \sum_{i=1}^{p+l} \sum_{j=1}^{n} \mathbb{E}|x_{ij}|^4 I(|x_{ij}| > \delta_n \sqrt{np}) = 0, \quad \delta_n \downarrow 0, \quad \delta_n \sqrt{np} \uparrow \infty.
\end{equation}

We first truncate $x_{ij}$ to $\hat{x}_{ij} = x_{ij}I(|x_{ij}| < \delta_n \sqrt{np})$ and then get the centralized version $\hat{x}_{ij} = \frac{\hat{x}_{ij} - \hat{\mathbb{E}}x_{ij}}{\sigma_i}$, where $\sigma_i$ is the standard deviation of $\hat{x}_{ij}$. It is easy to see that
\begin{equation}
\mathbb{P}(X \neq \hat{X}) \leq \sum_{i=1}^{p+l} \sum_{j=1}^{n} \mathbb{E}(|x_{ij}| \geq \delta_n \sqrt{np})
\end{equation}
\begin{equation}
\leq \frac{C}{np\delta_n^4} \sum_{i=1}^{p+l} \sum_{j=1}^{n} \mathbb{E}|x_{ij}|^4 I(|x_{ij}| > \delta_n \sqrt{np}) \to 0.
\end{equation}

It follows that
\begin{equation}
\mathbb{P}(U_1X(\lambda I - \frac{1}{n}X^T \Sigma X)^{-1}X^TU_1^T \neq U_1\hat{X}(\lambda I - \frac{1}{n}\hat{X}^T \Sigma \hat{X})^{-1}\hat{X}^TU_1^T) \to 0.
\end{equation}

For convenience, define $B_X(x) = x - \frac{1}{n}x^T \Sigma X$. Hence with probability tending to 1, the proofs of the above theorems based on (10.7) are equivalent to
\begin{equation}
\det(\Lambda^{-1} - \frac{1}{n}U_1\hat{X}B_X(\lambda I^{-1}X^TU_1^T) = 0.
\end{equation}

Note that
\begin{equation}
|1 - \sigma_i^2| \leq 2|\mathbb{E}(x_{ij}^2)I(|x_{ij}| > \delta_n \sqrt{np})|
\leq 2(np)^{-1/2} \delta_n^{-2} \mathbb{E}|x_{ij}|^4 I(|x_{ij}| > \delta_n \sqrt{np}),
\end{equation}
\begin{equation}
|\mathbb{E}\hat{x}_{ij}| \leq \delta_n^{-3} (np)^{-3/4} \mathbb{E}|x_{ij}|^4 I(|x_{ij}| > \delta_n \sqrt{np}),
\end{equation}

and
\begin{equation}
\frac{1}{n} \mathbb{E} tr(\hat{X} - \hat{X})(\hat{X} - \hat{X})^T \leq \sum_{i=1}^{p+l} \sum_{j=1}^{n} \mathbb{E}|\hat{x}_{ij} - x_{ij}|^2
\leq \frac{C}{n} \sum_{i=1}^{p+l} \sum_{j=1}^{n} \frac{(1 - \sigma_i^2)^2}{\sigma_i^2} \mathbb{E}|x_{ij}|^2 + \frac{1}{\sigma_i^2} \mathbb{E}|\hat{x}_{ij}|^2 = o\left(\frac{1}{n}\right).
\end{equation}

By (12.4), (12.5) and (12.6), replacing $\hat{X}$ by $X$, it is easy to show the perturbation is $o_p(Kn^{-1/2})$, which means that
\begin{equation}
\frac{1}{n} \|U_1\hat{X}B_X(\lambda I^{-1}X^TU_1^T) - U_1\hat{X}B_X(\lambda I^{-1}X^TU_1^T)\|_\infty = o_p(Kn^{-1/2} \mu_i^{-1}),
\end{equation}
and
\begin{equation}
\frac{1}{n} \|U_i^T\hat{X}B_X(\lambda I^{-1}X^TU_i^T) - U_i^T\hat{X}B_X(\lambda I^{-1}X^TU_i^T)\|_\infty = o_p(n^{-1/2} \mu_i^{-1}).
\end{equation}
Therefore, (10.7) can be rewritten as
\begin{equation}
\det (\Lambda_1^{-1} - \mu U_1 \hat{X} B_n (\lambda_i)^{-1} \hat{X}^T U_1^T + o_p(Kn^{-1/2} \mu_1^{-1})(11^T - e_i e_i^T) + o_p(n^{-1/2} \mu_1^{-1})e_i e_i^T) = 0,
\end{equation}
where \(o_p(.)\) is the entry wise order. One should notice that we deal with \((1/2) U_1 \hat{X} B_n (\lambda_i)^{-1} \hat{X}^T U_1^T)_{ii}\) independently with the other entries and hence we have the order \(o_p(n^{-1/2} \mu_1^{-1})e_i e_i^T\).

From the proof of Theorem 2.2, it is not hard to find out that the terms involving \(o_p(Kn^{-1/2})\) are negligible and does not affect CLT (see (10.12)), which means that we can prove Theorem 2.2 from the following equality
\begin{equation}
\det (\mu_1 \Lambda_1^{-1} - \mu U_1 \hat{X} (\lambda_i I - \hat{X}^T \Sigma \hat{X})^{-1} \hat{X}^T U_1^T) = 0.
\end{equation}

Checking on the proof of Theorem 2.2, all arguments hold for \(\hat{X}\) as well. Up to now, we have relaxed Assumption 7 and finish this section.

13. PROOF OF THEOREM 2.3.

The proof of Theorem 2.3 is almost the same as that of Theorem 2.2. We illustrate the joint distribution of the first \(n_1\) eigenvalues as an example. Checking on the proof of Theorems 2.2 and 2.4 carefully, we can get the following equality similar to (10.12)
\begin{equation}
\theta_1 \Lambda S^{-1} - \frac{\theta_1}{n} U_1 X B^{-1}(\theta_1) X^T U_1^T
\end{equation}

where \(\bar{S}_n\) is a \(n_1 \times n_1\) matrix such that \(\sqrt{n} \bar{S}_n \Rightarrow \mathcal{R}_1\). Here \(\mathcal{R}_1\) follows normal distribution with \(E \mathcal{R}_1 = 0\) and the covariance of the \((\mathcal{R}_1)_{k_1 l_1}\) and \((\mathcal{R}_1)_{k_2 l_2}\) is \(\lim_{n \to \infty} N^2 \times Cov(u_{k_1}^T x u_{l_1}^T x, u_{k_2}^T x u_{l_2}^T x)\). The asymptotic distribution of \(\mathcal{R}_1\) is ensured by the fact that the upper left \(n_1 \times n_1\) block of \(\theta_1 \Lambda S^{-1} - \frac{\theta_1}{n} U_1 X B^{-1}(\theta_1) X^T U_1^T\) is constructed by the entries with the expressions similar to (2.15) or (2.16). Therefore, by the Skorokhod strong representation and the corresponding arguments similar to page 464-465 of [6] we conclude Theorem 2.3.

14. PROOF OF THEOREM 4.1

Proof. Without loss of generality, we only consider the first spiked eigenvalue \(\lambda_1\). The other spiked eigenvalues \(\lambda_2, \ldots, \lambda_K\) can be handled similarly. By Cauchy’s integral theorem and the residue theorem, with high probability, we have
\[v_1^T \xi_1 v_1 \xi_1^T v_1 = - \frac{1}{2\pi i} \oint_{\Pi} v_1^T \hat{G}(z) v_1 dz,\]
where \(\hat{G}(z) = (S_n - z I)^{-1}\) and \(\Pi\) is a contour enclosing \(\lambda_1\) but the other eigenvalues \(\lambda_i\). The existence of the contour \(\Pi\) is ensured by Theorem 2.1 and Assumption 3.
In the sequel, we directly work on the integral \(-\frac{1}{2\pi i} \oint_{\Pi} \hat{G}(z) dz\). Write
\[
(14.1) \quad v_1^T \hat{G}(z)v_1 = v_1^T (S_n - z I)^{-1} v_1 = e_1^T \left( \frac{1}{n} \Lambda_1^{1/2} UXX^T \Lambda_1^{1/2} - z I \right)^{-1} e_1
\]

\[
= \left( \frac{1}{n} \lambda_1^2 u_1^T XX^T u_1 - z \right)^{-1} = \left( \frac{1}{n} \lambda_1^{1/2} u_1^T XX^T \tilde{U}_2 XX^T u_1 - z I \right)^{-1}
\]

\[
= \left( \frac{1}{n} \lambda_1 u_1^T XX^T u_1 - z \right)^{-1} = \left( \frac{1}{n} \lambda_1^{1/2} u_1^T XX^T \tilde{U}_2 XX^T u_1 - z I \right)^{-1}
\]

The aim is to prove \(\frac{1}{n} \lambda_1 u_1^T XX^T \tilde{U}_2 XX^T \tilde{U}_2 XX^T u_1 - z I\)^{-1} converges to 0 in probability. Not that \(\Lambda_2\) contains the remaining \(K-1\) spiked eigenvalues and the other non-spiked eigenvalues. Moreover, the non-spiked eigenvalues are all dominated by \(z\). Hinted by this observation, we write \(\Lambda_2 = \begin{pmatrix} \Lambda_{21} & 0 \\ 0 & \Lambda_p \end{pmatrix}\)

and \(\tilde{U}_2 = \begin{pmatrix} U_{21} \\ U_2 \end{pmatrix}\), where \(\Lambda_{21}\) is \((K-1) \times (K-1)\) diagonal matrix and \(U_{21}\) is the corresponding \((K-1) \times (p + l)\) eigenvector matrix. It follows that
\[
\left( \frac{1}{n} \Lambda_{21}^{1/2} \tilde{U}_2 XX^T \tilde{U}_2^{T} \Lambda_{21}^{1/2} - z I \right)^{-1} = \left( \frac{1}{n} \Lambda_{21}^{1/2} U_{21} XX^T U_{21}^{T} \Lambda_{21}^{1/2} - z I \right)^{-1}
\]

\[
= \left( \begin{pmatrix} A & B \\ B^T & C \end{pmatrix} \right)^{-1} = \begin{pmatrix} (A - BC^{-1}B^T)^{-1} & -(A - BC^{-1}B^T)^{-1}BC^{-1} \\ -C^{-1}B^T(A - BC^{-1}B^T)^{-1} & C^{-1} + C^{-1}B^T(A - BC^{-1}B^T)^{-1}BC^{-1} \end{pmatrix}
\]

(14.2)

where \(A, B\) and \(C\) are defined in an obvious way. By the definitions of \(A, B\) and \(C\) and the choice of \(\Pi\), it is easy to see that
\[
\|\Lambda_{21}^{-1/2} B\| = O_p(\sqrt{\frac{p}{n}}), \|C\| = O_p(1)
\]

and
\[
\|C^{-1}\| = O_p(\frac{1}{|z|}).
\]

Moreover, \(\|A - \Lambda_{21} + z I\| = o_p(1)\) since the dimension of \(A\) is \((K-1) \times (K-1)\). By (14.2), a straight forward calculation for block matrices yields
\[
X^T \tilde{U}_2^{T} \Lambda_{21}^{1/2} \frac{1}{n} \Lambda_{21}^{1/2} \tilde{U}_2 XX^T \tilde{U}_2^{T} \Lambda_{21}^{1/2} - z I \Lambda_{21}^{1/2} \tilde{U}_2 X
\]

\[
= X^T U_{21}^{T} \Lambda_{21}^{1/2} (A - BC^{-1}B^T)^{-1} \Lambda_{21}^{1/2} U_{21} X - X^T U_{21}^{T} \Lambda_{21}^{1/2} (A - BC^{-1}B^T)^{-1} BC^{-1} \Lambda_{21}^{1/2} U_{21} X
\]

\[
- X^T U_{21}^{T} \Lambda_{21}^{1/2} C^{-1} B^T (A - BC^{-1}B^T)^{-1} \Lambda_{21}^{1/2} U_{21} X
\]

\[
+ X^T U_{21}^{T} \Lambda_{21}^{1/2} (C^{-1} + C^{-1}B^T(A - BC^{-1}B^T)^{-1}BC^{-1}) \Lambda_{21}^{1/2} U_{21} X.
\]

Although the expression of (14.5) is complicated, it is not hard to conclude that all terms at the right hand side of (14.5) are \(o_p(1)\) in terms of the spectral norm. For
instance, we calculate one term \( X^T U_{21}^T A_{21}^{1/2} (A - BC^{-1}B^T)^{-1} A_{21}^{1/2} U_{21} X \). Note that
\[
\|A_{21}^{1/2} (A - BC^{-1}B^T)^{-1} A_{21}^{1/2}\| (14.6)
\]
with probability tending to 1, where we use the fact that \( A_{21}^{-1/2} B = \frac{1}{n} U_{21} X X^T U_{21}^T A_{21}^{1/2} \) and therefore \( \|A_{21}^{-1/2} B C^{-1} B^T A_{21}^{-1/2}\| = o_p(1) \) by (14.3)-(14.4). Hence,
\[
\frac{1}{n^2} u_i^T XX^T \tilde{U}_2 \tilde{A}_2 \frac{1}{n} u_i^T XX^T \tilde{U}_2 \tilde{A}_2 - z I) - 1 \|A_{21}^{1/2} \tilde{U}_2 XX^T u_1 \| (14.7) \leq o_p(\frac{1}{n^2} u_i^T XX^T U_{21} XX^T u_1) + o_p(1).
\]
By the fact that the rank of \( U_{21} \) is \( K - 1 \) and \( u_i^T U_{21}^T = 0 \), it suffices to consider such a term \( u_i^T XX^T u_2 u_3^T XX^T u_1 \), where \( u_i^T u_2 = u_i^T u_3 = 0 \). Since \( \frac{1}{n} E u_i^T XX^T u_2 u_3^T XX^T u_1 = O(n^{-1}) \), we conclude that
\[
(14.8) \frac{1}{n^2} \|u_i^T XX^T U_{21} XX^T u_1\| = \frac{1}{n^2} E u_i^T XX^T U_{21} U_{21} XX^T u_1 = O(\frac{K^2}{n}).
\]
Combining (14.2)-(14.8), we get that (14.1) \( \sim (\lambda_1 - z)^{-1} \) with probability tending to one. Noticing that (14.7) holds uniformly for \( z \in \Gamma \), we have (14.1) \( \sim (\lambda_1 - z)^{-1} \) holds uniformly for \( z \in \Gamma \), i.e. with probability tending to one and for all \( z \in \Gamma \), we have
\[
(14.9) v_i^T \xi_1 \xi_1^T v_1 \to 1.
\]

15. Proof of Corollary 2

Without loss of generality, we assume eigenvectors are real, otherwise we consider \( \sum_{j=1}^p |v_{ij}|^4 \). Since \( \xi_i \) and \( -\xi_i \) are regarded as the same eigenvectors in the eigenvector space, we always choose the direction such that \( v_i^T \xi_1 \geq 0 \). Therefore, by (14.9) we have
\[
v_i^T \xi_1 \xrightarrow{i.p.} 1.
\]
By Theorem 4.1, we have \( \sum_{j=1}^p |v_{ij} - \xi_{ij}|^2 = o_p(1) \), which implies that
\[
\max_j |v_{ij} - \xi_{ij}| = o_p(1).
\]
Therefore, we get
\[
\sum_{j=1}^p |v_{ij}^j - \xi_{ij}^j| \leq \sum_{j=1}^p (|v_{ij}| + |\xi_{ij}|)^3 \max_j |v_{ij} - \xi_{ij}| = o_p(1).
\]
This conclusion tells us that the sample eigenvector is a proper estimation of \( \sum_{j=1}^p |v_{ij}^j| \).
16. Proof of Theorem 2.5

Inspired by [11] and [22] in this section we establish asymptotic distribution of the largest non-spiked eigenvalues of the sample covariance matrices \( \frac{1}{n} \Gamma XX^T \Gamma^T \).

For simplicity and consistency with the papers such as [8] and [22], we absorb the \( \frac{1}{\sqrt{n}} \) into \( X \) and consider the eigenvalues of the matrix \( \Gamma XX^T \Gamma^T \) instead. That is to say, \( \text{var}(x_{ij}) = \frac{1}{n} \) and \( \mathbb{E}|x_{ij}|^k \leq \frac{C}{n^{\frac{k}{2}}} \). Without loss of generality, we assume that \( \mu_{K+1} > 1 \). Correspondingly, \( \nu_i \) is the \( i \)-th largest eigenvalue of \( X^T \Sigma_1 X \) in this section. Let \( D(z) = zI - X^T U_1^T \Lambda_p U_2 X \). As the first step of the proof of Theorem 2.5, by (10.6), we have the following Lemma.

**Lemma 2.** If \( \lambda \) is not the eigenvalue of \( X^T \Sigma_1 X \), then \( \lambda \) is the eigenvalue of \( \Gamma XX^T \Gamma^T \) equivalent to

\[
\det(I - A_S^{1/2} U_1 XD^{-1}(\lambda) X^T U_1^T \Lambda_S^{1/2}) = 0.
\]

In order to show the eigenvalue sticking, we need to prove the local law for

\[
(16.1) \quad U_1 XD^{-1}(z) X^T U_1^T,
\]

where \( U_1 U_2^T = 0 \). First of all, we consider the special case \( l = 0 \). To this end, we introduce the following linearization matrix

\[
(16.2) \quad H(z) := \begin{pmatrix}
\frac{z}{n} I & X^T U_2^T \Lambda_p^{1/2} & X^T U_1^T \\
A_p^{1/2} U_2 X & I & 0 \\
U_1 X & 0 & I
\end{pmatrix}^{-1}
\]

where the last equality follows from the assumption that \( L = 0 \) and \( \tilde{\Sigma} = \begin{pmatrix} \Lambda_p & 0 \\ 0 & 1 \end{pmatrix} \).

By simple calculation, it is easy to see that the lower right block of \( H(z) \) is equal to \((I - U_1 XD^{-1}(z) X^T U_1^T)^{-1} \). We introduce a definition before giving the local law.

**Definition 1.** Let

\( \xi = \{\xi^{(N)}(u) : N \in \mathbb{N}, u \in U^{(N)}\}, \quad \zeta = \{\zeta^{(N)}(u) : N \in \mathbb{N}, u \in U^{(N)}\} \)

be two families of nonnegative random variables, where \( U^{(N)} \) is a parameter set (can be either dependent on or independent of \( N \)). If for all small positive \( \epsilon \) and \( \sigma \), there exists a number \( N(\epsilon, \sigma) \) only depending on \( \epsilon \) and \( \sigma \) such that

\[
\sup_{u \in U^{(N)}} \mathbb{P} \left[ |\xi^{(N)}(u)| > N^\epsilon |\zeta^{(N)}(u)| \right] \leq N^{-\sigma}
\]

for large enough \( n \geq n(\epsilon, \sigma) \), then we say that \( \zeta \) stochastically dominates \( \xi \) uniformly in \( u \). We denote this relationship by \( \xi \prec \zeta \) or \( \xi = O_\prec(\zeta) \). Moreover, if there exists a constant \( C \) such that \( C^{-1} \leq \frac{\xi}{\zeta} \leq C \), then we say \( \xi \sim \zeta \).
By Theorem 3.7 of [24], we conclude that

\[(16.3) \quad \| (I - U_1 XD^{-1}(z)X^T U_1^T)^{-1} - (I + m_{\Sigma_1}(z))^{-1} \|_\infty \lesssim \sqrt{\frac{1}{n\kappa(z)}}, \]

where \( m_{\Sigma_1}(z) \) is the unique solution of the following equation

\[(16.4) \quad m_{\Sigma_1}(z) = -\frac{1}{z - \frac{1}{n} tr(I + m_{\Sigma_1}(z)\Sigma_1)^{-1}\Sigma_1}, \quad z \in \mathbb{C}^+, \]

\( \kappa(z) = |\Re z - \gamma_+|, n^{-2/3 + 5\epsilon} \leq |\Re z - \gamma_+| \leq 2\gamma_+ \) and \( \gamma_+ \) is the rightmost end point of the density determined by \( m_{\Sigma_1}(z) \). Similarly, it follows from Theorem 3.6 of [24] that

\[(16.5) \quad \| (I - U_1 XD^{-1}(z)X^T U_1^T)^{-1} - (I + m_{\Sigma_1}(z))^{-1} \|_\infty \lesssim \Phi(z), \]

where \( \Phi(z) = \sqrt{\frac{3m_{\Sigma_1}(z)}{n\kappa(z)}} \), \( \Im z \geq n^{-2/3 - \epsilon} \) and \( -c \leq |\Re z - \gamma_+| \leq n^{-2/3 + 5\epsilon} \) for some small constant \( c \). But this is not enough for the proof since \( z \) is very large when we consider the spiked eigenvalues. We below prove a stronger version of (16.3) instead.

Before doing it, note that our objective is \( U_1 XD^{-1}(z)X^T U_1^T \) instead of \( (I - U_1 XD^{-1}(z)X^T U_1^T)^{-1} \) by (16.1). Therefore, we first need to develop its upper bound from (16.3). By the formula that

\[ A^{-1} - B^{-1} = -A^{-1}(A - B)B^{-1}, \]

we have the following Neumann series

\[(16.6) \quad U_1 XD^{-1}(z)X^T U_1^T + m_{\Sigma_1}(z)I = (I + m_{\Sigma_1}(z)I) - (I - U_1 XD^{-1}(z)X^T U_1^T) = \sum_{r=1}^{\infty} (-1)^{r+1}(1 + m_{\Sigma_1}(z))^r \Delta^r, \]

where \( \Delta = (I - U_1 XD^{-1}(z)X^T U_1^T)^{-1} - (I + m_{\Sigma_1}(z)I)^{-1} \). By (16.3), we know that \( \| \Delta \|_\infty \lesssim \sqrt{\frac{1}{n\kappa}} \). Moreover, by the large deviation bound (see Lemma 3.4 of [9], [11] or [22]) we have

\[(16.7) \quad \| m_{\Sigma_1}(z)U_1XX^TU_1^T - m_{\Sigma_1}(z)I \|_\infty \lesssim \sqrt{\frac{1}{n}}, \]

The expansion at the right hand side of (16.6) is ensured by the fact that \( z \) is very close to or outside the support of \( X^T U_2^T \Lambda_P U_2 X \) and \( \| \Delta \| \ll 1 \). Together with the fact that \( K \ll n^{1/6} \ll \sqrt{n\kappa} \), we conclude that

\[(16.8) \quad \| U_1 XD^{-1}(z)X^T U_1^T + m_{\Sigma_1}(z)U_1^T XX^TU_1 \|_\infty \lesssim \sqrt{\frac{1}{n\kappa}} n^{-2/3 + 5\epsilon} \leq |\Re z - \gamma_+| \leq 2\gamma_+. \]

Up to now, we only show (16.8) holds for the case \( l=0 \). When \( l \neq 0 \), we can find a \( l \times (p + l) \) matrix \( U_3 \) such that \( U_3 U_1^T = 0 \) and \( U_3 U_2^T = 0 \). Let \( \tilde{U}_1 = (U_1^T, U_3^T)^T \).
Since the dimension of $\hat{\mathbf{U}}_1 \mathbf{X}^{-1}(z) \mathbf{X}^T \hat{\mathbf{U}}_1^T$ is $(l + K) \times (l + K)$ and $l + K \ll n^{1/6}$.

Then by similar arguments from (16.3) to (16.8) we have

\begin{equation}
\| \hat{\mathbf{U}}_1 \mathbf{X}^{-1}(z) \mathbf{X}^T \hat{\mathbf{U}}_1^T + m_{\Sigma_1}(z) \hat{\mathbf{U}}_1^T \mathbf{X} \mathbf{X}^T \hat{\mathbf{U}}_1 \|_\infty < \sqrt{\frac{1}{n\kappa}} \ n^{-2/3 + 5\varepsilon} \leq \Re z - \gamma_+ \leq 2\gamma_+.
\end{equation}

This implies that (16.8) also holds for the case $l \ll n^{1/6}$. Similarly, we also have (16.10)

\[\| \hat{\mathbf{U}}_1 \mathbf{X}^{-1}(z) \mathbf{X}^T \hat{\mathbf{U}}_1^T + m_{\Sigma_1}(z) \hat{\mathbf{U}}_1^T \mathbf{X} \mathbf{X}^T \hat{\mathbf{U}}_1 \|_\infty < \Phi(z), \ \exists z \geq n^{-2/3 - \varepsilon}, -\varepsilon \leq \Re z - \gamma_+ \leq n^{-2/3 + 5\varepsilon}.

In the sequel we prove the local law when $z$ is far away from $\gamma_+$.

**Theorem 16.1.** For all $\exists z \geq 0$, $\Re z = t \sim \varphi(n)$ and $\varphi(n) \to \infty$ when $n \to \infty$, we have

\begin{equation}
\| \mathbf{U}_1 \mathbf{X}^{-1}(z) \mathbf{X}^T \mathbf{U}_1^T + m_{\Sigma_1}(z) \mathbf{U}_1 \mathbf{X} \mathbf{X}^T \mathbf{U}_1^T \|_\infty < \frac{1}{\kappa(t) \sqrt{n}}.
\end{equation}

**Proof.** We prove

\[\mathbf{u}_1^T \mathbf{X}^{-1}(t) \mathbf{X}^T \mathbf{u}_1 + m_{\Sigma_1}(t) \mathbf{u}_1^T \mathbf{X} \mathbf{X}^T \mathbf{u}_1 < \frac{1}{\kappa(t) \sqrt{n}}.

as an example. The other entries of (16.11) can be shown similarly. Define

\[m^s(z) = -\mathbf{u}_1^T \mathbf{X}^{-1}(z) \mathbf{X}^T \mathbf{u}_1 - m_{\Sigma_1}(z) \mathbf{u}_1^T \mathbf{X} \mathbf{X}^T \mathbf{u}_1, \quad z \in \mathbb{C}^+, \ \Re z \gg 1,

\text{and}

\begin{equation}
F^s(x) = \sum_{i=1}^n \mathbf{u}_1^T \mathbf{X} \zeta_i \mathbf{X}^T \mathbf{u}_1 I(\nu_i \leq x) - F_0(x)(dx) \mathbf{u}_1^T \mathbf{X} \mathbf{X}^T \mathbf{u}_1,
\end{equation}

where $F_0(x)$ is the c.d.f. determined by $m_{\Sigma_1}(z)$, $\nu_i = \lambda_i(\mathbf{X}^T \Sigma_1 \mathbf{X})$ and $\zeta_i$ is the corresponding eigenvector. Hence, we have the steitjes transform

\begin{equation}
m^s(z) = \int \frac{\rho^s(dx)}{x - z}, \quad \exists z > 0.
\end{equation}

We next apply the Helffer-Sjöstrand formula to the following function

\[f_z(x) = \frac{1}{x - z}.

Let $\omega = x + yi \in \mathbb{C}$. Then define $\frac{\partial f(\omega)}{\partial \omega} = \frac{\partial f(\omega)}{\partial x} + i \frac{\partial f(\omega)}{\partial y}$. In order to apply the Helffer-Sjöstrand formula(referring to [17]), we need to look for a smooth version of $f_z(x)$, i.e. we define a smooth function $\chi(\omega) \in [0, 1], \omega \in \mathbb{C}^+$ satisfying $\frac{\partial \chi(\omega)}{\partial \omega} \leq C$, where $C$ is a constant. We choose a small constant $\omega' > 0$ and require $\chi(\omega) = 1$ for all $\omega$ belongs to $\omega'$-neighbourhood of $[-1, \gamma_+]$ and 0 outside the $2\omega'$-neighbourhood of $[-1, \gamma_+]$. By rigidity of the eigenvalues, i.e. $|\nu_1 - \gamma_+| < n^{-2/3}$, we conclude that $\text{supp} \rho^s \subset (-2\omega', \gamma_+ + 2\omega')$ with high probability. Therefore we can choose
suitable $z$ to be away from the support of $X^T \Sigma_1 X$, i.e. $z > \gamma_+ + 3\omega'$. Then by the Helffer-Sjöstrand formula, we have that for all $x \in \text{supp} \rho$,

$$f_z(x) = \frac{1}{\pi} \int_{\mathbb{C}} \frac{\partial_\omega (f_z(\omega))}{x - \omega} d\omega.$$

By the trivial fact that $\int \rho_s(dx) = 0$, we have

$$m^s(z) = \int \rho_s(dx) f_z(x) = \frac{1}{\pi} \int_{\mathbb{C}} f_z(\omega) \partial_\omega (\chi(\omega)) m^s(\omega) d\omega,$$

where the second equality follows from the fact that $f_z(\omega)$ is analytic away from $\text{supp} \rho$. By the definition of $\chi$, we have

$$\{ \frac{\partial}{\partial \omega} \neq 0 \} \subset \{ \omega : \text{dist}[-1, \gamma_+] \in [\omega', 2\omega'] \}$$

and on this interval we conclude that $|f_z(\omega)| \sim \kappa^{-1}(z)$. Moreover, following from (16.9), we have $m^s(\omega) \prec 1/\sqrt{n}$ in the set $\{ \frac{\partial}{\partial \omega} \neq 0 \}$. Therefore we have

$$m^s(z) \prec \frac{1}{\sqrt{n}} \kappa^{-1}(z).$$

Up to now, we have shown that (16.11) holds when $\Im z > 0$. To complete our proof, let $z = t + in^{-10}$. By the continuity of $m^{\Sigma_1}(z)$ and $X^T U_1^T \Lambda P U_2 X - 2I$, it is easy to conclude (16.11). \hfill \square

Immediately, we can get Corollary 4 from Theorem 16.1.

**Corollary 4.** Under the conditions of Theorem 16.1 we have

$$||U_1 XD^{-1}(t)X^T U_1^T + m_{\Sigma_1}(t)I||_\infty \prec \frac{1}{\kappa(t) \sqrt{n}}. \quad (16.16)$$

**Proof.** This corollary follows from Theorem 16.1 and the large deviation inequality that

$$||m_{\Sigma_1}(t)U_1 XX^T U_1^T - m_{\Sigma_1}(t)I||_\infty \prec \frac{1}{\kappa(t) \sqrt{n}}. \quad \square$$

By the singular value inequality, we have the following Lemma.

**Lemma 3.**

$$\sigma_{K+i}(\Lambda^{1/2}UX) \leq \sigma_i(\Lambda^{1/2}P \Sigma_1 P U_2 X), \quad i = 1, 2, ..., p - K,$$

where $\sigma_j(.)$ represents the $j$-th largest singular value.

In view of Lemma 3, there are at most $K$ spiked eigenvalues. Moreover, we need the eigenvalues of $X^T \Sigma_1 X$ to be distinct. To this end, we assume that the entries of $X$ are all absolutely continues. Otherwise we consider the matrix $X + e^{-n}Y$ instead, where $Y$ is a $(p + l) \times n$ matrix consisting of i.i.d. standard normal random variables. It is easy to see that such a perturbation doesn’t change the desired spectral properties and then the eigenvalues of $(X + e^{-n}Y)^T \Sigma_1 (X + e^{-n}Y)$ are all distinct almost surely.

In the sequel, we assume that the following events hold and all Lemmas below are based on these events:

1. All eigenvalues of $X^T \Sigma_1 X$ are distinct.
2. For all $\alpha = 1, 2, ..., n$, we have $U_1X\zeta_\alpha \neq 0$, where $\zeta_\alpha$ is the eigenvector of $X^T\Sigma_1X$ corresponding to the $\alpha$-th largest eigenvalue.

3. The rigidity result associated with $X^T\Sigma_1X$ holds for $\epsilon/2$ for all $\nu_i \geq \gamma_+ - n^{-2/3+5\epsilon}$, for example $|\nu_1 - \gamma_+| \leq n^{-2/3+\epsilon/2}$ and

$$
(16.17) \quad \|U_1XD^{-1}(z)X^TU_1^T + m\Sigma_i(z)\|_\infty \leq \frac{n^{t/2}}{\kappa(z)\sqrt{n}}, \quad \Re z \gg 1.
$$

Here Claims 1 and 2 hold by the absolutely continuous of the entries of $X$. Claim 3 is guaranteed by Corollary 4 and [8], [24]. In the sequel, define the intervals

$$
I_i = [\mu_i - \mu_i K n^{-1/2+2\epsilon}, \mu_i + \mu_i K n^{-1/2+2\epsilon}], \quad i = 1, ..., K.
$$

$I_0 = [\gamma_+ - n^{-2/3+2\epsilon}, \gamma_+ + n^{-2/3+2\epsilon}]$.

$$
\Gamma(d) = \bigcup_{i=0}^K I_i.
$$

The following proposition is to prove that $\Gamma(d)$ is the permission area for the spiked eigenvalues and the extremal bulk eigenvalues.

**Proposition 2.** Under Assumptions 2 or 5, the following holds:

$$
I_i \cap I_0 = \emptyset, \quad i = 1, ..., K,
$$

and

$$
(16.18) \quad \sigma(\Gamma XX^T \Gamma^T) \bigcap_{\gamma_+ - n^{-2/3+2\epsilon}, \infty} \subset \Gamma(d),
$$

where $\sigma(\Gamma XX^T \Gamma^T)$ represents the set of the eigenvalues of $\Gamma XX^T \Gamma^T$.

**Proof of Proposition 2.** First of all, it is trivial to get $I_i \cap I_0 = \emptyset$, $i = 1, ..., K$ by the definition of $I_i$. Therefore it suffices to show (16.18). We define a $K \times K$ matrix $M(t)$ with its entries being

$$
M_{ij}(t) = (U_1 XD^{-1}(t)X^TU_1^T)_{ij} - \delta_{ij} \mu_i^{-1}.
$$

By Lemma 2, we conclude that $t \in \sigma(\Gamma XX^T \Gamma^T)/\sigma(\Sigma_1^{1/2} XX^T \Sigma_1^{1/2})$ if and only if $M(t)$ is singular. Therefore we focus on the value $t \notin \sigma(\Sigma_1^{1/2} XX^T \Sigma_1^{1/2})$. First we consider the case when $t \geq \gamma_+ + n^{-2/3+2\epsilon}$. By Corollary 4 we have $M(t) = -m\Sigma_1(t)I - \Lambda_S^{-1} + O(\frac{n^{t/2}}{\kappa(t)\sqrt{n}})$, where $A = O(1)$ means $||A||_\infty = O(1)$. On the other hand, for all $t \in [\log \nu_K, \infty] \setminus \bigcup_{i=1}^K I_i$, by $m\Sigma_1(t) = -\frac{1}{2}(1 + o(1))$ we have

$$
\min_{k} \{|m\Sigma_1(t)I + \mu_k^{-1}|, k = 1, ..., K\} \geq \frac{Kn^\epsilon}{\kappa(t)\sqrt{n}}.
$$

Therefore any $t \in [\log \nu_K, \infty] \setminus \bigcup_{i=1}^K I_i$ is not an eigenvalue of $\Gamma XX^T \Gamma^T$ with high probability. Moreover, by Weyl’s inequality, we have

$$
|\sigma_i(\Lambda_1^{1/2} UX) - \sigma_i(\Lambda_S^{1/2} U_1X)| \leq \sigma_1(\Lambda_p^{1/2} U_2X) \sim 1,
$$

which implies that the first $K$ eigenvalues of $\Gamma XX^T \Gamma^T$ do not belong to $[\gamma_+ + n^{-2/3+2\epsilon}, \log \mu_K]$ with high probability by the fact that $\sigma_K(\Lambda_S^{1/2} U_1X) \geq \sqrt{nK}(1 - \ldots
}
Proposition 3. Under Assumption 2, for large enough $n$, each interval $I_i$, $i = 1, \ldots, K$ contains exactly one eigenvalue of $\Gamma XX^T \Gamma^T$.

Proof. We choose a positive oriented contours $C = \bigcup_{i=1}^{K} C_i \subset \mathbb{C} \setminus [\gamma_-, \gamma_+]$ such that each contour $C_i$ encloses $d_i$ but no other points of $\mu_j$, $j \neq i$. Moreover, the radius of each contour enclosing $\mu_i$ is of the same order of $\mu_i$. By Proposition 3, such contours exist. In view of Proposition 2, it suffices to prove that there exists exactly one eigenvalue of $\Gamma XX^T \Gamma^T$ in each contour. Recalling that $M(z)$ in (16.19), we define the following two functions

$$F_n(z) = \det(M(z)), \quad f_n(z) = \det(m_{\Sigma}^1(z)I + \Lambda_S^{-1}).$$

By the definition of $C$, the functions $F_n$ and $f_n$ are holomorphic in $C$. Furthermore, the construction of $C_i$ ensures that each $C_i$ contains exactly one root of $f_n(z) = 0$. For instance, we look at the first contour $C_1$ containing $\mu_1$. For any $z \in C_1$, $\exists z \neq 0$, it is easy to see that $\Im f_n(z) \neq 0$. If $z \in C_1, \Im z = 0$, then $m_{\Sigma}^1(z)$ is an increasing function of $z$. Combining with the fact that $m_{\Sigma}^1(z)I + \Lambda_S^{-1}$ is a diagonal matrix, we conclude that there is only one root of $f_n(z) = 0$ in $C_1$. By (16.17) and Lebniz’s formula for the determinant, it is not hard to see that

$$|f_n(z) - F_n(z)| \leq \frac{K^2 n^{T/2}}{\sqrt{n}} \min_{z \in \partial C_i} |f_n(z)|,$$

which implies that $F_n(z)$ also contains exactly one root of $F_n(z) = 0$ in $C_i$ by Rouché’s theorem. Notice that this arguments hold uniformly for $i = 1, \ldots, K$, by Proposition 2 and $I_i \subset C_i$. We finish our proof. \qed

Similarly, we have

Proposition 4. Under Assumption 5, for large enough $n$, each interval $\bigcup_{j=m_i+1}^{m_{i+1}} I_j = I_{m_i+1}$, $i = 0, \ldots, L$ contains exactly one eigenvalue of $\Gamma XX^T \Gamma^T$.

Assume that $\Gamma XX^T \Gamma^T$ and $\Sigma_1^{1/2} XX^T \Sigma_1^{-1/2}$ do not have the same eigenvalue. Before considering the phase transition, we show the following delocalization result, which is used in the eigenvalue counting arguments.

Lemma 4. Assume that $\zeta_i$ is the eigenvector of $(X^T U_2^T \Lambda_P U_2 X - tI)^{-1}$ corresponding to the eigenvalue $\nu_i \geq \gamma_+ - n^{-2/3 + 5\epsilon}$ for a sufficiently small constant $\epsilon$. We have

$$e_k^T U_1^T X \zeta_i \asymp \frac{1}{\sqrt{n}}.$$

Proof. By (16.8) with $z = v_i + in^{-1+\epsilon}$, $0 < \epsilon$, we have

$$e_k^T U_1^T X D^{-1}(z) X^T U_1^T e_k + m_{\Sigma}_i(z)e_k^T U_1^T X X^T U_1 e_k \asymp \frac{1}{nk} \leq n^{-1/8}.$$
Therefore, with high probability \( e_k^T U_1 XD^{-1}(z) X^T U_1^T e_k = O(1) \). Moreover,

\[
\begin{align*}
(16.21) \quad \exists e_k^T U_1 XD^{-1}(z) X^T U_1^T e_k &= n^{-1+\epsilon} \sum_j e_k^T U_1 X \zeta_j \zeta_j^T X^T U_1^T e_k \\
&\geq n^{-1+\epsilon} \frac{e_k^T U_1 X \zeta \zeta^T X^T U_1^T e_k}{|\nu_k - z|^2} = \frac{(e_k^T U_1^T X \zeta_k)^2}{n^{-1+\epsilon}}.
\end{align*}
\]

Since \( \epsilon \) can be arbitrary small, the proof of this Lemma is complete. \( \square \)

16.1. The Non-spiked eigenvalues. Considering the non-spiked eigenvalues, we prove the following area is forbidden for the eigenvalues of \( \Gamma XX^T \Gamma^T \).

\[
(16.22) \quad t \in [\gamma_+ - n^{-2/3+2\epsilon}, \gamma_+ + n^{-2/3+2\epsilon}], \quad \text{dist}(t, \sigma(\Sigma_1^{1/2} XX^T \Sigma_1^{1/2})) \geq n^{-2/3-2\epsilon}.
\]

Similar to the arguments of Proposition 2, we aim at showing that for \( t \) satisfying (16.22), \( M(t) \) is non singular. Choosing \( \eta = n^{-2/3-\epsilon} \) and \( z = t + i\eta \), we have

\[
(16.23) \quad |(U_1 XD^{-1}(t) X^T U_1^T - U_1 XD^{-1}(z) X^T U_1^T)_{ij}| \\
\leq \sum_{a} \frac{|(X^T U_1^T e_i, \zeta_a)^2 + (X^T U_1^T e_j, \zeta_a)^2|}{2} \left| \frac{1}{\lambda_a - t} - \frac{1}{\lambda_a - z} \right| \\
\leq \sum_{a} \frac{|(X^T U_1^T e_i, \zeta_a)^2 + (X^T U_1^T e_j, \zeta_a)^2|}{2} \frac{\eta}{\eta^2 + (\lambda_a - t)^2} \\
= -3(U_1 XD^{-1}(z) X^T U_1^T)_{ij} - 3(U_1 XD^{-1}(z) X^T U_1^T)_{jj},
\]

where \( \zeta_a \) is the eigenvector of \( X^T \Sigma_1 X \) corresponding to the \( a \)-th largest eigenvalue. Therefore, by local law we have

\[
(16.24) \quad M(t) = -m_{\Sigma_1}(z)I - \Lambda_{S}^{-1} + O(n^{1/3} \gamma_1(z) + \frac{n^{1/2}}{\eta}) = -m_{\Sigma_1}(z)I - \Lambda_{S}^{-1} + O(n^{-1/3+2\epsilon}).
\]

Since \( |m_{\Sigma_1}(z)| \sim 1 \), we have \( |m_{\Sigma_1}(z) + \mu_i^{-1}| \sim 1, \quad i = 1, ..., K \) uniformly. Therefore, it is easy to see that \( M(t) \) is non singular for \( t \) satisfying (16.22). Up to now, we are ready to prove Theorem 2.5.

Actually, once the tools and results including Lemma 2–(16.22) are available, the proof of Theorem 2.5 is almost the same as the proof of Proposition 6.8 in [22]. The only difference is that we only prove that the eigenvalues are sticking with the order \( n^{-2/3-\epsilon} \) instead of \( n^{-1+\epsilon} \), which is caused by allowing \( K \) to tend to infinity. Hence we ignore the details.

The detailed proof is similar to Proposition 6.8 in [22] and thus we omit it.
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