Estimation of the number of spiked eigenvalues in a covariance matrix by bulk eigenvalue matching analysis

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Abstract

The spiked covariance model has gained increasing popularity in high-dimensional data analysis. A fundamental problem is determination of the number of spiked eigenvalues, $K$. For estimation of $K$, most attention has focused on the use of top eigenvalues of sample covariance matrix, and there is little investigation into proper ways of utilizing bulk eigenvalues to estimate $K$. We propose a principled approach to incorporating bulk eigenvalues in the estimation of $K$. Our method imposes a working model on the residual covariance matrix, which is assumed to be a diagonal matrix whose entries are drawn from a gamma distribution. Under this model, the bulk eigenvalues are asymptotically close to the quantiles of a fixed parametric distribution. This motivates us to propose a two-step method: the first step uses bulk eigenvalues to estimate parameters of this distribution, and the second step leverages these parameters to assist the estimation of $K$. The resulting estimator $\hat{K}$ aggregates information in a large number of bulk eigenvalues. We show the consistency of $\hat{K}$ under a standard spiked covariance model. We also propose a confidence interval estimate for $K$. Our extensive simulation studies show that the proposed method is robust and outperforms the existing methods in a range of scenarios. We apply the proposed method to analysis of a lung cancer microarray data set and the 1000 Genomes data set.

Keywords. Empirical null; factor model; Kaiser’s criterion; latent dimension; Machenko-Pastur distribution; parallel analysis; Principal Component Analysis; unsupervised learning.

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1 Introduction

The spiked covariance model [Johnstone 2001] has been widely used to model the covariance structure of high-dimensional data. In this model, the population covariance matrix has $K$ large eigenvalues, called spiked eigenvalues, where $K$ is presumably much smaller than the dimension. Estimation of $K$ is of great interest in practice, as it helps determination of the latent dimension of data. For example, in a clustering model with $K_0$ clusters [Jin et al. 2017], the pooled covariance matrix has $(K_0 - 1)$ spiked eigenvalues; therefore, an estimate of $K$ tells the number of clusters. Similarly, in Genome-Wide Association Studies (GWAS), the number of spiked eigenvalues of a genetic covariance matrix reveals the number of ancestry groups in the study [Patterson et al. 2006]. In high-dimensional covariance matrix estimation, $K$ is often required as input for factor-based covariance estimation [Fan et al. 2013].

In this paper, we assume the data vectors $\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_n \in \mathbb{R}^p$ are independently generated from a multivariate distribution with covariance matrix $\Sigma \in \mathbb{R}^{p \times p}$, which has positive values $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_K$ and mutually orthogonal unit-norm vectors $\xi_1, \xi_2, \ldots, \xi_K \in \mathbb{R}^p$ such that

$$\Sigma = \sum_{k=1}^{K} \mu_k \xi_k \xi_k^\top + D,$$

(1)

Here, $D$ is called the residual covariance matrix. The goal is to estimate $K$ from $\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_n$.

We are primarily interested in the settings where $K$ is finite and $p/n \to \gamma$, for a constant $\gamma > 0$. Throughout the paper, we denote by $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_p$ the eigenvalues of $\Sigma$, and denote by $\hat{\lambda}_1 \geq \hat{\lambda}_2 \geq \ldots \geq \hat{\lambda}_n$ the nonzero eigenvalues of the sample covariance matrix.

In the literature, there are several approaches for estimating $K$. The first is the information criterion approach, which finds $\hat{K}$ that minimizes an objective of the form $L_n(K) + P_n(K)$, where $L_n(K)$ is a measure of goodness-of-fit and $P_n(K)$ is a penalty on $K$. An influential work is Bai and Ng (2002), who let $L_n(K)$ be the sum of squared residuals after fitting a $K$-factor model and studied a few choices of the penalty function $L_n(K)$. Other examples include Wax and Kailath (1985), where $L_n(K)$ is a function of the arithmetic and geometric means of $(n - K)$ smallest eigenvalues. However, the information criterion approach requires the spiked eigenvalues to be sufficiently large. In Bai and Ng (2002), the spiked eigenvalues are at the order of $p$, which is much larger than the necessary order. It has been recognized that correct estimation of $K$ is possible even when the spiked eigenvalues are at the constant order [Baik et al. 2005].

The second approach finds a big “gap” between eigenvalues of the sample covariance matrix. Recall that $\hat{\lambda}_k$ is the $k$th eigenvalue of the sample covariance matrix. Onatski (2009) introduced a test statistic, $\max_{K_0 < k \leq K_{\max}} (\hat{\lambda}_i - \hat{\lambda}_{i+1})/(\hat{\lambda}_{i+1} - \hat{\lambda}_{i+2})$, for testing against the null hypothesis $K = K_0$ and then applied it sequentially to estimate $K$. Cai et al. (2019) proposed an iterative algorithm for estimating $K$ that searches for a gap of $\gtrsim O(n^{-2/3})$ between eigenvalues. Such methods rely on sharp limiting distributions of the first $K$ empirical eigenvalues, which
theoretically requires the magnitude of the spiked eigenvalues to tend to infinity. Additionally, while utilizing eigengap is a neat idea in theory, its practical use is challenging, since the actual eigengaps in many real data sets are slowly varying, without a clear cut.

The last approach estimates $K$ by thresholding the empirical eigenvalues. For this approach, the key is to calculate a proper data-driven threshold. The threshold should reflect the “scaling” of the residual matrix $D$. One idea is to first standardize the data matrix so that each variable has a unit variance and then use a scale-free threshold. Examples include the empirical Kaiser’s criterion (Bräken and Van Assen 2017) and parallel analysis (Horn 1965), where the scale-free threshold is determined by asymptotic behavior of the largest eigenvalue of sample covariance matrix associated with $X_i \overset{iid}{\sim} N(0, I_p)$. Another idea is to estimate $D$ by the diagonal of the sample covariance matrix and then calculate the threshold via a deterministic algorithm (Dobriban 2015). The success of both ideas rely on regularity conditions to ensure that the low-rank part in Model (1) has a negligible effect on the diagonal of $\Sigma$; for example, the population eigenvalues cannot be enormously large and the population eigenvectors have to satisfy “delocalization” conditions. Dobriban and Owen (2019) improved the algorithm in Dobriban (2015) by a recursive procedure to remove leading eigenvalues and eigenvectors, but their method still requires some “delocalization” conditions on eigenvectors. Other related work includes Onatski (2010), which used a convex combination of $\hat{\lambda}_{K_{\max}+1}$ and $\hat{\lambda}_{2K_{\max}+1}$ as the threshold, and Fan et al. (2019), which introduced an unbiased estimator for each of the first few eigenvalues of the population correlation matrix, and estimated $K$ by thresholding these unbiased estimators at $1 + \sqrt{p/n}$.

To address the limitations of these methods, we propose a new estimator of $K$. Different from the existing work, our attention is largely focused on how to better utilize the bulk empirical eigenvalues in the estimation of $K$, especially those eigenvalues in the middle range:

$$\{\hat{\lambda}_k : \alpha(n \wedge p) \leq k \leq (1-\alpha)(n \wedge p)\}, \text{ for some constant } \alpha \in (0,1/2).$$

It is well-known in random matrix theory that these bulk eigenvalues are almost not affected by the low-rank part in Model (1) (e.g., see Bloemendal et al. (2016)). We can use these eigenvalues to gauge the “scaling” of $D$ and determine an appropriate threshold for top eigenvalues. To this end, we impose a working model on the diagonal matrix $D$. Let $\text{Gamma}(a, b)$ denote the gamma distribution with shape parameter $a$ and rate parameter $b$. Fixing $\sigma > 0$ and $\theta > 0$, we assume

$$\sigma_j^2 \overset{iid}{\sim} \text{Gamma}(\theta, \theta/\sigma^2), \quad 1 \leq j \leq p. \quad (2)$$

The mean and variance of $\text{Gamma}(\theta, \theta/\sigma^2)$ is $\sigma^2$ and $\sigma^4/\theta$, respectively. As a result, the diagonal entries of $D$ are centered around $\sigma^2$, where the level of dispersion is controlled by $\theta$. As $\theta \to \infty$, $\text{Gamma}(\theta, \theta/\sigma^2)$ converges to a point mass at $\sigma^2$, and it yields $D = \sigma^2 I_p$. This case corresponds to the standard spiked covariance model which is frequently studied in the literature (Johnstone, 2001).
Combining Model (2) with Model (1), we now have a flexible spiked covariance model that includes the standard spiked covariance model as a special case.

Under Models (1)-(2), the empirical spectral distribution (ESD) converges to a limit, which is a fixed distribution with two parameters \((\sigma^2, \theta)\) (Silverstein 2009). Since the empirical eigenvalues are nothing but quantiles of the ESD, we expect that all the bulk eigenvalues are asymptotically close to the corresponding quantiles of the limit of ESD. We thus estimate \((\sigma^2, \theta)\) by minimizing the sum of squared differences between bulk eigenvalues and quantiles of the limiting distribution. Once \((\hat{\sigma}^2, \hat{\theta})\) are available, we borrow the idea of parallel analysis (Horn 1965) to decide a threshold for the top eigenvalues by Monte Carlo sampling. This gives rise to a new method for estimating \(K\), which we call \textit{bulk eigenvalue matching analysis} (BEMA). Analogous to the orators’ bema in Athens, our BEMA is a platform for gathering a large number of bulk eigenvalues and utilizing them efficiently in the estimation of \(K\). Additional to the point estimator, we also propose a confidence interval for \(K\).

Our method has an intuitive explanation in terms of a scree plot. Figure 1 shows the scree plot of a simulated example. There are multiple elbow points, and it is hard to decide where the true \(K\) is. The core idea of our method is to explore the “shape” of the scree plot in the middle range and fit it with a parametric curve; this curve is determined by the theoretical quantiles of the limit of ESD, governed by two parameters \(\sigma^2\) and \(\theta\). Then, this curve can be extended to the left boundary of the scree plot to produce a threshold for top eigenvalues.

The goodness-of-fit check of Model (2) on real datasets can also be done via the scree plot. If the middle range of the scree plot can be well approximated by the estimated parametric curve, then it suggests that the model indeed fits the real data. In Section 6 we shall see that Model (2) is well suited to gene microarray data and GWAS data. We remark that assuming the diagonal entries of \(D\) are generated from a fixed distribution is only a mild assumption. Similar conditions appear in the literature (often implicitly as regularity conditions in the theory); e.g., Dobriban and Owen (2019) and Fan et al. (2019) assume that the histogram of population eigenvalues...
of $D$ converges to a fixed limit. Here, we make one step ahead by assuming that this fixed distribution is a gamma distribution. At the first glance, restricting to the gamma family seems restrictive, but Model (2) is in fact much more flexible than what one expects. With only two parameters ($\sigma^2, \theta$), it can accommodate various kinds of real data and even misspecified models (see Section 5).

The special case of $\theta = \infty$ is of independent interest. It corresponds to the standard spiked covariance model (Johnstone 2001), where $D = \sigma^2 I_p$. This model has attracted a lot of attention (Baik et al. 2005, Paul 2007, Donoho et al. 2018). In this special case, BEMA reduces to a simpler algorithm. We conduct theoretical analysis under this model. First, we give an explicit error bound for estimating $\sigma^2$. This is connected to the robust estimation of $\sigma^2$ in the literature of reconstruction of spiked covariance matrices (Donoho et al. 2018, Shabalin and Nobel 2013). These works proposed robust estimators of $\sigma^2$ as part of their matrix reconstruction algorithms, but did not study these estimators. In our method, we obtain a new robust estimator of $\sigma^2$ as a byproduct, and we study it theoretically. Second, we prove the consistency of estimating $K$ under minimal conditions. Our results impose no assumptions on the population eigenvectors $\xi_1, \ldots, \xi_K$ and only require that the spiked eigenvalues $\lambda_1, \ldots, \lambda_K$ are larger than a constant. In comparison, many papers in the literature either require some regularity conditions on eigenvectors or need spiked eigenvalues to be much larger. See Section 4 for detailed discussions.

The remaining of this paper is organized as follows: In Section 2, we describe BEMA for the standard spiked covariance model (i.e., $\theta = \infty$); in this case, the idea is easier to understand and the algorithm is simpler. In Section 3, we describe BEMA for the general case. Section 4 states the theoretical properties. Section 5 and Section 6 provide simulation study results and real data analysis, respectively. Section 7 concludes the paper. Proofs are relegated to the appendix.

2 BEMA for the standard spiked covariance model

In this section, we consider the standard spiked covariance model (Johnstone 2001), a special case of Models (1)-(2) with $\theta = \infty$. Since each $\sigma_j^2$ is equal to $\sigma^2$, the model is re-written as

$$\Sigma = \sum_{k=1}^{K} \mu_k \xi_k \xi_k^\top + \sigma^2 I_p. \quad (3)$$

The first $K$ eigenvalues of $\Sigma$ are $\lambda_k = \mu_k + \sigma^2$, and the remaining eigenvalues are $\sigma^2$. The sample covariance matrix is $S = \frac{1}{n} \sum_{i=1}^{n} (X_i - \bar{X})(X_i - \bar{X})^\top$, where $\bar{X} = \frac{1}{n} \sum_{i=1}^{n} X_i$. With probability 1, $S$ has $n \wedge p$ distinct nonzero eigenvalues (Uhlig 1994), denoted as $\hat{\lambda}_1 > \hat{\lambda}_2 > \ldots > \hat{\lambda}_{n \wedge p}$.

We first review some existing results about the asymptotic behavior of empirical eigenvalues. We focus on nonzero eigenvalues only, hence, when $p > n$, our definitions of the Machenko-Pastur (MP) distribution and ESD (see below) are slightly different from the conventional definition. This is for notation convenience.
Definition 1. Given a parameter $\gamma > 0$, the Machenko-Pastur (MP) distribution is defined by the density

$$f_{\gamma}(x; \sigma^2) = \frac{1}{2\pi\sigma^2} \frac{1}{x(\gamma \wedge 1)} \sqrt{(x - \sigma^2h_-)(\sigma^2h_+ - x)} \cdot 1\{\sigma^2h_- < x < \sigma^2h_+\}, \quad (4)$$

where $h_{\pm} = (1 \pm \sqrt{\gamma})^2$. We let $F_{\gamma}(x; \sigma)$ denote its cumulative distribution function.

The empirical spectral distribution (ESD) is $F_n(x) = \frac{1}{n \wedge p} \sum_{i=1}^{n \wedge p} 1\{\hat{\lambda}_i \leq x\}$, which is the empirical distribution associated with nonzero eigenvalues of $S$. When $\Sigma$ satisfies (3), if $K$ is fixed, $p/n \to \gamma$ for a constant $\gamma \in (0, \infty)$, and $\mu_K > \sigma^2 \sqrt{\gamma}$, under mild regularity conditions, the following statements are true (Bloemendal et al., 2016):

- The ESD converges to the MP distribution with parameter $\gamma$; more precisely, for any fixed $x$, $\|F_n(x) - F_{\gamma}(x; \sigma^2)\|_{\infty} \to 0$ with probability 1.
- The first $K$ empirical eigenvalues are located outside the support of the MP distribution with high probability.

See Figure 2 for an illustration via simulated data ($n = 1000, p = 500$).

![Figure 2: The asymptotic behavior of empirical eigenvalues. The histogram of bulk eigenvalues converges to an MP distribution, and $K$ top eigenvalues are outside the support.](image)

Inspired by the asymptotic behavior of empirical eigenvalues, we propose a two-step approach to estimating $K$. In the first step, we use bulk eigenvalues to fit an MP distribution. The density $f_{\gamma}(x; \sigma^2)$ in (4) has two parameters ($\gamma, \sigma^2$), where $\gamma$ can be approximated by $\gamma_n = p/n$. It reduces to considering $f_{\gamma_n}(x; \sigma^2)$, for all possible $\sigma^2$. We aim to find $\hat{\sigma}^2$ such that $f_{\gamma_n}(x; \hat{\sigma}^2)$ is the best fit to the histogram of empirical eigenvalues. In the second step, we determine $K$ by comparing top eigenvalues with the right boundary of the support of the estimated MP density, namely, $\hat{\sigma}^2(1 + \sqrt{\gamma_n})^2$.

Now, we describe the method in detail. First, consider the estimation of $\sigma^2$. Fixing a constant $\alpha \in (0, 1/2)$, we take only a faction of nonzero eigenvalues:

$$\{\hat{\lambda}_k : \alpha(n \wedge p) \leq k \leq (1 - \alpha)(n \wedge p)\}.$$  

Since $K$ is fixed and $n \wedge p \to \infty$, any $\alpha$ guarantees that the first $K$ eigenvalues are excluded. The choice of $\alpha$ does not matter. We usually set $\alpha = 0.2$, so that 60% of the nonzero eigenvalues
in the middle range are used. Write for short \( \tilde{p} = n \wedge p \). By definition, \( \hat{\lambda}_k \) is the \((k/\tilde{p})\)-upper-quantile of the ESD. Let \( q_k = q_k(\gamma_n) \) denote the \((k/\tilde{p})\)-upper-quantile of the MP distribution associated with \( \gamma = \gamma_n \) and \( \sigma^2 = 1 \), that is,

\[
q_k \text{ is the unique value such that } \int_{q_k}^{(1+\sqrt{n})^2} f_{\gamma_n}(x; 1) dx = k/\tilde{p}.
\]

These \( q_k \)'s can be easily computed (e.g., via the R package RMTstat). For an MP distribution with a general \( \sigma^2 \), its \((k/\tilde{p})\)-upper-quantile equals to \( \sigma^2 q_k \). Since the ESD is asymptotically close to the MP distribution, we expect that

\[
\hat{\lambda}_k \approx \sigma^2 \cdot q_k.
\]

It motivates us to use \( \{(q_k, \hat{\lambda}_k)\}_{\alpha\tilde{p} \leq k \leq (1-\alpha)\tilde{p}} \) to fit a line without intercept, and this can be done by a simple least-squares. The slope of this line is an estimator of \( \sigma^2 \).

Next, we use \( \hat{\sigma}^2 \) to determine a threshold for the top eigenvalues. A natural choice of threshold is \( \hat{\sigma}^2 (1 + \sqrt{n})^2 \), but it has a considerable probability of over-estimating \( K \). We slightly increase this threshold by taking an advantage of another result in random matrix theory. When \( \mu_K > \sigma^2 \sqrt{n} \), it is known that \( \hat{\lambda}_{K+1} - \sigma^2 (1 + \sqrt{n})^2 \sigma^{-2} n^{-\frac{2}{3}} \gamma_n^{-\frac{1}{2}} \) \( \sim \) Tracy-Widom distribution.

\[
\frac{\hat{\lambda}_{K+1} - \sigma^2 (1 + \sqrt{n})^2}{\sigma^2 n^{-\frac{2}{3}} \gamma_n^{-\frac{1}{2}} (1 + \sqrt{n})^{\frac{1}{2}}} \quad \Rightarrow \quad \text{Tracy-Widom distribution.}
\]

We propose thresholding the top eigenvalues at

\[
\hat{T} = \hat{\sigma}^2 \left[ (1 + \sqrt{n})^2 + t_{1-\beta} \cdot n^{-\frac{2}{3}} \gamma_n^{-\frac{1}{2}} (1 + \sqrt{n})^{\frac{1}{2}} \right],
\]

where \( t_{1-\beta} \) denotes the \((1-\beta)\)-quantile of the Tracy-Widom distribution. Then, the probability of over-estimating \( K \) is controlled by \( \beta \).

**Algorithm 1.** BEMA for the standard spiked covariance model.

**Input:** Nonzero eigenvalues \( \hat{\lambda}_1, \ldots, \hat{\lambda}_{n \wedge p} \), \( \alpha \in (0, 1/2) \) and \( \beta \in (0, 1) \).

**Output:** An estimate of \( K \).

**Step 1:** Write \( \tilde{p} = n \wedge p \). For each \( \alpha \tilde{p} \leq k \leq (1-\alpha)\tilde{p} \), obtain \( q_k \), the \((k/\tilde{p})\)-upper-quantile of the MP distribution associated with \( \sigma^2 = 1 \) and \( \gamma_n = p/n \). Compute

\[
\hat{\sigma}^2 = \frac{\sum_{\alpha \tilde{p} \leq k \leq (1-\alpha)\tilde{p}} q_k \hat{\lambda}_k}{\sum_{\alpha \tilde{p} \leq k \leq (1-\alpha)\tilde{p}} q_k^2}.
\]

**Step 2:** Obtain \( t_{1-\beta} \), the \((1-\beta)\)-quantile of Tracy-Widom distribution. Estimate \( K \) by

\[
\hat{K} = \# \{ 1 \leq k \leq \tilde{p} : \hat{\lambda}_k > \hat{\sigma}^2 \left[ (1 + \sqrt{n})^2 + t_{1-\beta} \cdot n^{-\frac{2}{3}} \gamma_n^{-\frac{1}{2}} (1 + \sqrt{n})^{\frac{1}{2}} \right] \}.
\]

Algorithm 1 has two tuning parameters \((\alpha, \beta)\). The output of the algorithm is insensitive to \( \alpha \) if \( \alpha \) is not too small, and we set \( \alpha = 0.2 \) by default. \( \beta \) controls the probability of over-estimating
and is specified by the user. In theory, the ideal choice of $\beta$ should satisfy that $\beta \to 0$ at a properly slow rate (see Section 4). In practice, choosing a moderate $\beta$ often yields the best finite-sample performance. Our numerical experiments suggest that $\beta = 0.1$ is a good choice for most settings.

**A simulation example.** We illustrate Algorithm 1 on a simulation example. Fix $(n,p,K) = (1000,500,10)$. We generate $X_i \overset{iid}{\sim} N(0, \Sigma)$, where $\Sigma$ is a diagonal matrix whose first $K$ diagonals equal to 5.4 and the remaining diagonals equal to $\sigma^2 = 2$. In the left panel of Figure 3 we plot $\hat{\lambda}_k$ versus $q_k$. Except for a few top eigenvalues, it fits well to a straight line crossing the origin. We use 300 bulk eigenvalues $\{\hat{\lambda}_k\}_{100 < k \leq 400}$ (the blue dots) to fit a regression line (the red dotted line). The slope of this line gives the estimate $\hat{\sigma}^2 = 2.04$. In the middle panel of Figure 3 we plot $\hat{\lambda}_k$ versus $k$. The red solid line is the curve of $\hat{\sigma}^2 q_k$ versus $k$. Although it is estimated using the blue dots only, we can extend this curve to the left boundary, which gives rise to the value $\hat{\sigma}^2 (1 + \sqrt{\gamma n})^2$. We then use this value and the Tracy-Widom distribution to calculate a threshold for the top eigenvalues. The estimator $\hat{K}$ equals to the number of top eigenvalues that exceed this threshold. The right panel of Figure 3 is a zoom-in of the middle panel. As $k$ gets smaller (e.g., $k < 50$), the eigenvalues stay above the fitted MP quantile curve. This is because these $\hat{\lambda}_k$ are influenced by the spiked eigenvalues of $\Sigma$. Such eigenvalues are already excluded in the estimation of $\sigma^2$. The right panel can also be viewed as a scree plot. Finding the elbow point of the scree plot is a common ad-hoc method for estimating $K$. In this plot, the elbow points are $\{6, 7, 10, 11\}$. It is hard to decide which is the true $K$. In contrast, our method correctly picks $\hat{K} = 10$.

Figure 3: Illustration of BEMA for the standard spiked covariance model (simulated data, $n = 1000$, $p = 500$, $K = 10$). The left panel plots $\hat{\lambda}_k$ versus $q_k$, where $q_k$ is the $(k/\tilde{p})$-upper-quantile of the standard MP distribution. The dashed red line is the fitted regression line on bulk eigenvalues (blue dots), whose slope is an estimate of $\sigma^2$. The middle panel plots $\hat{\lambda}_k$ versus $k$, which is the scree plot. The red solid line is $\hat{\sigma}^2 q_k$ versus $k$. It fits the bulk eigenvalues (blue dots) very well. When this curve is extended to the left boundary, it hits $\hat{\sigma}^2 (1 + \sqrt{\gamma n})^2$. Our threshold for the top eigenvalues, which is the $(1 - \beta)$-quantile of the Tracy-Widom distribution, is slightly larger than this value and shown by the dotted red line. The right panel zooms into the grey square area of the middle panel. It shows that 10 empirical eigenvalues exceeds the threshold, resulting in $\hat{K} = 10$. 
Remark (Connection to the robust estimation of $\sigma^2$). As a byproduct, the BEMA algorithm yields a new estimator for $\sigma^2$ in the standard spiked covariance model, which can be useful for other problems such as reconstruction of spiked covariance matrices. Gavish and Donoho (2014) proposed a robust estimator of $\sigma^2$, which is the ratio between the median of eigenvalues and the median of a standard MP distribution. Viewed in the Q-Q plot (left panel of Figure 3), their method is equivalent to using a single point to decide the slope. In comparison, our method uses a number of bulk eigenvalues to decide the slope and is thus more robust. Kritchman and Nadler (2009) proposed an estimator of $\sigma^2$ by solving a non-linear system of equations, and Shabalin and Nobel (2013) estimated $\sigma^2$ by minimizing the Kolmogorov-Smirnov distance between the ESD and its theoretical limit. In comparison, our estimator of $\sigma^2$ is from a simple least-squares and is much easier to compute. In Section 4 we also give an explicit error bound for our estimator.

3 BEMA for the general spiked covariance model

We now consider the general case where the residual covariance matrix can have unequal diagonal entries. We shall modify Algorithm 1 to accommodate this general setting. Re-write Models (1)-(2) as

$$
\Sigma = \sum_{k=1}^{K} \mu_k \xi_k \xi_k^\top + \text{diag}(\sigma_1^2, \sigma_2^2, \ldots, \sigma_p^2), \quad \text{where } \sigma_k \overset{iid}{\sim} \text{Gamma}(\theta, \theta/\sigma_k^2). \quad (7)
$$

Same as before, let $\hat{\lambda}_1 > \hat{\lambda}_2 > \ldots > \hat{\lambda}_{n \wedge p}$ denote the nonzero eigenvalues of the sample covariance matrix. Below, in Section 3.1, we first state some well-known results from random matrix theory and motivate our methodology idea. In Section 3.2 we formally introduce the BEMA algorithm. In Section 3.3 we provide an asymptotic confidence interval for $K$.

3.1 The asymptotic behavior of empirical eigenvalues

Under Model (7), the asymptotic behavior of bulk eigenvalues and top eigenvalues exhibit some similarity to the case of standard spiked covariance model:

- The empirical spectral distribution (ESD) converges to a fixed limit.
- The first $K$ empirical eigenvalues stand out of the bulk.

However, the precise statement is more sophisticated.

We first consider the ESD. When $K$ is finite and $p/n \to \gamma$, the ESD converges to a distribution $F_{\gamma}(x; \sigma^2, \theta)$. This distribution is parametrized by $(\sigma^2, \theta)$, but it does not have an explicit form. It is defined implicitly by an equation about its Stieltjes transform (Silverstein, 2009). Let $H_{\sigma^2, \theta}(t)$ denote the CDF of $\text{Gamma}(\theta, \theta/\sigma^2)$. Let $m = m(x, \gamma, \sigma^2, \theta) \in \mathbb{C}^+$ be the unique solution to the equation

$$
x = -\frac{1}{m} + \gamma \int \frac{t}{1 + tm} dH_{\sigma^2, \theta}(t). \quad (8)
$$
The density of \( F_\gamma(x;\sigma^2,\theta) \), denoted by \( f_\gamma(x;\sigma^2,\theta) \), satisfies that
\[
f_\gamma(x;\sigma^2,\theta) = \frac{1}{\gamma \pi} \Im(m(x,\gamma,\sigma^2,\theta)),
\]
(9)
where \( \Im(\cdot) \) denotes the imaginary part of a complex number.

We aim to estimate \((\sigma^2,\theta)\) by comparing the bulk eigenvalues with the corresponding quantiles of \( F_\gamma(x;\sigma^2,\theta) \). In the special case of \( \theta = \infty \), \( F_\gamma(x;\sigma^2,\theta) \) reduces to the MP distribution. Therefore, we can compute its quantiles explicitly and estimate \( \sigma^2 \) by a simple least-squares. For the general case, we have to compute the quantiles of \( F_\gamma(x;\sigma^2,\theta) \) numerically. There are two approaches, one is solving the density from equations (8)-(9) and then computing the quantiles, and the other is using Monte Carlo simulations. We relegate the details to Section 3.2 and the appendix.

Next, we consider the top eigenvalues. It requires a precise definition of “standing out” of the bulk. We use the distribution of \( \hat{\lambda}_{K+1} \) under Model (7) as a benchmark, i.e., \( \hat{\lambda}_k \) needs to be much larger than a high-probability upper bound of \( \hat{\lambda}_{K+1} \) in order to be called “standing out.” Fortunately, the behavior of \( \hat{\lambda}_{K+1} \) has been studied in the literature of random matrix theory. We define the following null model, which is a special case of Model (7) with \( K = 0 \):
\[
\Sigma = \text{diag}(\sigma_1^2,\sigma_2^2,\ldots,\sigma_p^2), \quad \text{where } \sigma_k^2 \overset{iid}{\sim} \text{Gamma}(\theta, \theta/\sigma^2).
\]
(10)
Let \( \hat{\lambda}_1^* \) denote the largest eigenvalue of the sample covariance matrix under this null model. The eigenvalue sticking result (e.g., see Bloemendal et al. (2016)) tells that the distribution of \( \hat{\lambda}_{K+1} \) is asymptotically close to the distribution of \( \hat{\lambda}_1^* \). We now re-frame the statement that “the first \( K \) empirical eigenvalues stand out” as follows: Under some regularity conditions, each of \( \hat{\lambda}_1,\ldots,\hat{\lambda}_K \) is significantly larger than \( \hat{\lambda}_1^* \) associated with Model (10).

We aim to threshold the top eigenvalues by the \((1-\beta)\)-quantile of the distribution of \( \hat{\lambda}_1^* \), where \( \beta \) controls the probability of over-estimating \( K \). In the special case of \( \theta = \infty \), the distribution of \( \hat{\lambda}_1^* \) converges to a Tracy-Widom distribution, so that we have a closed-form expression for the threshold. In the general case, we calculate this threshold by Monte Carlo simulation, where we simulate data from the null model to approximate the distribution of \( \hat{\lambda}_1^* \). We relegate the details to Section 3.2.

### 3.2 The algorithm of estimating \( K \)

Same as before, the BEMA algorithm has two steps: Step 1 estimates \((\sigma^2,\theta)\) from bulk eigenvalues, and Step 2 calculates a threshold for the top eigenvalues.

Consider Step 1. Write \( \hat{p} = p \wedge n \) and \( \gamma_n = p/n \). For a constant \( \alpha \in (0,1/2) \), we take the \((1-2\alpha)\)-fraction of bulk eigenvalues in the middle range, i.e., \( \{\hat{\lambda}_k : \alpha \hat{p} \leq k \leq (1-\alpha)\hat{p}\} \). Each empirical eigenvalue \( \hat{\lambda}_k \) is also the \((k/\hat{p})\)-upper-quantile of the ESD. We recall that \( F_{\gamma_n}(x;\sigma^2,\theta) \)
Let \( \hat{\lambda}_k \) with \( \hat{\lambda}_k \) being obtained by regressing \( \theta \). As long as we can compute \( \hat{\lambda}_k \), the theoretical limit of the ESD should be the same as that for Gaussian \( X \). It is known that \( F_{\gamma_n}(x; \sigma^2, \theta) \) is also the theoretical limit of the ESD of the null model \( \sigma^2 \). Since \( \sigma^2 = \text{Gamma}(\theta, \theta/\sigma^2) \) is equivalent to \( \sigma^2 \gamma^2 \sim \text{Gamma}(\theta, \theta) \), we conclude that Model \( \sigma^2 \) can be re-written as \( \Sigma = \sigma^2 \Sigma_0 \), where \( \Sigma_0 \) follows the same null model but with \( \sigma^2 = 1 \). When \( X_i \)'s follow a multivariate normal distribution, multiplying the covariance matrix by a factor of \( \sigma^2 \) yields the same effect on eigenvalues and on the theoretical limit of ESD. We immediately have

\[
\hat{\lambda}_k \approx \tilde{\lambda}^{-1}_{\gamma_n}(k/\tilde{p}; \sigma^2, \theta).
\]

It motivates the following estimator of \( (\sigma^2, \theta) \):

\[
(\hat{\sigma}^2, \hat{\theta}) = \arg\min_{(\sigma^2, \theta)} \left\{ \sum_{\alpha \tilde{p} \leq k \leq (1-\alpha)\tilde{p}} \left[ \hat{\lambda}_k - \tilde{\lambda}^{-1}_{\gamma_n}(k/\tilde{p}; \sigma^2, \theta)^2 \right] \right\}, \tag{11}
\]

We now describe how to solve \( \hat{\sigma}^2 \). This is a two-dimensional optimization. As long as we can evaluate the objective function for arbitrary \( (\sigma^2, \theta) \), we can solve it via a simple grid search. To further simplify the objective, we first get rid of \( \sigma^2 \) and reduce it to an optimization on \( \theta \) only. It is known that \( F_{\gamma_n}(x; \sigma^2, \theta) \) is also the theoretical limit of the ESD of the null model \( \sigma^2 \). When \( X_i \)'s follow a multivariate normal distribution, multiplying the covariance matrix by a factor of \( \sigma^2 \) yields the same effect on eigenvalues and on the theoretical limit of ESD. We immediately have

\[
\tilde{\lambda}^{-1}_{\gamma_n}(k/\tilde{p}; \sigma^2, \theta) = \sigma^2 \cdot \tilde{\lambda}^{-1}_{\gamma_n}(k/\tilde{p}; 1, \theta).
\]

When the distribution of \( X_i \) is nonGaussian, as long as the eigenvalue universality theory holds \( \text{Pillai and Yin, 2014} \), the theoretical limit of the ESD should be the same as that for Gaussian data, so that the above equality still holds. Given this equality, we can re-write \( \hat{\sigma}^2 \) as

\[
\min_{\theta} H(\theta), \quad \text{where} \quad H(\theta) = \min_{\sigma^2} \left\{ \sum_{\alpha \tilde{p} \leq k \leq (1-\alpha)\tilde{p}} \left[ \hat{\lambda}_k - \sigma^2 \tilde{\lambda}^{-1}_{\gamma_n}(k/\tilde{p}; 1, \theta)^2 \right] \right\}.
\]

As long as we can compute \( \tilde{\lambda}^{-1}_{\gamma_n}(y; \sigma^2, \theta) \) for any \( \theta > 0 \) and \( y \in [0, 1] \), we can obtain \( H(\theta) \) for each \( \theta \) by least squares. Given \( H(\theta) \), we can solve the optimization by a grid search on \( \theta \).

This is described in Step 1 of Algorithm 2. Suppose there is an available algorithm GetQT that computes \( \tilde{\lambda}^{-1}_{\gamma_n}(y; 1, \theta) \) for any \( \theta > 0 \) and \( y \in [0, 1] \). Fix a grid \( \{\theta_j\}_{j=1}^N \). For each \( \theta_j \), we first compute \( \tilde{\lambda}^{-1}_{\gamma_n}(k/\tilde{p}; 1, \theta_j) \) for all \( \alpha \tilde{p} \leq k \leq (1-\alpha)\tilde{p} \). Given \( \theta_j \), the value of \( \sigma^2 \) that minimizes \( \hat{\sigma}^2 \) is obtained by regressing \( \{\lambda_k\}_{\alpha \tilde{p} \leq k \leq (1-\alpha)\tilde{p}} \) on \( \{\tilde{\lambda}^{-1}_{\gamma_n}(k/\tilde{p}; 1, \theta_j)\}_{\alpha \tilde{p} \leq k \leq (1-\alpha)\tilde{p}} \) with a least-squares. Let \( \hat{\sigma}^2(\theta_j) \) denote this optimal value of \( \sigma^2 \), and let \( v_j \) denote the objective in \( \hat{\sigma}^2(\theta_j) \) associated with \( (\theta_j, \hat{\sigma}^2(\theta_j)) \). We select \( j^* \) so that \( v_j \) is minimized and set \( \tilde{\theta} = \theta_{j^*} \), and \( \hat{\sigma}^2 = \hat{\sigma}^2(\theta_{j^*}) \).

What remains is the design of an algorithm GetQT \((y, \gamma_n, \theta)\) to compute the \( y \)-upper-quantile of the distribution \( F_{\gamma_n}(:,1,\theta) \) for arbitrary \( (\theta, y) \). We note that \( F_{\gamma_n}(x;1,\theta) \) only has an implicit definition through equations \( (8) \). In the appendix, we propose two algorithms that serve for this purpose:

- GetQT1 first utilizes the definition \( (8) \) to solve the density \( f_{\gamma_n}(x;1,\theta) \) and then uses the density to compute quantiles.
the sampling distribution of $\hat{\lambda}_1 \ldots, \hat{\lambda}_n$; $\alpha \in (0, 1/2), \beta \in (0, 1)$, a grid of values $0 < \theta_1 < \theta_2 < \ldots < \theta_N$, an algorithm GetQT, and an integer $M \geq 1$.

Output: An estimate of $K$.

Step 1: Write $\tilde{\rho} = n \wedge p$ and $\gamma_n = p/n$. For each $1 \leq j \leq N$:

- For each $\alpha \tilde{\rho} \leq k \leq (1 - \alpha) \tilde{\rho}$, run the algorithm GetQT($k / \tilde{\rho}, \gamma_n, \theta_j$) to obtain $q_{kj}$.
- Compute $\hat{\sigma}^2(\theta_j) = (\sum_{\alpha \tilde{\rho} \leq k \leq (1 - \alpha) \tilde{\rho}} q_{kj} \hat{\lambda}_k) / (\sum_{\alpha \tilde{\rho} \leq k \leq (1 - \alpha) \tilde{\rho}} q_{kj}^2)$.
- Let $v_j = \sum_{\alpha \tilde{\rho} \leq k \leq (1 - \alpha) \tilde{\rho}} [\hat{\lambda}_k - \hat{\sigma}^2(\theta_j) \cdot q_{kj}]^2$.

Find $j^* = \arg\min_{1 \leq j \leq N} v_j$. Let $\hat{\theta} = \theta_{j^*}$ and $\hat{\sigma}^2 = \hat{\sigma}^2(\theta_{j^*})$.

Step 2: For $1 \leq m \leq M$:

- Sample $d^*_j \sim \text{Gamma}(\hat{\theta}, \hat{\theta})$, independently for $1 \leq j \leq p$. Sample $X^*_i(j) \sim N(0, \sigma^2 d^*_j)$, independently for $1 \leq i \leq n$ and $1 \leq j \leq p$.
- Compute $\hat{\lambda}^*_{(m)}$; the first eigenvalue of $S^* \equiv (1/n) \sum_{i=1}^n X^*_i(X^*_i)^\top$.

Let $T$ be the $(1 - \beta)$-quantile of $\{\hat{\lambda}^*_{(m)}\}_{1 \leq m \leq M}$. Output $\tilde{K} = \#\{1 \leq k \leq \tilde{\rho} : \hat{\lambda}_k > T\}$.

- GetQT2 takes advantage of the fact that $F_{\gamma_n}(x; \sigma^2, \theta)$ is also the theoretical limit of the ESD of the null model (10). This algorithm simulates data from Model (10) with $\sigma^2 = 1$ to get the Monte Carlo approximation of the target quantile.

The two GetQT algorithms have comparable numerical performance, but each has an advantage on running time in some cases; see the appendix for more discussions.

Consider Step 2. We estimate $K$ by comparing each top eigenvalue with the $(1 - \beta)$-quantile of the distribution of $\hat{\lambda}^*_1$ under the null model (10), with $(\hat{\sigma}^2, \hat{\theta})$ plugged in. The threshold is

$$\hat{T} = \begin{cases} \text{(1 - $\beta$)-quantile of the distribution of $\hat{\lambda}^*_1$ under the null model} \\ \Sigma = \text{diag}(\sigma^2_1, \sigma^2_2, \ldots, \sigma^2_p), \text{ where } \sigma^2_j \text{ iid } \text{Gamma}(\hat{\theta}, \hat{\theta} / \hat{\sigma}^2) \end{cases}. \quad (12)$$

The $\hat{T}$ here generalizes the threshold in Algorithm 1. The threshold in Algorithm 1 is a special case of $\hat{T}$ at $\hat{\theta} = \infty$, which happens to have an explicit formula.

We compute $\hat{T}$ via Monte Carlo simulations. We first draw $\Sigma$ from the null model in (12), and then draw the data matrix from multivariate normal distributions and compute the largest eigenvalue of the sample covariance matrix. By repeating these steps multiple times, we obtain the sampling distribution of $\hat{\lambda}^*_1$ in (12). This is described in Step 2 of Algorithm 2.

The BEMA algorithm has three tuning parameters $(\alpha, \beta, M)$. $\alpha$ controls the percentage of bulk eigenvalues used for estimating $(\sigma^2, \theta)$ and $M$ is the number of Monte Carlo repetitions for approximating $\hat{T}$. The performance of the algorithm is insensitive to $(\alpha, M)$. We set $\alpha = 0.2$ and $M = 500$ by default. $\beta$ controls the probability of over-estimating $K$. Theoretically, if the
spiked eigenvalues are large enough, we should use a diminishing \( \beta \) (i.e., \( \beta \to 0 \) as \( n \to \infty \)) so that the probability of over-estimating \( K \) tends to zero. In practice, it often happens that the spiked eigenvalues are only moderately large, we thus need a moderate \( \beta \) to strike a balance between the probability of over-estimating \( K \) and the probability of under-estimating \( K \). We leave it to the users to decide. It is analogous to the situation in false discovery rate control, where the users select the target false discovery rate. In our numerical experiments, we find that \( \beta = 0.1 \) is a good choice.

**A simulation example.** We illustrate Algorithm 2 on a simulation example. Fix \((n, p, K) = (1000, 200, 5)\) and \((\sigma^2, \theta) = (1, 10)\). We generate \( X \) iid from \( N(0, \Sigma) \), where \( \Sigma \) satisfies model \( \text{(7)} \) with \( \lambda_k = 2.3 \) for \( 1 \leq k \leq K \). The left panel of Figure 4 shows the plot of \( \hat{\lambda}_k \) versus the MP quantiles \( q_k \). It does not fit a line crossing the origin, suggesting that Algorithm 1 is not working for this general covariance model. The middle panel contains the plot of \( \hat{\lambda}_k \) versus \( \bar{F}_n^{-1}(k/\tilde{p}; 1, \hat{\theta}) \), where \( \hat{\theta} \) is an estimate of \( \theta \) by Algorithm 2. Except for a few top eigenvalues, it fits very well a line crossing the origin, suggesting that Algorithm 2 is successful in this setting. The estimated parameters are \( (\hat{\sigma}^2, \hat{\theta}) = (1.02, 10.39) \), which is close to the true values. The right panel contains the plot of \( \hat{\lambda}_k \) versus \( k \), and the fitted curve of \( \hat{\sigma}^2 \cdot \bar{F}_n^{-1}(k/\tilde{p}; 1, \hat{\theta}) \) versus \( k \) (solid red line). The threshold \( \hat{T} \) is also shown by the dashed line. It yields \( \hat{K} = 5 \), which is the same as the ground truth.

Remark (**Connection to parallel analysis**). The parallel analysis (Horn, 1965) is a popular method for estimating the number of spiked eigenvalues in real applications. It samples data from a null covariance model that has no spiked eigenvalues, and estimates \( K \) by comparing the distribution of top empirical eigenvalues on simulated data to those actually observed from the original data. The most common version of parallel analysis first standardizes the data matrix
so that each variable has a unit variance and then uses $\Sigma = I_p$ as the null model. Our algorithm has a similar spirit as parallel analysis, but we adopt a more sophisticated null covariance model, Model (10), and estimate parameters of this null model carefully from bulk eigenvalues.

**Remark (Memory use of BEMA).** The input of BEMA includes nonzero eigenvalues of the sample covariance matrix. These eigenvalues can be computed by eigen-decomposition on either the $p \times p$ matrix $X^\top X$ or the $n \times n$ matrix $XX^\top$. Therefore, the memory use depends on the minimum of $n$ and $p$. In many real applications, $p$ is very large but $n$ is relatively small, and BEMA is still implementable under even strict memory constraints.

### 3.3 A confidence interval of $K$

By varying $\beta$ in Algorithm 2, we get different estimators of $K$, where the over-shooting probability is controlled at different levels. We use these estimators to construct a confidence interval for $K$.

**Definition 2 (Confidence interval of $K$).** Denote the output of Algorithm 2 by $\hat{K}_\beta$ to indicate its dependence on $\beta$. Given any $\omega_0 \in (0, 1)$, we introduce the following $(1 - \omega_0)$-confidence interval of $K$:

$$[\hat{K}_{\omega_0/2}, \hat{K}_{1-\omega_0/2}].$$  \hspace{1cm} (13)

We explain the rationale of the confidence interval. Let $\hat{T} = \hat{T}_\beta$ be the threshold in (12), and let $\hat{\lambda}_1^*$ be the largest eigenvalue of sample covariance matrix when data are generated from the null model (10). We use $P_0$ to denote the probability measure associated with Model (10). By definition of $\hat{T}_\beta$,

$$P_0\{\hat{\lambda}_1^* \leq t\}_{t=\hat{T}_\beta} = 1 - \beta.$$  

At the same time, the eigenvalue sticking result [Bloemendal et al., 2016] says that, under some regularity conditions, the distribution of $\hat{\lambda}_{K+1}$ is asymptotically close to the distribution $\hat{\lambda}_1^*$. It follows that

$$P\{\hat{K}_{\omega_0/2} > K\} \leq P\{\hat{\lambda}_{K+1} > \hat{T}_{\omega_0/2}\} \approx P_0\{\hat{\lambda}_1^* > t\}_{t=\hat{T}_{\omega_0/2}} = \omega_0/2,$$

$$P\{\hat{K}_{1-\omega_0/2} < K\} \leq P\{\hat{\lambda}_K \leq \hat{T}_{1-\omega_0/2}\} \leq P\{\hat{\lambda}_{K+1} \leq \hat{T}_{1-\omega_0/2}\} \approx P_0\{\hat{\lambda}_1^* \leq t\}_{t=\hat{T}_{1-\omega_0/2}} = \omega_0/2.$$  

This justifies that (13) is indeed an asymptotically valid confidence interval.

### 4 Theoretical properties

The standard spiked covariance model [Johnstone, 2001] serves as a common theoretical platform to compare and evaluate methods. We focus our theoretical study on this model for two reasons: First, it facilitates a fair comparison with existing methods. Most existing methods were not designed for our general covariance model, but almost every method is applicable to the standard
spiked covariance model. It is an ideal platform for comparing different methods. Second, the theoretical study of this model is already non-trivial. We have to borrow a few advanced results from random matrix theory to get the desired conclusions.

In the study of the standard spiked covariance model, it is common to assume that the data vectors $X_1, X_2, \ldots, X_n$ are actually generated from a factor model:

**Assumption 1** (Factor model). Let $Y = [Y_1, Y_2, \ldots, Y_n]^T \in \mathbb{R}^{n \times (p+K)}$ be a random matrix with independent but not identically distributed entries, where $\mathbb{E}[Y_i(j)] = 0$ and $\text{Var}(Y_i(j)) = 1$, for all $1 \leq i \leq n$ and $1 \leq j \leq p + K$. Given $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_K > 0$ and a set of orthonormal vectors $\xi_1, \xi_2, \ldots, \xi_K \in \mathbb{R}^p$, the data vectors $X_1, X_2, \ldots, X_n$ satisfy that

$$X_i(j) = \sigma \cdot Y_i(j) + \sum_{k=1}^{K} \sqrt{\mu_k} \xi_k(j) \cdot Y_i(p + k), \quad 1 \leq i \leq n, 1 \leq j \leq p.$$ 

The factor model is a special case of the standard covariance model, since the covariance matrix of $X$ automatically satisfies Model 3. When the entries of $Y$ are Gaussian variables, these two models are equivalent. For non-Gaussian data, the factor model is theoretically more tractable and commonly used in the literature (Bai and Ng, 2002).

We first give an error bound on estimating $\sigma^2$.

**Theorem 1** (Estimation error of $\hat{\sigma}^2$). Suppose $X_1, X_2, \ldots, X_n$ follow the factor model, where $K \geq 1$ is fixed and $p/n \to \gamma \in (0, \infty)$ as $n \to \infty$. Suppose, for each integer $m \geq 1$, there exists a universal constant $C_m > 0$ such that $\sup_{1 \leq i \leq n, 1 \leq j \leq p} \mathbb{E}[|Y_i(j)|^m] \leq C_m$. Let $\hat{\sigma}^2$ be the estimator of $\sigma^2$ by Algorithm 1, where the tuning parameter $\alpha$ is set to be an arbitrary constant in $(0, 1/2)$. Then, there is a constant $C = C(\alpha, \gamma, \sigma^2, K)$ such that, for any $\epsilon > 0$ and $s > 0$,

$$\mathbb{P}\left\{ |\hat{\sigma}^2 - \sigma^2| > C n^{-(1-\epsilon)} \right\} \leq n^{-s}.$$ 

This result is connected to the robust estimation of $\sigma^2$ in a standard spiked covariance model (Gavish and Donoho, 2014; Kritchman and Nadler, 2009; Shabalin and Nobel, 2013). In these works, there are only consistency results available (Donoho et al., 2018) which say that $\hat{\sigma}^2 \to \sigma^2$ almost surely, but there are no explicit error rates. Thanks to the recent advancement in random matrix theory on sharp large-deviation bounds for individual empirical eigenvalues (see Ke, 2016 for a survey), we can repackage those results to obtain an explicit bound for $|\hat{\sigma}^2 - \sigma^2|$. In this error bound, $\epsilon$ can be arbitrarily close to 0, so that the bound for $|\hat{\sigma}^2 - \sigma^2|$ can get close to $O(n^{-1})$.

We then establish the consistency on estimating $K$.

**Theorem 2** (Consistency of $\hat{K}$). Suppose $X_1, X_2, \ldots, X_n$ follow the factor model, where $K \geq 1$ is fixed, $p/n \to \gamma$, and $\mu_K \geq \sigma^2 (\sqrt{\gamma} + \tau)$, for positive constants $\gamma$ and $\tau$. Suppose, for each integer $m \geq 1$, there exists a universal constant $C_m > 0$ such that $\sup_{1 \leq i \leq n, 1 \leq j \leq p} \mathbb{E}[|Y_i(j)|^m] \leq C_m$. 


Let $\hat{K}$ be the estimator of $K$ by Algorithm 1, where the tuning parameters satisfy that $\alpha \in (0, 1/2)$ is a fixed constant and $\beta \to 0$ at a properly slow rate as $n \to \infty$. Then,

$$P\{\hat{K} = K\} = 1 - o(1).$$

We compare the conditions required for consistent estimation of $K$ with those in other work. Recall that $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_p$ denote the eigenvalues of $\Sigma$. In our model, $\lambda_k = \mu_k + \sigma^2$ for $1 \leq k \leq K$, and $\lambda_k = \sigma^2$ for $k > K$. The condition in Theorem 2 translates to $\lambda_K > \sigma^2(1 + \sqrt{\gamma} + \tau)$, for an arbitrarily small constant $\tau > 0$. This is weaker than the conditions for spiked eigenvalues in Bai and Ng (2002) and Cai et al. (2019), where the former requires $\lambda_K$ to be at the order of $p$ (see their Assumption B) and the latter needs $\lambda_K \to \infty$ (see their Assumption 2). Our condition on spiked eigenvalues matches with the critical phase transition threshold in Baik et al. (2005) and is hardly improvable: If $\lambda_K \leq \sigma^2(1 + \sqrt{\gamma})$, no method is able to consistently estimate $K$ (Fan et al., 2019). Dobriban and Owen (2019) require the same lower bound condition on $\lambda_K$, but they need stronger conditions on population eigenvectors. The “delocalization” condition in their paper says that $\|\Xi \Lambda_{1/2}\|_\infty \to 0$, where $\Xi = [\xi_1, \ldots, \xi_K]$, $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_K)$, and $\|\cdot\|_\infty$ is the maximum absolute row sum of a matrix. It requires that the eigenvectors are incoherent (i.e., $\max_{1 \leq k \leq K} \|\xi_k\|_\infty$ is sufficiently small) and that the eigenvalues cannot be enormously large. Examples such as the equal-correlation covariance matrix (i.e., $\Sigma(i,j) = a$, for all $i \neq j$, where $a \in (0, 1)$ is a constant) are unfortunately excluded. In contrast, our result requires no conditions on eigenvectors.

The proof of Theorem 2 is an application of the eigenvalue sticking theory (Bloemendal et al., 2016). It compares the distribution of empirical eigenvalues $\{\hat{\lambda}_k\}$ under the spiked covariance model with the distribution of empirical eigenvalues $\{\hat{\lambda}_k^*\}$ under the null model $\Sigma = \sigma^2 I_p$. The claim is that the distribution of $\hat{\lambda}_{K+s}$ is asymptotically close to the distribution of $\hat{\lambda}_s^*$, for a wide range of $s$. We use this result to study the thresholding step in Algorithm 1.

5 Simulation studies

We examine the performance of our methods in simulations. To differentiate between Algorithm 1 and Algorithm 2, we call the former BEMA0 and the latter BEMA. BEMA0 is a simplified version of BEMA, specifically designed for the standard spiked covariance model. The tuning parameters are fixed as $(\alpha, \beta) = (0.2, 0.1)$ for BEMA0 and $(\alpha, \beta, M) = (0.2, 0.1, 500)$ for BEMA.

We compare our methods with a few existing methods in the literature, including the deterministic parallel analysis (DDPA) from Dobriban and Owen (2019), the empirical Kaiser’s cri-

\footnote{We remark that the comparison is for the standard spiked covariance model only. For this model, our method has the weakest conditions for consistent estimation of $K$. On the other hand, other methods apply to some other settings, which are not considered in the comparison.}
Figure 5: Result of Simulation 1. $K = 5$. From left to right, $(n, p) = (10000, 1000)$, $(1500, 5000)$, and $(1500, 1500)$. The top three panels show the estimator $\hat{K}$ along with the 95% confidence upper/lower bound, where each quantity is the average of 100 repetitions. The bottom three panels show the probability of correctly estimating $K$ (correct rate) and the coverage probability of 95% confidence interval (coverage rate). In each panel, the red dotted line indicates the critical value of $\rho = 1$.

Simulation 1. This experiment is for the standard spiked covariance model, where we investigate the performance of BEMA0 and the confidence interval for $K$ as described in Section 3.3. We generate data from $X_i \overset{iid}{\sim} N(0, \Sigma)$, $1 \leq i \leq n$, where $\Sigma$ satisfies Model (3) with

$$
\mu_1 = \mu_2 = \cdots = \mu_K = \rho \cdot \sigma^2 \sqrt{p/n},
$$

for some $\rho > 0$.

The value of $\rho$ controls the magnitude of spiked eigenvalues. $\rho \leq 1$ is the region where consistent estimation of $K$ is impossible (Baik et al., 2005; Fan et al., 2019). We examine the performance of BEMA0 in the region of $\rho > 1$.

Fix $K = 5$ and $\sigma^2 = 1$. We consider three settings, where $(n, p)$ are $(10000, 1000)$, $(1500, 5000)$, and $(1500, 1500)$, respectively. They cover different cases of size relationship between $p$ and $n$. The eigenvector matrix $\Xi$ is drawn uniformly from the Stiefel manifold (which is the collection of all $p \times K$ matrices that have orthonormal columns). For each of the three settings, we vary the value of $\rho$ and report the average of $\hat{K}$ and upper/lower boundary of a 95% confidence interval, based on 100 repetitions; the results are in the top three panels of Figure 5. We also report the probability of correctly estimating $K$ (correct rate) and the coverage probability of the 95%
| $(n, p, K, \lambda, \theta)$ | BEMA0 | BEMA | DDPA | EKC | Bai & Ng |
|-----------------------------|-------|-------|------|-----|---------|
| (100, 500, 5, 9, $\infty$) | 4.996 (99.9%) | 4.99 (99%) | 6.422 (40%) | 5.57 (58.2%) | 0 (0%) |
| (100, 500, 5, 49, $\infty$) | 5 (100%) | 5 (100%) | 7.802 (37.4%) | 6.454 (26.6%) | 5 (100%) |
| (500, 100, 5, 1.5, $\infty$) | 4.998 (99.8%) | 4.944 (94.4%) | 5.854 (44.4%) | 5.032 (96.8%) | 0 (0%) |
| (500, 100, 5, 3, $\infty$) | 5 (100%) | 5 (100%) | 5.996 (40.8%) | 5.074 (92.6%) | 0 (0%) |
| (100, 500, 5, 15, 3) | – | 5.174 (85.8%) | 10.1 (18.6%) | 5.944 (39.2%) | 0.062 (0%) |
| (100, 500, 5, 50, 3) | – | 5.178 (86.2%) | 9.492 (21%) | 10.22 (6.8%) | 5 (100%) |
| (500, 100, 5, 4.5, 3) | – | 4.756 (81.8%) | 63.34 (23.2%) | 5.624 (48.6%) | 3.362 (39.4%) |
| (500, 100, 5, 6, 3) | – | 5.03 (95.8%) | 45.01 (39.2%) | 6.208 (22.2%) | 5.006 (99.4%) |

Table 1: Result of Simulation 2. The top four rows (with $\theta = \infty$) correspond to the standard spiked covariance model, and the bottom four rows correspond to the general spiked covariance model. The number in each cell is the average $\hat{K}$, and the number in brackets is the probability of correctly estimating $K$ (correct rate).

It agrees with our theoretical understanding that $\rho = 1$ is the critical phase transition point. When $\rho$ slightly departs from 1, the coverage rate starts to increase from 0% and quickly reaches the target of 95%. The increase of the correct rate is slightly slower, but it reaches 100% before $\rho = 1.5$, for all three settings. According to Theorem 2, the correct rate should be asymptotically 100% as long as $\rho > 1$. In terms of finite-sample performance, to get a 100% correct rate we need $\rho$ to be larger than 1 by a proper constant. Furthermore, as $\rho$ increases, the estimated $\hat{K}$ increases from 0 to 5, with a sharp change at around $\rho = 1$. The length of the 95% confidence interval initially decreases with $\rho$ and then stays almost constant.

**Simulation 2.** In this simulation, we compare BEMA0 and BEMA with other methods. We consider both the standard spiked covariance model (3) and the general spiked covariance model (7). BEMA0 and BEMA are designed for these two settings, respectively. We note that BEMA can also be applied to Model (3), which simply ignores the prior knowledge of equal diagonal in the residual covariance matrix. We thereby also include BEMA in the numerical comparison on the standard spiked covariance model.

Given $(n, p, K, \lambda, \theta)$, we generate data $X_i \overset{iid}{\sim} N(0, \Sigma)$, $1 \leq i \leq n$, where $\Sigma$ satisfies Model (7) with $\sigma^2 = 1$ and $\mu_k = \lambda$, for $1 \leq k \leq K$. The eigenvector matrix $\Xi$ is drawn uniformly from the Stiefel manifold. We allow $\theta$ to take the value of $\infty$; when $\theta = \infty$, it indicates that $\Sigma$ follows the standard spiked covariance model (3). We consider 8 different settings which cover a wide range of parameter values. The results are shown in Table 1 where the average $\hat{K}$ and the probability of correctly estimating $K$ (correct rate) are reported based on 500 repetitions.

We have a few observations. First, in the standard spiked covariance model ($\theta = \infty$, top four rows of Table 1), BEMA0 has the best performance. Interestingly, BEMA has nearly comparable performance. The reason is that the algorithm will automatically output a very large $\hat{\theta}$, so that the estimator is similar to that of knowing $\theta = \infty$. This suggests that we do not have to choose...
between BEMA0 and BEMA in practice. We can always use BEMA, even when the data come from the standard spiked covariance model. On the other hand, BEMA0 is conceptually simpler and computationally much faster, hence, it is still the better choice if we are confident that the standard spiked covariance model holds. We note that the “delocalization” condition in DDPA is not satisfied here (see more explanations below), and so DDPA does not perform well.

Second, in the general spiked covariance model ($\theta < \infty$, bottom four rows of Table 1), BEMA outperforms both DDPA and EKC in all the considered settings, and it outperforms Bai&Ng in two out of four settings. Especially, BEMA is the only method whose correct rate is above 80% in all settings. In comparison, although Bai&Ng outperforms BEMA in some cases, its correct rate in the other cases is very low. In terms of the overall performance, BEMA is the best.

The unsatisfactory performance of DDPA is because the “delocalization” condition is not satisfied. The “delocalization” condition requires that $\|\Xi \Lambda^{1/2}\|_\infty \to 0$. In our simulations, $\Xi$ is uniformly drawn from the Stiefel manifold. There is a considerable probability that $\|\Xi \Lambda^{1/2}\|_\infty$ is not sufficiently small. When the “delocalization” condition is violated, DDPA tends to over-estimate $K$.

The performance of Bai&Ng is sensitive to the magnitude of spikes. When $\lambda$ is sufficiently large, this method can achieve a 100% correct rate, outperforming all the other methods. However, when $\lambda$ is only moderately large, the correct rate quickly drops to a very low level and the method tends to under-estimate $K$. This is consistent with the theoretical understanding, since the theory of this method imposes a strong condition on the magnitude of spiked eigenvalues.

The performance of EKC is also sensitive to the magnitude of spikes. Different from Bai&Ng, EKC performs better when the spiked eigenvalues are not very large. EKC does not use a single threshold for all eigenvalues. It uses a smaller threshold for $\hat{\lambda}_2$ than that for $\hat{\lambda}_1$, and a further smaller threshold for $\hat{\lambda}_3$, and so on. When some spiked eigenvalues are not sufficiently large, the thresholding scheme of EKC makes it easier for the corresponding empirical eigenvalues to stand out. However, when the spiked eigenvalues are all sufficiently large (e.g., Row 6 of Table 1), such a thresholding scheme can yield an over-estimation of $K$.

**Simulation 3.** In this simulation, we change the generation process of eigenvectors, so that they satisfy the “delocalization condition” ([Dobriban and Owen, 2019]) with a higher probability. Recall that the “delocalization condition” means $\|\Xi \Lambda^{1/2}\|_\infty$ is sufficiently small.

Given $(n, p, K, s_1, \cdots, s_K, \theta)$, we generate $X_i \overset{iid}{\sim} N(0, \Sigma)$, $1 \leq i \leq n$, where $\Sigma = BB^\top + D$. The matrix $D = \text{diag}(\sigma_1^2, \sigma_2^2, \ldots, \sigma_p^2)$ is generated in the same way as in Model (7), and $B$ is a $p \times K$ matrix obtained by first generating a $p \times K$ matrix with independent $N(0,1)$ entries and then re-normalizing each column to have an $\ell^2$-norm equal to $s_k \sqrt{p/n}$. Under this setting, the $L_\infty$-norm of each population eigenvector is only $O(p^{-1/2} \sqrt{\log(p)})$, so the “delocalization”
Table 2: Result of Simulation 3. The top four rows (with \( \theta = \infty \)) correspond to the standard spiked covariance model, and the bottom four rows correspond to the general spiked covariance model. The number in each cell is the average \( \hat{K} \), and the number in brackets is the probability of correctly estimating \( K \) (correct rate).

| \((n, p, K, s_1, \theta)\) | BEMA0 | BEMA | DDPA | EKC | Bai&Ng |
|--------------------------|-------|------|------|-----|--------|
| (100, 500, 1, 1, \infty) | 0.99 (98.2%) | 0.952 (95.2%) | 1.102 (89%) | 1.06 (91%) | 0 (0%) |
| (100, 500, 1, 3, \infty) | 1.026 (97.4%) | 1.004 (99.6%) | 1.174 (84.4%) | 3.94 (84%) | 1 (100%) |
| (500, 100, 1, 3, \infty) | 1.008 (99.2%) | 1 (100%) | 1.124 (88.4%) | 1.046 (95.4%) | 0 (0%) |
| (500, 100, 1, 6, \infty) | 1.014 (98.6%) | 1 (100%) | 1.122 (88.6%) | 1.13 (87.4%) | 1 (100%) |
| (100, 500, 1, 2, 10) | – | 1.092 (91%) | 1.282 (75.8%) | 1.162 (83.2%) | 0.378 (37.8%) |
| (100, 500, 1, 6, 10) | – | 1.058 (94.2%) | 1.224 (81%) | 1.646 (55%) | 1 (100%) |
| (500, 100, 1, 6, 3) | – | 1.068 (93.6%) | 1.248 (95.6%) | 1.222 (78.6%) | 1.004 (99.6%) |
| (500, 100, 1, 12, 3) | – | 1.078 (92.4%) | 1.432 (97%) | 3.694 (2.6%) | 1.008 (99.2%) |

condition is satisfied. The numbers \( s_1, \ldots, s_K \) control the magnitude of spiked eigenvalues. The simulation setting here is similar to that in Dobriban and Owen (2019). We fix \( K = 1 \) and let \((n, p, s_1, \theta)\) vary. The results are shown in Table 2.

Compared with the result of Simulation 2, the performance of DDPA has significantly improved. The performance of EKC is slightly better. Bai&Ng behaves similarly as before: It either performs extremely well, when the spiked eigenvalue is sufficiently large, or unsatisfactorily, when the spiked eigenvalue is only moderately large.

The performance of BEMA0 and BEMA is insensitive to the generating process of eigenvectors. In almost every setting, they attain comparable performance with the best method in that setting. This is consistent with our theoretic understanding. In Section 4, we have seen that the success of BEMA0 requires no conditions on eigenvectors.

Simulation 4. In this simulation, we investigate the case of model misspecification. We still assume that \( \Sigma \) is a low-rank matrix plus a residual covariance matrix \( D \). However, we no longer let \( D \) be a diagonal matrix. Below, we consider three misspecified models, where \( D \) is a Toeplitz matrix, a block-wise diagonal matrix, and a sparse matrix, respectively.

- In the first model, \( D(i, j) = (1 + |i - j|)^{-t} \), for \( 1 \leq i, j \leq p \). Here, \( D \) is a Toeplitz matrix with polynomial decays in the off-diagonal. The larger \( t \), the closer to a diagonal matrix.

- In the second model, \( D(i, i) = 1 \) for \( 1 \leq i \leq p \), and \( D(2j - 1, 2j) = D(2j, 2j - 1) = b \) for \( 1 \leq j \leq p/2 \). \( D \) is a block-wise diagonal matrix which has many \( 2 \times 2 \) diagonal blocks. The smaller \( b \), the closer to a diagonal matrix.

- In the third model, \( D(i, i) = 1 \) for \( 1 \leq i \leq p \), and \( D(i, j) = D(j, i) \sim s \cdot \text{Bernoulli}(0.1) \) for \( i \neq j \). The matrix \( D \) has approximately \( 0.1p \) nonzero entries in each row. The smaller \( s \), the closer to a diagonal matrix.
Table 3: Results of Simulation 4. Data are generated from three misspecified models, where the residual covariance matrix is a Toeplitz matrix, a block diagonal matrix, and a sparse matrix, respectively. The number in each cell is the average $\hat{K}$, and the number in brackets is the probability of correctly estimating $K$ (correct rate).

| $\lambda$ | residual covariance | BEMA0 | BEMA | DDPA | EKC | Bai&Ng |
|-----------|----------------------|-------|------|------|-----|--------|
| 6         | Toeplitz($t=4$)      | 1.092 (90.8%) | 1 (100%) | 1.436 (66.4%) | 1.398 (63.0%) | 1 (100%) |
| 3         | Toeplitz($t=2$)      | 9.25 (0%) | 0.878 (82.6%) | 100 (0%) | 1.941 (0%) | 0 (0%) |
| 6         | block diagonal($b=0.1$) | 1.316 (69.2%) | 1 (100%) | 2.492 (31.2%) | 1.928 (31.4%) | 1 (100%) |
| 3         | block diagonal($b=0.2$) | 3.726 (0%) | 0.818 (81.6%) | 100 (0%) | 6.37 (0%) | 0 (0%) |
| 6         | sparse($s=0.05$)     | 1.788 (28.2%) | 1.006 (99.4%) | 4.246 (7.2%) | 2.494 (6.8%) | 1 (100%) |
| 3         | sparse($s=0.08$)     | 3.354 (0%) | 1.004 (98.8%) | 97.77 (0%) | 5.13 (0%) | 0 (0%) |

The low-rank part of $\Sigma$ is generated in the same way as before: We let all $\mu_k$ equal to $\lambda$ and let the eigenvector matrix $\Xi$ be drawn uniformly from the Stiefel manifold. Fix $(n, p, K) = (500, 100, 1)$. The results are shown in Table 3.

For each misspecified model, we consider two settings, where $D$ is closer to a diagonal matrix in the first setting (Rows 1, 3, 5 of Table 3) than in the second one (Rows 2, 4, 6 of Table 3). Every method performs better in the first case, suggesting that the diagonal assumption on $D$ is indeed critical. In comparison, BEMA is least sensitive to a non-diagonal $D$. In Rows 2, 4, 6 of Table 3, the correct rate of BEMA is still above 80%, while the correct rate of other methods is only 0%.

To try to understand this phenomenon, we first note that one can always apply an orthogonal transformation to data vectors $X_1, \ldots, X_n$, so that the post-transformation data follow a different spiked covariance model whose residual covariance matrix $\tilde{D}$ is a diagonal matrix containing the eigenvalues of $D$. This orthogonal transformation is unknown in practice. However, if a method uses the empirical eigenvalues only, it does not matter whether or not we know this orthogonal transformation, because any orthogonal transformation does not change eigenvalues of the sample covariance matrix and thus it does not change the estimator of $K$. It implies that, for methods that only use eigenvalues, we can treat the misspecified model as if $D$ is replaced by the diagonal matrix $\tilde{D}$. Therefore, the surprising robustness of BEMA can be interpreted as the capability of the gamma model (2) in approximating the eigenvalue structure in $D$. The flexibility of this gamma model comes from the parameter $\theta$. In comparison, such strong robustness is not observed for BEMA0, where $\theta$ is fixed as $\infty$.

The method of DDPA uses empirical eigenvectors in the procedure, thus, it is more sensitive to the diagonal assumption of $D$. EKC uses eigenvalues only, but its thresholding scheme is too conservative. In these misspecified models, some bulk empirical eigenvalues can get large; EKC gives too small thresholds to non-leading eigenvalues and yields over-estimation of $K$. 

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6 Real applications

We apply BEMA to two real datasets. We compare our method with EKC (Braeken and Van As- sen, 2017), Bai&Ng (Bai and Ng, 2002), and DDPA and its variants (Dobriban and Owen, 2019). DDPA has three versions: DPA is the original version that is equivalent to parallel analysis (Horn, 1965) but is a deterministic algorithm; DDPA is an improvement of DPA aiming to resolve the issue of “eigenvalue shadowing,” that is, an extremely large spiked eigenvalue shadows the other spiked eigenvalues and causes an under-estimation of $K$; DDPA+ is a robust version of DDPA recommended for real data analysis. We include all three versions in comparison.

6.1 The Lung Cancer data

The Lung Cancer dataset was collected and cleaned by Gordon et al. (2002). The original data set contains the expression data of 12,533 genes and 181 subjects. The subjects divide into two groups, the diseased group and the normal group. Jin and Wang (2016) processed this data set by removing genes that are not differentially expressed across subject groups and resulted in a new data matrix with $(p,n) = (251,181)$. The selection of these 251 “influential genes” used no information of true groups, including the number of groups. We use this processed data matrix, because the original data matrix contains too many features (genes) that are irrelevant to the clustering structure, where no method gives meaningful results.

It was argued in Jin and Wang (2016) that this data matrix follows a clustering model. As a result, the covariance matrix has $(K_0 - 1)$ spiked eigenvalues, where $K_0$ is the number of clusters. Here, the ground-truth is $K_0 = 2$, i.e., the true number of spiked eigenvalues is $K = 1$.

We apply BEMA with $(\alpha, \beta, M) = (0.2, 0.1, 500)$, i.e., $60\% (1 - 2\alpha)$ of the bulk eigenvalues in the middle range are used to estimate model parameters, the probability of over-estimating $K$ is controlled by 0.1, and 500 Monte Carlo samples are used to determine the ultimate threshold for eigenvalues. The BEMA algorithm outputs $(\hat{\theta}, \hat{\sigma}^2) = (0.288, 0.926)$. In Figure 6(a), we check the goodness-of-fit. If the proposed spiked covariance model (7) is suited for the data, we expect to see $\hat{\lambda}_k \approx \hat{\sigma}^2 \cdot F^{-1}_{\gamma}(k/\hat{p}; 1, \hat{\theta})$, except for a few small $k$. The left panel of Figure 6(a) plots $\hat{\lambda}_k$ versus $F^{-1}_{\gamma}(k/\hat{p}; 1, \hat{\theta})$, suggesting a good fit to a line crossing the origin. The right panel contains the scree plot, i.e., $\hat{\lambda}_k$ versus $k$. We also plot the curve of $F^{-1}_{\gamma}(k/\hat{p}; \hat{\sigma}^2, \hat{\theta})$ versus $k$. This curve is a good fit to the scree plot in the middle range. These plots suggest that Model (7) is well-suited for this dataset.

The estimator of $K$ by BEMA is $\hat{K} = 1$, which is exactly the same as the ground truth. This is the output of the algorithm by setting $\beta = 0.1$. Using the argument in Section 3.3, this is also a confidence lower bound for $K$. By setting $\beta = 0.9$ in the algorithm, we get a confidence upper bound which is 4. This gives an 80% confidence interval for $K$ as $[1, 4]$. Figure 6(b) contains the scatter plots of the left singular vectors of $X$, colored by the true group label. The first singular
vector clearly contains information for separating two groups, but other singular vectors also contain some information. This explains why the confidence upper bound is larger than 1.

The comparison with other methods is summarized in Table 4. Except for BEMA and DPA, the other methods over-estimate $K$. The behavior of EKC is consistent with our observation in simulation studies. In this dataset, the eigenvalues of the residual covariance matrix vary widely (this can be seen from the estimated $\theta$ by BEMA, $\hat{\theta} = 0.288$, which is far from $\infty$); as a result, EKC gives too small threshold to non-leading eigenvalues. The behavior of Bai&Ng is different from what we observe in simulations. One possible reason is that we have to use the effective $p$ after the data processing by Jin and Wang (2016), where the dimension reduces from 12,533 to 251. With the reduced $p$, the penalty on $K$ in the information criterion is weaker than that in simulations, and so the method significantly over-estimates $K$. Among DDPA and its variants, DPA (which is a deterministic algorithm to implement parallel analysis) performs the best. A possible reason is that DPA does not use empirical eigenvectors and is more stable than DDPA and DDPA+. We note that $K = 1$ in this dataset, so there is no “eigenvalue shadowing.” When the shadowing effect happens (e.g., in the 1000 Genomes dataset below), DPA tends to under-estimate $K$.

Different from all other methods, BEMA not only outputs an estimator of $K$ but also yields a fitted model, $\text{Gamma}(\hat{\theta}, \hat{\theta}/\hat{\sigma}^2) = \text{Gamma}(0.288, 0.311)$, for eigenvalues of the residual covariance matrix. This can be useful for many other statistical inference tasks.

### 6.2 The 1000 Genomes data

The 1000 Genomes Phase 3 dataset (Consortium, 2015) consists of the genotypes of 2504 subjects for over 84.4 million variants. There are 26 self-reported ethnicity groups, coming from five super-populations: African (AFR), Ad Mixed American (AMR), East Asian (EAS), European (EUS), and South Asian (SAS).

In view of high linkage disequilibrium (LD) among some variants, which can distort the eigenvector and eigenvalue structure (Patterson et al., 2006), we first performed LD pruning. We used an independent pair-wise LD pruning, with window size 1000, step size 50 and a threshold 0.02 for R-squared. Restricting to LD pruned markers, we obtain a data matrix with $p = 24,248$ and $n = 2,504$. The number of spiked eigenvalues equals to the number of true ancestry groups minus one (Patterson et al., 2006). We treat the self-reported ethnicity groups

|                  | BEMA | EKC | Bai&Ng | DDPA | DPA | DDPA+ | truth |
|------------------|------|-----|--------|------|-----|-------|-------|
| Lung Cancer Data | 1    | 56  | 180    | 180  | 1   | 11    | 1     |
| 1000 Genomes Data| 28   | 2503| 4      | 85   | 20  | 4     | 25    |

Table 4: Comparison of methods on two real data sets.
(a) The goodness-of-fit of BEMA on the Lung Cancer data. The left panel plots $\hat{\lambda}_k$ versus $F^{-1}_{\gamma_n}(k/\tilde{p}; 1, \hat{\theta})$ (which is quantile of the theoretical limit of ESD with estimated $\theta$), where the first 4 eigenvalues are removed for better visualization. It fits well a line crossing the origin. The right panel plots $\hat{\lambda}_k$ versus $k$, where the red solid curve is $F^{-1}_{\gamma_n}(k/\tilde{p}; \hat{\sigma}^2, \hat{\theta})$ versus $k$. The curve fits the bulk eigenvalues (blue dots). These two plots together suggest that the spiked covariance model (7) is suitable for this dataset.

(b) The plots of singular vectors of $X$.

Figure 6: Results for the Lung Cancer data.

as the ground truth, which gives $K = 25$.

We apply BEMA with $(\alpha, \beta, M) = (0.1, 0.1, 500)$. First, we check the goodness-of-fit. BEMA outputs $(\hat{\theta}, \hat{\sigma}^2) = (4.256, 0.377)$. Figure 7(a) shows the Q-Q plot and the scree plot, with reference curves from the BEMA fitting. The meaning of these plots is the same as described in Section 6.1 and is also explained in the caption of this figure, which we do not repeat here. The conclusion is that our proposed spiked covariance model (7) is an excellent fit to this dataset.

The estimated model for eigenvalues of the residual covariance matrix is $\text{Gamma}(\hat{\theta}, \hat{\theta}/\hat{\sigma}^2) = \text{Gamma}(4.256, 11.3)$. We note that the variance of the genotype on each SNP is $2q(1-q)$, where $q$ is the null Minor Allele Frequency (MAF) of this SNP. We thus interpret the BEMA fitting as follows: After the ancestry effect is removed, the null MAF $q_j$ (on LD pruned SNPs) satisfy that $2q_j(1-q_j) \overset{iid}{\sim} \text{Gamma}(4.256, 11.3)$. The mean and standard deviation of this gamma distribution is 0.377 and 0.14, respectively.

Next, we look at the estimation of $K$. The BEMA algorithm outputs $\hat{K} = 28$, which is very close to the ground truth $K = 25$. The 98% confidence interval of $K$ is [27, 31], which is obtained by running the algorithm for $\beta = 0.01$ and $\beta = 0.99$, respectively.

The comparison with other methods is summarized in Table 4 where BEMA is closest to the ground truth. EKC and DDPA give $\hat{K} = 2, 503$ and $\hat{K} = 85$, which is significant over-estimation. Bai&Ng and DDPA+ both give $\hat{K} = 4$, which is significant under-estimation. DPA gives $\hat{K} = 20$, which is also under-estimation. DPA is the only competitor that locates $\hat{K}$ in a reasonable range. Its under-estimation is due to that the “eigenvalue shadowing” effect is severe in this dataset:
The goodness-of-fit of BEMA on the 1000 Genomes data. The left panel is the plot of $\hat{\lambda}_k$ versus $F_{\gamma n}(k; \hat{p}; 1, \hat{\theta})$ (which is quantile of the theoretical limit of ESD with estimated $\theta$) for $\alpha n \leq k \leq (1 - \alpha)n$. It fits well a line crossing the origin. The right panel plots $\hat{\lambda}_k$ versus $k$, where the red solid curve is the curve of $F_{\gamma n}(k; \hat{p}; \hat{\sigma}^2, \hat{\theta})$ versus $k$; for better visualization, this curve is only plotted for $11 \leq k \leq 2504$. It fits well the bulk eigenvalues (blue dots). These two plots suggest that the spiked covariance model (7) is suitable for this dataset.

(a) The plots of singular vectors of $X$.

(b) The goodness-of-fit of BEMA on the 1000 Genomes data.

The first a few eigenvalues are far larger than the remaining. DDPA aims to overcome this issue, but it is sensitive to the diagonal assumption on the residual covariance matrix (see Experiment 4 in Section 5), which explains why the performance of DDPA is unsatisfactory. In comparison, BEMA estimates $K$ from exploring the variability in bulk eigenvalues. It is almost not affected by “eigenvalue shadowing” and relatively insensitive to the diagonal assumption.

Last, we validate the results by investigating the singular vectors of $X$. We first measure the association between each singular vector and the true ethnicity labels by the Rayleigh quotient. Let $\tilde{\eta}_k \in \mathbb{R}^n$ be the $k$th left singular vector of the centralized data matrix; we treat its entries as $n$ data points and compute the ratio of between-cluster-variance and within-cluster-variance, denoted as $RQ_k$. The larger $RQ_k$, the more correlated $\tilde{\eta}_k$ with true ethnicity labels. Figure 8(a) plots $RQ_k$ versus $k$. The first a few singular vectors have very high association with the ethnicity labels. These singular vectors capture the super population structure. The pairwise scatter plots of first 4 singular vectors are contained in Figure 7(b), which show clearly that super populations are well separated on these singular vectors. Besides the first few singular vectors, the remaining singular vectors capture more of the sub-structure within each super population. Figure 8(b) is the parallel coordinate plot. The largest $k$ that shows a clear separation of super populations is $k = 23$, which explains the peak at $k = 23$ in the Rayleigh quotient plot. For $k > 23$, the Rayleigh
The association between singular vectors of $X$ and the true ethnicity labels.

The parallel coordinate plot of singular vectors, color-coded by five super-populations.

The parallel coordinate plots of singular vectors for each super-population, color-coded by the ethnicity groups within each super-population. The five super-populations are EAS (top left), EUR (top right), AFR (middle left), AMR (middle right), and SAS (bottom left).

Figure 8: Interpretation of results for the 1000 Genomes data.

Quotient is mainly contributed by the separation of ethnicity groups within super populations. In Figure 8c, we re-generate parallel coordinate plots by restricting to each super population. Within the super population AMR, there is still separation of ethnicity groups for $k$ as large as 27. This explains why BEMA outputs a $\hat{K}$ that is slightly larger than the ground truth.
7 Discussion

We propose a new method for estimating the number of spiked eigenvalues in a large covariance matrix. The novelty of our method lies in a systematic approach to incorporating bulk eigenvalues in the estimation of \( K \). Under a working model which assumes the diagonal entries of the residual covariance matrix are \( iid \) drawn from a gamma distribution, we fit a parametric curve on bulk eigenvalues. The estimated parameters of this curve are then used to decide a threshold for top eigenvalues and produce an estimator of \( K \). We study the theoretical properties of our method under a standard spiked covariance model, and show that our estimator requires weaker conditions for consistent estimation of \( K \) compared with the existing methods. We examine the performance of our method using both simulated data and two real data sets. Our empirical results show that the proposed method outperforms other competitors in a variety of scenarios.

Our approach is conceptually connected to the empirical null (Efron, 2004) in multiple testing. The empirical null imposes a working model (e.g., a normal distribution) on \( Z \)-scores of individual null hypotheses and estimates the parameters of this distribution from a large number of \( Z \)-scores. The fitted null model is then used to correct \( p \)-values and help identify the non-null hypotheses. Similarly, we impose a working model (i.e., a gamma distribution) on non-spiked population eigenvalues and estimate the parameters of this distribution from a large number of bulk empirical eigenvalues. The fitted null model is then used to assist estimation of \( K \).

From this perspective, our method can be regarded as a conceptual application of the empirical null approach to eigenvalues. Meanwhile, our setting is much more complicated than that in multiple testing. The bulk eigenvalues are highly correlated, and their marginal distribution has no explicit form. These impose great challenges on algorithm design and theoretical analysis.

In theory, we analyze a special case when \( \theta = \infty \). It corresponds to the well-known standard spiked covariance model (Johnstone, 2001), which has attracted many theoretical interests. Our theory contributes to this literature with an explicit error bound on estimating \( \sigma^2 \) and consistency theory on estimating \( K \). The theoretical study for a general \( \theta \) is of great interest but is technically challenging. The analysis relies on sharp large deviation bounds for each individual eigenvalue.

In the standard spiked covariance model, we are equipped with the eigenvalue universality theory and eigenvalue sticking theory, which have already been developed in a series of papers in random matrix theory (Bloemendal et al., 2016). For the general spiked covariance model proposed here, there are no such available results. The theoretical investigation of this setting will need to use more sophisticated techniques in random matrix theory. Since the main focus of this paper is development of new methodology for estimating \( K \), we leave such tedious theoretical investigation to future work.

The method can be extended in multiple directions. Here we assume that the diagonal entries of the residual covariance matrix are from a gamma distribution. It can be generalized to other
parametric distributions. For example, we can use a truncated gamma distribution to eliminate extremely large variances for the residuals, and we can also use a mixture of gamma distributions to accommodate heterogeneous feature groups. Our main algorithm can be conveniently adapted to these cases. The thresholding scheme in our method can also be modified. We currently apply a single threshold to all eigenvalues. Alternatively, we may use different thresholds for different eigenvalues. One proposal is using the $(1-\beta)$-quantile of the distribution of $\hat{\lambda}_k^*$ in the null model (12) as a threshold for $\hat{\lambda}_k$. We leave these extensions into future work.

In the numerical experiments, our method exhibits robustness to model misspecification. It is suggested by Simulation 4 of Section 5 that our method continues to work when the residual covariance matrix is a Toeplitz matrix, or a block-wise diagonal matrix, or a sparse matrix. A theoretical understanding to this phenomenon will be useful. As stated in Section 5, we have observed empirically that there always exist $(\sigma^2, \theta)$ such that the theoretical limit of ESD induced by the gamma model (2) can accurately approximate the theoretical limit of ESD induced by a Toeplitz or block-wise diagonal or sparse covariance matrix. It remains an interesting question how to justify it theoretically. We leave it to future work.

8 Appendix

A GetQT algorithms

We present details of the GetQT algorithms used in BEMA. Under the general spiked covariance model (7), the empirical spectral distribution (ESD) converges to a fixed distribution $F_{\gamma}(\cdot; \sigma^2, \theta)$. Write $\gamma_n = p/n$. The purpose of the algorithm GetQT$(y, \gamma_n, \theta)$ is as follows: Fixing $\sigma = 1$, given any $\theta > 0$ and $y \in [0, 1]$, it outputs the $y$-upper-quantile of the distribution $F_{\gamma_n}(\cdot; 1, \theta)$.

A.1 The Monte Carlo simulation algorithm GetQT1

As explained in Section 3.1, $F_{\gamma_n}(\cdot; 1, \theta)$ is also the theoretical limit of the ESD under the following null covariance model:

$$\Sigma = \text{diag}(\sigma_1^2, \ldots, \sigma_p^2), \quad \text{where } \sigma_k^2 \overset{\text{iid}}{\sim} \text{Gamma}(\theta, \theta).$$

(14)

We can simulate data from (14) and use its ESD as a numerical approximation to $F_{\gamma_n}(\cdot; 1, \theta)$.

Write $\tilde{p} = \min\{n, p\}$ and $y = k/\tilde{p}$. When the population covariance matrix satisfies (14), the $k$th eigenvalue of the sample covariance matrix, $\hat{\lambda}_k$, is asymptotically close to the $y$-upper-quantile of $F_{\gamma_n}(\cdot; 1, \theta)$. We thereby use the mean of $\hat{\lambda}_k$, obtained by sampling the data matrix multiple times, to estimate the desired quantile. We note that model (14) only specifies how to sample $\Sigma$, but it does not specify how to sample $X_i$’s. Due to universality theory of eigenvalues
(e.g., see Pillai and Yin (2014)), the choice of distribution of $X_i$’s does not matter much. For convenience, we sample $X_i$’s from multivariate normal distributions. See Algorithm 3.

**Algorithm 3.** GetQT1.

Input: $n$, $p$, $\theta$, $k$, and an integer $B$.

Output: An estimate of the $(k/\hat{p})$-upper-quantile of $F_{\gamma_n}(\cdot; 1, \theta)$.

1. For $b = 1, 2, \ldots, B$, repeat: First generate $\Sigma^{(b)}$ from (14), and then generate $X^{(b)}_i \overset{iid}{\sim} N(0, \Sigma^{(b)})$, $1 \leq i \leq n$. Write $X^{(b)} = [X^{(b)}_1, \ldots, X^{(b)}_n]^\top \in \mathbb{R}^{n \times p}$. Construct the sample covariance matrix $S^{(b)} = (1/n)(X^{(b)})^\top X^{(b)}$ and obtain its $k$th eigenvalue $\hat{\lambda}_k^{(b)}$.

2. Output $\frac{1}{B} \sum_{b=1}^{B} \hat{\lambda}_k^{(b)}$ as the estimated $(k/\hat{p})$-upper-quantile.

In the practical implementation, we use the following strategies to further reduce computation time and memory use: (i) When $n$ is smaller than $p$, we no longer construct the $p \times p$ covariance matrix $S^{(b)}$. Instead, we construct an $n \times n$ matrix $(1/n)X^{(b)}(X^{(b)})^\top$. This matrix shares the same nonzero eigenvalues as $S^{(b)}$ but requires much less memory in eigen-decomposition. This strategy is especially useful for genomic data, where $n$ is typically much smaller than $p$. (ii) In the main algorithm, Algorithm 2, GetQT1 is applied multiple times to compute the $(k/\hat{p})$-upper-quantile for a collection of $k$. We let the sampling step, Step 1 above, be shared across different values of $k$: For each $b = 1, 2, \ldots, B$, we obtain and store $\hat{\lambda}_k^{(b)}$ for all values of $k$; next, in Step 2, we output the estimated $(k/\hat{p})$-upper-quantile simultaneously for all values of $k$. This strategy can significantly reduce the actual running time.

**A.2 The deterministic algorithm GetQT2**

This algorithm directly uses the definition of $F_{\gamma_n}(\cdot; 1, \theta)$. Let $H_\theta(t)$ be the CDF of Gamma($\theta, \theta$). Let $m = m(y, \gamma_n, \theta) \in \mathbb{C}^+$ be the unique solution to the equation

$$y = -\frac{1}{m} + \gamma_n \int \frac{t}{1 + tm}dH_\theta(t).$$

Then, the density of $F_{\gamma_n}(\cdot; 1, \theta)$, denoted by $f_{\gamma_n}(y; 1, \theta)$, satisfies that

$$f_{\gamma_n}(y; 1, \theta) = \frac{1}{\gamma_n \pi} \Im(m(y, \gamma_n, \theta)),$$

where $\Im(\cdot)$ denotes the imaginary part of a complex number.

The above motivates a three-step algorithm.

1. Fix a grid $y_1 < y_2 < \ldots < y_N$. Solve equation \[15\] to obtain $m(y_j, \gamma_n, \theta)$ for $1 \leq j \leq N$.

2. Use equation \[16\] to obtain $f_{\gamma_n}(y_j; 1, \theta)$, for $1 \leq j \leq N$. Obtain the whole density curve $\hat{f}_{\gamma_n}(y; 1, \theta)$ by linear interpolation.

3. Find $q$ such that $\int_q^{(1+\sqrt{m})^2} \hat{f}_{\gamma_n}(z; 1, \theta)dz = y$. Output $q$ as the estimated $y$-upper-quantile.
Step 2 is straightforward. Step 3 is also easy to implement, because \( \hat{f}_{\gamma_n}(y;1, \theta) \) is nothing but a piece-wise linear function. Below, we describe Step 1 with more details.

In Step 1, fix \( y \) and write \( m = a + bi \), where \( i = \sqrt{-1} \), and \( a \in \mathbb{R} \) and \( b \in \mathbb{R}^+ \) are the real and imaginary parts of \( m \), respectively. We aim to find \((a, b)\) so that \( m \) solves the complex equation \((15)\). The equation \((15)\) can be re-written as a set of real equations:

\[
\begin{align*}
\begin{cases}
 y = \gamma_n \int \frac{t}{1+2at+(a^2+b^2)t^2} \, dH_\theta(t), \\
\frac{1}{a^2+b^2} = \gamma_n \int \frac{t^2}{1+2at+(a^2+b^2)t^2} \, dH_\theta(t),
\end{cases}
\end{align*}
\]

\[
\iff
\begin{align*}
\begin{cases}
 2ay = \gamma_n \int \frac{2at}{1+2at+(a^2+b^2)t^2} \, dH_\theta(t), \\
 1 = \gamma_n \int \frac{2at^2}{1+2at+(a^2+b^2)t^2} \, dH_\theta(t).
\end{cases}
\end{align*}
\]

First, by combining the above equations with \( \gamma_n = \gamma_n \int \frac{1+2at+(a^2+b^2)t^2}{1+2at+(a^2+b^2)t^2} \, dH_\theta(t) \), we have

\[
\gamma_n - 1 - 2ay = \gamma_n \int \frac{1}{1+2at+(a^2+b^2)t^2} \, dH_\theta(t) > 0.
\]

It yields that \( a < (\gamma_n - 1)/2y \). Second, by Cauchy-Schwarz inequality, \( \left[ \int \frac{1}{1+2at+(a^2+b^2)t^2} \, dH_\theta(t) \right]^2 \leq \int \frac{1}{1+2at+(a^2+b^2)t^2} \, dH_\theta(t) \cdot \int \frac{t^2}{1+2at+(a^2+b^2)t^2} \, dH_\theta(t) \). It follows that

\[
y^2 \leq (\gamma_n - 1 - 2ay) \cdot \frac{1}{a^2+b^2}.
\]

Re-arranging the terms gives \( (a - 1/y)^2 + b^2 \leq \gamma_n/y^2 \). So far, we have obtained a feasible set of \((a, b)\) for the solution of \((15)\):

\[
S_{y, \gamma_n} = \{(a, b) : (a - 1/y)^2 + b^2 \leq \gamma_n/y^2, a < (\gamma_n - 1)/2y\} \tag{17}
\]

This is a bounded set. Therefore, we can take a grid on this feasible set and solve \((15)\) via grid search. See Algorithm 4.

### A.3 Comparison

We compare the performance of two GetQT algorithms on a numerical example where \((n, p, \theta) = (10000, 1000, 1)\). The results are in Figure 6. To generate this figure, first, we simulate eigenvalues \( \hat{\lambda}^{(b)}_k \) for \( B = 20 \) and plot the histogram of eigenvalues. Next, we plot the estimated density \( \hat{f}_{\gamma_n}(y;1, \theta) \) from GetQT2 (tuning parameter is \( \delta = 0.05 \)). The estimated density fits the histogram well, suggesting that the steps in GetQT2 for estimating \( \hat{f}_{\gamma_n}(y;1, \theta) \) are successful. Furthermore, the estimated quantiles from two algorithms are very close to each other.

In terms of numerical performance, the two GetQT algorithms are similar. We now discuss the computing time. The main computational cost of GetQT1 comes from computing the eigenvalues of \( S^{(b)} \) at each iteration. As we have mentioned in the end of Section A.1 if \( p < n \), we conduct eigen-decomposition on an \( p \times p \) matrix; if \( n < p \), we conduct eigen-decomposition on an \( n \times n \) matrix. Therefore, as long as \( \min\{n, p\} \) is not too large, GetQT1 is fast.

Compared with GetQT1, the advantage of GetQT2 is that it does not need to compute any eigen-decomposition. As a result, when \( \min\{n, p\} \) is large, GetQT2 is much faster than GetQT1.
It follows that we need to choose \( \delta \) to be the number of grid points in the algorithm, governed by the tuning parameter \( \text{GetQT2} \) (and \( \text{GetQT1} \) only in the case that \( \min \text{GetQT2} \) significantly increases the cost of grid search. Our experience suggests that \( \text{Let} \). \( \text{B.1 Proof of Theorem} \)

**Algorithm 4. GetQT2.**

*Input*: \( n, p, \theta, \) and \( y \in [0, 1] \).

*Output*: An estimate of the \( y \)-upper-quantile of \( F_n(.; \theta) \).

**Step 1:** Write \( \tilde{\rho} = n \wedge p \) and \( \gamma_n = p/n \). Fix a grid \( y_1 < y_2 < \ldots y_{N-1} < y_N \). For each \( 1 \le j \le N \), compute \( \hat{m}(y, \gamma_n, \theta) \) as follows:

- For a tuning parameter \( \delta > 0 \), construct the set of grid points in \( \mathbb{R} \times \mathbb{R}_+ \):
  \[
  S_{y, \gamma_n, \delta} = \{(a, b) : a = k\delta, b = \ell\delta, \ k, \ell \in \mathbb{Z}, \ (a - 1/y_j)^2 + b^2 \le \gamma_n/y_j^2, \ a < (\gamma_n - 1)/2y_j\}.
  \]

- For each \( (a, b) \in S_{y, \gamma_n, \delta} \), compute
  \[
  \Delta(a, b) = \left| y + \frac{1}{m} - \gamma_n \int \frac{t}{1 + tm} dH_\theta(t) \right|,
  \]
  where \( H_\theta(t) \) is the CDF of Gamma(\( \theta, \theta \)). The integral above can be computed via standard Monte Carlo approximation (by sampling data from Gamma(\( \theta, \theta \)).

- Find \( (\hat{a}, \hat{b}) = \arg \min_{(a, b) \in S_{y, \gamma_n, \delta}} \Delta(a, b) \). Let \( \hat{m}(y, \gamma_n, \theta) = \hat{a} + \hat{b} \).

**Step 2:** Let \( \hat{f}_{\gamma_n}(y_j; 1, \theta) = \frac{1}{\gamma_n} \mathbb{E}(\hat{m}(y, \gamma_n, \theta)) \), for \( 1 \le j \le N \). For any \( y_{j-1} < z < y_j \), let

\[
\hat{f}_{\gamma_n}(z; 1, \theta) = \frac{y_j - z}{y_j - y_{j-1}} \hat{f}_{\gamma_n}(y_{j-1}; 1, \theta) + \frac{z - y_{j-1}}{y_j - y_{j-1}} \hat{f}_{\gamma_n}(y_j; 1, \theta).
\]

**Step 3:** Find \( q \) such that \( \int_q^{(1+\sqrt{n})^2} \hat{f}_{\gamma_n}(z; 1, \theta) = y \). Output \( q \) as the estimated \( y \)-upper-quantile.

(and \( \text{GetQT2} \) also requires less memory use). The computational cost of \( \text{GetQT2} \) is proportional to the number of grid points in the algorithm, governed by the tuning parameter \( \delta \). Sometimes, we need to choose \( \delta \) sufficiently small to guarantee the accuracy of computing \( \hat{m}(y, \gamma_n, \theta) \), which significantly increases the cost of grid search. Our experience suggests that \( \text{GetQT2} \) is faster than \( \text{GetQT1} \) only in the case that \( \min\{n, p\} \) is larger than \( 10^4 \).

### B Proofs

#### B.1 Proof of Theorem \[1\]

Let \( z_k = \lambda_k - \sigma^2 q_k \), for all \( 1 \le k \le \tilde{\rho} \). It follows that

\[
\hat{\sigma}^2 = \frac{\sum_{\alpha \tilde{\rho} \le k \le (1-\alpha)\tilde{\rho}} q_k (\sigma^2 q_k + z_k)}{\sum_{\alpha \tilde{\rho} \le k \le (1-\alpha)\tilde{\rho}} q_k^2} = \sigma^2 + \frac{\sum_{\alpha \tilde{\rho} \le k \le (1-\alpha)\tilde{\rho}} q_k z_k}{\sum_{\alpha \tilde{\rho} \le k \le (1-\alpha)\tilde{\rho}} q_k^2}.
\]

It follows that

\[
|\hat{\sigma}^2 - \sigma^2| \le \frac{\sum_{\alpha \tilde{\rho} \le k \le (1-\alpha)\tilde{\rho}} |q_k|}{\sum_{\alpha \tilde{\rho} \le k \le (1-\alpha)\tilde{\rho}} q_k^2} \times \max_{\alpha \tilde{\rho} \le k \le (1-\alpha)\tilde{\rho}} |z_k|.
\]

\[\equiv B_{n, p}(\alpha)\]
We recall that $q_k$ is the $(k/p)$-upper-quantile of a standard Machenko-Pastur distribution associated with $\gamma_n = p/n$. Note that $p/n \to \gamma$ and $\alpha \leq k/p \leq 1 - \alpha$, where $\gamma > 0$ and $\alpha \in (0, 1/2)$ are constants. It follows immediately that there is a constant $C_1 = C_1(\alpha, \gamma)$ such that $B_n, p(\alpha) \leq C_1$.

As a result,

$$|\hat{\sigma}^2 - \sigma^2| \leq C_1 \max_{\alpha \leq k \leq (1 - \alpha)p} |\hat{\lambda}_k - \sigma^2 q_k|. \tag{18}$$

We bound the right hand side of (18). By Assumption 1, the data vectors $X_1, X_2, \ldots, X_n$ are generated from a random matrix

$$Y = [Y_1, Y_2, \ldots, Y_n]^\top \in \mathbb{R}^{n \times (p + K)}$$

where the entries of $Y$ are independent variables with zero mean and unit variance. Given $Y$, define $X^*_1, X^*_2, \ldots, X^*_n$ as follows:

$$X^*_i(j) = \sigma \cdot Y_i(j), \quad 1 \leq i \leq n, 1 \leq j \leq p.$$ 

Then, $X^*_1, \ldots, X^*_n$ follow a “null” model that is similar to the factor model in Assumption 1 but corresponds to $K = 0$. Let $S^*$ be the sample covariance matrix of $X^*_1, \ldots, X^*_n$. Then, $S^*$ serves as a reference matrix for $S$. The eigenvalue sticking result says that eigenvalues of $S$ “stick” to eigenvalues of the reference matrix. The precise statement is as follows: Let $\hat{\lambda}_1^* > \hat{\lambda}_2^* > \ldots > \hat{\lambda}_p^*$ be the nonzero eigenvalues of $S^*$. When the entries of $Y$ satisfy the regularity conditions stated in Theorem 1 by Theorem 2.7 of [Bloemendal et al., 2016], there is a constant $C_2 = C_2(\alpha, \gamma, \sigma^2)$ such that, for any $\epsilon > 0$ and $s > 0$,

$$\mathbb{P} \left\{ \max_{(1/2)p \leq j \leq (1 - 1/2)p} |\hat{\lambda}_{j + K_1} - \hat{\lambda}_j^*| > C_2 n^{-(1 - \epsilon)} \right\} \leq n^{-s}, \tag{19}$$

where $K_1$ is the total number of spiked eigenvalues in Model (3) such that $\lambda_k = \sigma^2 (\sqrt{\gamma} + \tau_k)$ for some $\tau_k \geq n^{-1/3}$. It remains to study $\hat{\lambda}_j^*$. Its large deviation bound can be found in [Pillai and Yin, 2014] (also, see Theorem 3.3 of [Ke, 2016]). There is a constant $C_3 = C_3(\alpha, \gamma, \sigma^2) > 0$ such that, for any $\epsilon > 0$ and $s > 0$,

$$\mathbb{P} \left\{ \max_{(1/2)p \leq j \leq (1 - 1/2)p} |\hat{\lambda}_j^* - \sigma^2 q_j| > C_3 n^{-(1 - \epsilon)} \right\} \leq n^{-s}. \tag{20}$$
Furthermore, since $K_1 \leq K$ and $K$ is fixed, there is a constant $C_4 = C_4(\gamma, K)$ such that
\begin{equation}
\max_{(\alpha/2)\bar{p} \leq j \leq (1-\alpha/2)\bar{p}} |q_j - q_{j+K_1}| \leq C_4n^{-1}.
\end{equation}
Combining (24)-(25) gives that, for sufficiently large $n$, appropriately such that for a constant $\epsilon > 0$ and $s > 0$,
\begin{equation}
\mathbb{P}\left\{ \max_{(\alpha/2)\bar{p} \leq j \leq (1-\alpha/2)\bar{p}} |\hat{\lambda}_j + \lambda_{k+1} - \sigma^2 q_{j+K_1}| > Cn^{-(1-\epsilon)} \right\} \leq n^{-s}.
\end{equation}
We plug it into (18). The claim follows immediately.

\section*{B.2 Proof of Theorem 2}

Denote by $T_{n,p}(\hat{\sigma}^2, \beta_n)$ the threshold used in Algorithm 1. It satisfies that
\begin{equation}
T_{n,p}(\hat{\sigma}^2, \beta_n) = \hat{\sigma}^2[(1 + \sqrt{\gamma_n})^2 + \omega_n], \quad \text{where } \omega_n = O(n^{-2/3} t_{1-\beta_n}).
\end{equation}
Here, $t_{1-\beta_n}$ is the $(1 - \beta_n)$-quantile of the Tracy-Widom distribution. We can choose $\beta_n$ appropriately such that for a constant $c_0 \in (0, 1/3),
\begin{equation}
n^{-2/3 - c_0} \leq \omega_n \leq n^{-c_0}.
\end{equation}

First, we derive a lower bound for $\hat{\lambda}_K$ and show that $\hat{K} \geq K$ with probability $1 - o(1)$. Recall that $\lambda_k$ denotes the $k$th largest eigenvalue of $\Sigma$. In view of Model (3), it is true that $\lambda_k = \mu_k + \sigma^2$ for $1 \leq k \leq K$ and $\lambda_k = \sigma^2$, for $K < k \leq p$. Introduce
\begin{equation}
\lambda_k^* = \lambda_k \left(1 + \frac{\gamma_n}{\lambda_k/\sigma^2 - 1}\right), \quad 1 \leq k \leq K.
\end{equation}
Let $g(t) = (1 + t)(1 + \gamma_n/t)$ and rewrite $\lambda_k^* = \sigma^2 \cdot g(\lambda_k/\sigma^2 - 1)$. The function $g$ satisfies that $g(\sqrt{\gamma_n}) = (1 + \sqrt{\gamma_n})^2$ and $g'(t) \geq 1 - \sqrt{\gamma_n}/t$. Hence, it is monotone increasing in $(\sqrt{\gamma_n}, \infty)$. For any $\tau > 0$ and $t > \sqrt{\gamma_n} + \tau$, we have $g(t) \geq g(\sqrt{\gamma_n}) + g'(\sqrt{\gamma_n} + \tau) \cdot \tau \geq (1 + \sqrt{\gamma_n})^2 + \tau^2/\sqrt{\gamma_n} + \tau$. By our assumption, $\lambda_K/\sigma^2 - 1 \geq \sqrt{\gamma_n} + \tau$. It follows that
\begin{equation}
\lambda_k^* \geq \sigma^2 \left[1 + \sqrt{\gamma_n}^2 + C_5\right],
\end{equation}
where $C_5 = C_5(\tau, \gamma) = \tau^2/(\sqrt{\gamma_n} + \tau)$. We apply Theorem 2.3 of Bloemndal et al. (2016): There is a constant $C_6 = C_6(\gamma, \sigma^2, \tau)$ such that, for any $\epsilon > 0$ and $s > 0$,
\begin{equation}
\mathbb{P}\left\{ |\hat{\lambda}_K - \lambda_k^*| > \lambda_k^* \cdot C_6 n^{-(1-\epsilon)} \right\} \leq n^{-s}.
\end{equation}
Combining (24)-25 gives that, for sufficiently large $n$,
\begin{equation}
\mathbb{P}\left\{ \hat{\lambda}_K > \sigma^2 \left[1 + \sqrt{\gamma_n}^2 + 2C_5/3\right] \right\} = 1 - o(1).
\end{equation}
Furthermore, by Theorem 1 $|\hat{\sigma}^2 - \sigma^2| = O(n^{-0.9})$ with probability $1 - n^{-2}$. It yields that
\begin{equation}
\mathbb{P}\left\{ \hat{\lambda}_K > \sigma^2 \left[1 + \sqrt{\gamma_n}^2 + C_5/3\right] \right\} = 1 - o(1).
\end{equation}
We compare $\hat{\lambda}_K$ with the threshold in (22). Since $\omega_n \leq n^{-\epsilon_0}$, it is implied from (26) that $\hat{\lambda}_K$ exceeds this threshold with probability $1 - o(1)$. Therefore,

$$P\{\hat{K} \geq K\} = 1 - o(1).$$

Next, we derive an upper bound for $\hat{\lambda}_{K+1}$ and show that $\hat{K} \leq K$ with probability $1 - o(1)$. We apply Theorem 2.3 of [Bloemendal et al. 2016] again: For any $\epsilon > 0$ and $s > 0$,

$$P\left\{|\hat{\lambda}_{K+1} - \sigma^2(1 + \sqrt{\gamma n})^2| > \sigma^2 n^{-2/3 - \epsilon}\right\} \leq n^{-s}. \tag{27}$$

Let $\epsilon = \epsilon_0/2$ and use the large deviation bound for $\hat{\sigma}^2$ in Theorem [1]. We immediately find that

$$P\left\{\hat{\lambda}_{K+1} < \hat{\sigma}^2 \left[(1 + \sqrt{\gamma n})^2 + n^{-2/3 - \epsilon_0/2}\right]\right\} = 1 - o(1). \tag{28}$$

We compare $\hat{\lambda}_{K+1}$ with the threshold in (22). Since $\omega_n \geq n^{-(2/3 - \epsilon_0)}$, it follows that $\hat{\lambda}_{K+1}$ is below this threshold with probability $1 - o(1)$. Therefore,

$$P\{\hat{K} \leq K\} = 1 - o(1).$$

The claim follows immediately.

\[ \square \]

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