Confidence Intervals for the Number of Components in Factor Analysis and Principal Component Analysis via Subsampling

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Abstract

Factor analysis (FA) and principal component analysis (PCA) are popular statistical methods for summarizing and explaining the variability in multivariate datasets. By default, FA and PCA assume the number of components or factors to be known \emph{a priori}. However, in practice the users first estimate the number of factors or components and then perform FA and PCA analyses using the point estimate. Therefore, in practice the users ignore any uncertainty in the point estimate of the number of factors or components. For datasets where the uncertainty in the point estimate is not ignorable, it is prudent to perform FA and PCA analyses for the range of positive integer values in the confidence intervals for the number of factors or components. We address this problem by proposing a subsampling-based data-intensive approach for estimating confidence intervals for the number of components in FA and PCA. We study the coverage probability of the proposed confidence intervals and provide non-asymptotic theoretical guarantees concerning the accuracy of the confidence intervals. As a byproduct, we derive the first-order \emph{Edgeworth expansion} for spiked eigenvalues of the sample covariance matrix when the data matrix is generated under a factor model. We also demonstrate the usefulness of our approach through numerical simulations and by applying our approach for estimating confidence intervals for the number of factors of the genotyping dataset of the Human Genome Diversity Project.

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1 Introduction

1.1 Motivation

Factor analysis (FA) and principal component analysis (PCA) are well-established statistical techniques for explaining the variability in multivariate datasets. More precisely, for a data matrix $X$ consisting of $p$ features collected on $n$ samples, researchers use FA for attributing the dependencies among the $p$ features to few latent factors, whereas they use PCA for explaining the variability observed in terms of the first few principal components (see Anderson (1958) pg 569 [1]). Moreover, FA and PCA are increasingly becoming popular as dimension reduction techniques for large multivariate datasets (see [2], [3], [4], [5]). Although FA and PCA continue to remain popular statistical techniques, the concern related to selecting the number of factors or components in FA and PCA remains, see Costello and Osborne (2005) [6]. For the sake of simplicity, henceforth we use components for denoting both factors and components in FA and PCA.

By default, FA and PCA assume the true number of components to be known a priori. However, in practice the users use the point estimate as a substitute for the true number of components and thereby ignore any uncertainty in the point estimate. Therefore, for all practical purposes, estimating the number of components is the most important decision for effectively performing FA and PCA analyses, (see [6], [7], [8], [9], [10], [11],[12]). Zwick and Velicer (1986) [8] put this in context. They pointed out that the under-specification of the number of components will result in the loss of information of components either by ignoring a component or by combining multiple components. This loss, due to the under-specification, is rather grave if significant resources were expended to collect a large dataset only to throw away significant signals during dimension reduction. On the other hand, the over-specification of the number of components will weaken the estimated signal strength by combining the true signal with noise and may result in an incorrect understanding of the underlying data generating process. Rather than ignoring the uncertainty in the point estimate, it is prudent to quantify the uncertainty in the point estimate using a high confidence interval for the number of components and then perform FA and PCA analyses for all positive integer values in the confidence interval (i.e., the confidence set for the number of components). In this paper, we propose a subsampling-based data-intensive approach for estimating confidence intervals for the number of components in FA and PCA.
1.2 Existing methods for estimating the number of components

The existing methods for estimating the number of components in FA and PCA can be grouped into three categories. The first approach considers the problem of estimating the number of components as a model selection problem. The main idea is that the true model (i.e., the model with the true number of components) will maximize a penalized likelihood function or some other information criteria. Bai and Ng (2002) [13] proposed an information criterion-based approach for estimating the number of components. Later, Bai et al. (2018) [14] proved that the methods maximizing Akaike information criteria (AIC) and Bayesian information criteria (BIC) are also consistent for estimating the number of components in PCA.

The second approach is motivated by the scree test (Cattell (1966) [15]) method. The scree test entails visually inspecting the scree plot (i.e., the line plot of ordered eigenvalues of the sample correlation matrix in the descending order) for an elbow. The number of components to the left of the elbow in the scree plot is the estimate of the number of components. Onatski (2009) [16] quantified the elbow in the scree plot using the maximum ratio of consecutive eigenvalue gap statistics and used it for estimating the number of components.

The third approach estimates the number of components by comparing eigenvalues of the sample covariance matrix against an empirical threshold. The number of eigenvalues that are larger than the empirical threshold is the estimate of the number of components. Horn (1965)’s parallel analysis prescribed computing the empirical threshold as the mean of eigenvalues of sample correlation matrices generated from Monte Carlo (MC) simulations under the null hypothesis. Buja and Eyboglu (1992) [18]’s PA estimated the empirical threshold as the mean of the eigenvalues of sample correlation matrices of permuted data matrices, where permuted data matrices were generated by independently permuting column entries of the data matrix. Hong, Sheng, and Dobriban (2020) [19] extended parallel analysis for estimating the number of components in PCA under heterogeneous noise using the sign flip method. Recently, several authors have used the random matrix theory (RMT) for estimating the threshold. Dobriban and Owen (2019) [20] proposed three different methods, namely: DPA, DDPA, and DDPA+ for estimating the number of components that estimated the threshold using the Marchenko-Pastur (MP) distribution. Cai, Han, and Pan (2020) [21] estimated the threshold using the upper-endpoint of the scale-adjusted Tracy-Widom (TW) high confidence interval. Ke, Ma, and Lin (2020) [22] estimated the threshold using a weighted sum of quantiles of the Marchenko-Pastur distribution. Fan, Guo, and Zheng (2020) [23] estimated
the number of components by thresholding the unbiased estimators of the largest few eigenvalues of the population correlation matrix at the phase-transition threshold of \((1 + \sqrt{\gamma})\), where \(\gamma_n \to \gamma\) as \(n \to \infty\) and the aspect ratio \(\gamma_n\) is the ratio of the number \(p\) of columns of the data matrix \(X\) to the number \(n\) of rows of the data matrix \(X\).

1.3 Other related works

1. Larsen and Warne [11] discussed two methods for constructing confidence intervals for eigenvalues of the population covariance matrix in exploratory factor analysis. The two methods use the asymptotic distribution of the eigenvalues in classical low-dimensional asymptotics (i.e., \(\gamma_n = p/n \to \gamma = 0\)) [1, 24]. As we discuss, these two methods do not yield a good approximation of the spiked eigenvalues of the sample covariance matrix (i.e., spiked eigenvalue of the sample covariance matrix is an eigenvalue whose corresponding population eigenvalue is larger than the phase transition threshold of \((1 + \sqrt{\gamma})\)) when the underlying data matrix \(X\) is generated from a factor model.

2. Recently, Saccenti and Timmerman (2017) [25] compared parallel analysis and the sequential TW tests of Johnstone (2001) [26] that refit the variance and the number of features of the TW distribution to the deflated data. They showed that for the maximum eigenvalue \(\lambda_1\) of the sample covariance matrix parallel analysis is equivalent to a test based on the TW distribution. For the further eigenvalues, parallel analysis can be viewed as relying on the joint distribution of eigenvalues, as opposed to the conditional distributions given the previous ones. They observed that under an alternative when the maximum eigenvalue \(\lambda_1\) is small, parallel analysis can have a much larger false positive rate than the nominal one. We can understand this heuristically as the empirical second largest eigenvalue may be larger in this case than under the global null. They argue that the sequential TW tests are empirically more accurate, while still being heuristic methods.

3. Recently, Ke, Ma, and Lin (2020) [22] proposed an approach for estimating confidence intervals for the number of components in FA and PCA using bulk eigenvalue matching analysis. Their approach rely on smoothing the bulk eigenvalues of the residual covariance matrix using quantiles of the Marchenko-Pastur distribution (i.e., eigenvalue matching analysis). In particular, they use the eigenvalue matching analysis and the assumption that the diagonal entries of the residual covariance matrix follow a gamma distribution for estimating confidence
intervals for the number of components. As we discuss, we see that the coverage probability of their proposed confidence interval is not close to the nominal confidence level. We discuss this in the Section 4. Moreover, their approach do not provide any theoretical guarantees for the coverage probability of their proposed confidence intervals for finite-sample cases, i.e., non-asymptotic cases.

1.4 Overview

Let \( X = (x_1, \ldots, x_n)^\top \) denote a data matrix comprising of measurements taken on \( p \) features for \( n \) independent units. Then for the \( i^{th} \) unit, the standard linear factor model (see [1],[27]) is given as follows

\[
x_i = \mu + \Lambda \eta_i + \varepsilon_i,
\]

(1)

where \( \mu = (\mu_1, \ldots, \mu_p)^\top \), \( \Lambda \) is the factor loading matrix of dimension \( p \times r \), \( \eta_i = (\eta_{i1}, \ldots, \eta_{ir})^\top \) are the factor scores for the \( i^{th} \) sample, and \( \varepsilon_i = (\varepsilon_{i1}, \ldots, \varepsilon_{ip})^\top \) is the residual vector. Assume that the data matrix \( X \) is centered, then the matrix version of the above factor model is as follows

\[
X = Z \Theta^{1/2} \Lambda^\top + \mathbb{E},
\]

(2)

where \( Z \) is the \( n \times r \) matrix containing the standardized factor values, \( \Theta \) is a diagonal matrix with diagonal elements controlling the scale of variability for each component, \( \Lambda \) is the loading matrix of dimension \( p \times r \), and \( \mathbb{E} \) is the residual matrix with \( \varepsilon_i \) as the \( i^{th} \) row of \( \mathbb{E} \).

Our approach is a subsampling-based data-intensive approach that uses eigenvalues of conditionally independent submatrices (conditional independent given \( X \)) to estimate confidence intervals for the number of components. The detailed approach is as follows. We sample \( b \) conditionally independent submatrices (conditional on the data matrix \( X \)) of the same dimensions that share the aspect ratio with the data matrix \( X \), i.e., \( \gamma_n = \frac{p}{n} \), where \( b \) is a positive integer greater than one. Subsequently, we divide \( b \) conditionally independent submatrices into a set of \( (b-1) \) submatrices and the remaining submatrix (henceforth, we will refer to it as the lone submatrix). Assume that the eigenvalues of any Hermitian matrix are always arranged in the decreasing order from the largest eigenvalue to the smallest eigenvalue. Using the eigenvalues of sample covariance matrices of the \( (b-1) \) submatrices, we construct empirical confidence intervals for the (unknown) eigenvalues of the population covariance submatrix at the confidence level \( \beta \), where \( 0.5 < \beta < 1 \). Then, our preliminary estimate for the number of components is one less than the first index of the empirical
confidence intervals that does not contain corresponding eigenvalue of the sample covariance matrix of the lone submatrix. For example, in the Figure 3, the first index of the eigenvalues of the sample covariance matrix of the lone submatrix that does not lie in the corresponding empirical confidence intervals is second. Therefore, the preliminary estimate is one. The preliminary estimate is comparable to the third approach in Section 1.2 in the following manner. Rather than comparing eigenvalues against an empirical threshold (i.e., testing whether eigenvalues lie in a one-sided confidence interval), we use the test whether eigenvalues lie in two-sided confidence intervals for estimating the number of components. However, the preliminary estimate is weak because we have discarded a large portion of the data matrix $X$. For improving the estimate and estimating confidence intervals for the number of components, we average the preliminary estimate independently (conditional on the data matrix $X$) across sets of $(b-1)$ submatrices and sets of lone submatrix thus estimating confidence interval for the number of components at the confidence level $\beta$, see Section 2 for details. For optimizing the performance of our method, we need to appropriately select our hyperparameters, including the choice of $b$ and $\beta$. As we show later, the optimum selection of the hyperparameters $b$ and $\beta$ in our approach is connected with the first-order Edgeworth expansion of the spiked eigenvalues of the sample covariance matrix of the lone submatrix.

We briefly discuss our main theoretical result. Consider the setup of spiked PCA, first considered by [26]. Suppose the eigenvalues of the population covariance matrix $\Sigma$ of the data matrix $X$ generated under PCA consists of $r$ eigenvalues that are greater than one and $(p-r)$ eigenvalues that are one. For high-dimensional asymptotic regime (i.e., $\gamma_n = p/n \to \gamma \in (0, \infty)$ as $n \to \infty$), Baik, Arous, and Pêché (2005) [28] proved phase transition for eigenvalues of the sample covariance matrix. In particular, they proved that in the high-dimensional asymptotic regime when an eigenvalue $l$ of the population covariance matrix $\Sigma$ is smaller than the phase-transition threshold $(1+\sqrt{\gamma})$, the corresponding estimated eigenvalue, after appropriately scaling and centering, converges to the TW distribution with a convergence rate of $n^{2/3}$. Moreover, they proved that in the high-dimensional asymptotic regime when the eigenvalue $l$ is greater than the phase-transition threshold $(1+\sqrt{\gamma})$, (i.e., a spiked eigenvalue), the corresponding estimated spiked eigenvalue $\hat{l}$, after appropriately centering and scaling, converges in distribution to a normal distribution with a convergence rate of $n^{1/2}$, i.e.,

$$n^{1/2} \left( \frac{\hat{l} - \rho(l, \gamma_n)}{\sigma(l, \gamma_n)} \right) \xrightarrow{\mathcal{L}} N(0,1),$$

where $\mathcal{L}$ denotes converges in distribution, and the centering and scaling parameter has the following
analytical form (see [28, 29, 30])

$$\rho(l, \gamma) = l + \frac{\gamma l}{(l - 1)}, \quad \sigma^2(l, \gamma) = 2l^2 \left( 1 - \frac{\gamma}{(l - 1)^2} \right).$$  \hfill (3)

Improving upon this result, Yang and Johnstone [29] derived a first-order *Edgeworth* correction result for the spiked eigenvalues of the sample covariance matrix. Moreover for FA, the above *phase transition* also occurs, but the exact analytical form of centering and scaling parameters are difficult to compute in a general case, (see Theorem 11.11 of [31] (pg 234-235, Chapter 11)). Recently, Cai, Han, and Pan (2020) showed that, in that case of FA, the $i^{th}$ (spiked) eigenvalue of the sample covariance matrix asymptotically converges to a normal distribution provided the $i^{th}$ eigenvalue $l_i$ of the population covariance matrix $\Sigma$ is larger than the phase transition threshold $(1 + \sqrt{\gamma})$ and $\gamma_n/l_i \to 0$ as $n \to \infty$.

We use a subsampling approach for estimating the centering and scaling parameters. In particular, we independently sample $M$ (conditional on the data matrix $X$) submatrices of size $\lceil n/b \rceil \times \lceil p/b \rceil$. Then, we numerically compute $\rho^*_j$ and $\sigma^*_j$ as the average and standard deviation of the $j^{th}$ largest eigenvalues of the subsampled covariance matrices (i.e., sample covariance matrices of the subsampled matrices). Then, the centering and scaling parameter is given as follows

$$\rho_j(\lceil n/b \rceil, \gamma_n) = \rho^*_j, \quad \sigma_j(\lceil n/b \rceil, \gamma_n) = \sigma^*_j.$$  \hfill (4)

As we discuss, we see the centering and scaling parameter in (4) leads to a better density approximation of spiked eigenvalues of subsampled covariance matrix, see Figure 2. Analytically, we derive a first-order *Edgeworth expansion* result for the spiked eigenvalues of the sample covariance matrix of the lone submatrix. The main idea behind the proof is that a substitution covariance matrix can be written as a sum of two positive semidefinite matrices. We exploit this structure to first solve the determinant equation and then obtain the first-order *Edgeworth expansion* for the spiked eigenvalues of the substitution covariance matrix. Thereafter, we use the Delta theorem to extend this result to the spiked eigenvalues of the sample covariance matrix.

Our theoretical result guaranteeing the non-asymptotic coverage accuracy of our proposed confidence intervals follow from the following observations. We observe that the preliminary estimate is essentially a convolution of a lone spiked (sample) eigenvalue and the mean of $(b - 1)$ conditionally independent spiked (sample) eigenvalues. Also, we have the first-order *Edgeworth expansion* for the spiked eigenvalues of the sample covariance matrix of the lone submatrix. From Theorem 2.2 of Hall (1993) [32], the mean of $(b - 1)$ spiked eigenvalues of sample covariance matrices of $(b - 1)$
Figure 1: Visual representation of the subsampling data matrix. The shaded part on the left denotes the original data matrix $X$ whereas the shaded and dotted part denote submatrices. The submatrices are selected in the manner such that they do not overlap and have the same dimensions while sharing the aspect ratio with the data matrix $X$.

submatrices also has a first-order Edgeworth expansion. Then, our proposed confidence interval is obtained by independently averaging over the choice of lone submatrix and a set of $(b-1)$ independent submatrix conditional on $X$. Then, we use the Berry-Esseen inequality and the convolution of the above-mentioned first-order Edgeworth correction of lone spiked eigenvalue and the mean of $(b-1)$ spiked eigenvalues to get an error bound of the coverage accuracy of the proposed confidence interval. As a consequence, the hyperparameters are obtained by minimizing the above error bound. The optimum choice of the hyperparameter $b$ is $\lfloor n^{1/3} \rfloor$, whereas the optimum hyperparameter $\beta$ is obtained by optimizing the conditional likelihood over a grid of $\beta$ values. We also discover that our proposed confidence intervals have greater accuracy for high confidence levels.

Organization of the paper. Our contributions are the following: i) We propose a new likelihood-based estimator for estimating the number of components in FA and PCA. ii) We propose a subsampling-based approach for estimating confidence intervals for the number of components in FA and PCA. iii) We also derive a non-asymptotic upper bound for the coverage accuracy for our proposed confidence intervals. iv) As a byproduct, we also derive a first-order Edgeworth expansion for the spiked eigenvalues of the sample covariance matrix generated under a factor model. v) Furthermore, we obtain a sharp upper bound on the spectral norm of a cross-product of two
random matrices. The rest of the paper is organized as follows. In Section 2, we describe the set up of our problem. Moreover in Section 2, we propose a subsampling algorithm for estimating confidence intervals for the number of components while also proposing a likelihood-based approach for estimating the number of components. In Section 3, we derive a first-order Edgeworth correction result for the spiked eigenvalues of the sample covariance matrix when the underlying data matrix was generated under a factor model. In addition, we derive a non-asymptotic bound for the coverage accuracy for our proposed confidence intervals of the number of components. In Section 4, we perform numerical evaluation of our approach through various simulation scenarios. In Section 5, we demonstrate the usefulness of our approach for carrying out FA and PCA on the genotyping data of Human Genome Diversity Project. Section 6 ends with the discussion of our proposed approach.

2 Methods

2.1 Notations and Preliminaries

For any two sequences \( \{a_n\} \) and \( \{b_n\} \), we say \( b_n = O(a_n) \) when there exist constants \( C \) and \( n_0 \) such that \( |b_n| \leq Ca_n \) for all \( n \geq n_0 \). Likewise, we denote \( b_n = o(a_n) \) when for any arbitrarily small \( \epsilon > 0 \) there exist \( n_0 \) such that \( |b_n| < \epsilon a_n \) for all \( n \geq n_0 \). For the rest of the discussion, we assume that the eigenvalues of any Hermitian matrix are always ordered in the decreasing order (i.e., arranged from the largest to the smallest). We also denote the greatest integer function by \( \lfloor \cdot \rfloor \).

The matrix factor model in (2) is overparametrized and therefore not identifiable. To make the model identifiable, we need to impose condition A.1 on the loading matrix \( \Lambda \), see [33] for review of identifiability conditions in FA. Moreover, for estimating the model parameters of FA in (2), we assume that the signal and the error matrices are independent, see assumption A.2. Further, we assume that the signal matrix and the error matrix are centered, see assumption A.3.

A.1 (Identifiability) Assume that the factor loading matrix \( \Lambda \) satisfies \( \Lambda^\top \Lambda = I_r \), where \( I_r \) is the identity matrix of dimension \( r \times r \).

A.2 (Independence) Assume that the signal matrix \( Z\Theta^{1/2}\Lambda^\top \) and the noise matrix \( E \) are independent.

A.3 (Centering) Assume that the expected signal and expected noise are zero matrices, i.e., \( \mathbb{E}(Z\Lambda^\top) = 0_{n \times p} \) and \( \mathbb{E}(E) = 0_{n \times p} \), where \( 0_{n \times p} \) denotes a matrix of dimension \( n \times p \) with all
of its entries as zero.

Furthermore, we impose additional assumptions (A.4)-(A.6) on the matrix factor model in (2) for obtaining theoretical guarantees for our proposed confidence intervals.

A.4 (Score Normality) Assume that the elements of factor score $Z$ are independent realizations from the standard normal distribution, i.e., $N(0, 1)$.

A.5 (Error Normality) Assume that the elements of noise matrix $E$ are independent realizations from the standard normal distribution.

A.6 (Signal Strength) Assume that $\Theta = \text{diag}(\theta_1, \cdots, \theta_r)$ the diagonal matrix controlling the scale of variability for each factor consists of $\theta_j$ that are at least of the order $O(p^{1+\delta})$ for any $j = 1, \cdots, r$ and arbitrarily small $\delta > 0$.

Assumption A.4 ensures that all the elements of factor values matrix $Z$ are independent realizations from the standard normal distribution. Intuitively, assumption A.4 assumes that the component signals are distorted uniformly across the $n$ sample units. Assumption A.5 assumes that the residuals are independent realizations from the standard normal distribution. Note that the data matrix $X$ can be appropriately centered and scaled to ensure that the elements of $E$ (i.e., error terms) in (2) are normally distributed with mean zero and variance one. Assumption A.6 prescribes the minimum order of the scale of variability. As the scale factor of every component becomes large, the signal components will overwhelm the noise. A common assumption in this context is to assume that the eigenvalues of $Z\Theta Z^\top$ increases with $p$. Bai and Ng (2003)[34] and Fan, Yuan, and Mincheva (2013) [35] estimated the number of factors under the assumption that the leading eigenvalues of $Z\Theta Z^\top$ increases with $p$. Onatski (2009) [36] proposed a sequential hypothesis test for estimating the number of factors when the leading eigenvalues of $Z\Theta Z^\top$ increased with $p^\theta$, where $0 < \theta < 1$. Recently, Cai, Han, and Pan (2020) [21] obtained the asymptotic distribution of the spiked eigenvalues of the sample covariance matrix under the assumption that $p/(nl_i) \to 0$, where $l_i$ denote $i^{th}$ spiked eigenvalue of the population covariance matrix of $X$. In assumption A.6, we assume that the scale factor, the diagonal elements of $\Theta$, increased at the rate of $p^{1+\delta}$ for any arbitrarily small $\delta > 0$, i.e., $O(p^{1+\delta})$. Equivalently, in our setup, this means that the eigenvalues corresponding to the signal matrix are atleast $O(p^{1+\delta})$. The rest of the analysis is carried when $\gamma_n = p/n \to \gamma \in (0, 1]$. For $\gamma \in [1, \infty)$, we can proceed further by taking the transpose of the data matrix $X$. 

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2.2 Likelihood-based estimator

We propose a sequential likelihood procedure for estimating the number of components in the matrix factor model in (2). We know from Lee and Schnelli (2016) [37] that the largest eigenvalue of the residual sample covariance matrix (sample covariance matrix computed after removing all signals) follows a TW distribution. We use this result to estimate the number of components in the matrix factor model in (2). In particular, our estimate of the number of components is one less than the first index for which TW density evaluated at the \((r + 1)^{th}\) eigenvalue is greater than an arbitrarily small positive number \(\delta_0\). An insight into the above observation follows from noting that for spiked eigenvalues that are well above the phase transition threshold of \((1 + \sqrt{\gamma})\), the TW likelihood would approach zero.

Algorithm 1 Likelihood Based Estimator for the Number of Spikes

1: Column-wise center and scale the data matrix \(X\).
2: Assume the eigenvalues of the sample covariance matrix of \(X\) is given as \(\hat{l}_1 > \hat{l}_2 > \cdots > \hat{l}_p\).
3: Initialize \(\hat{r} = 0\).
4: Choose \(\delta_0\) to be an arbitrarily small positive number, say \(\delta_0 = 0.01\).
5: If Tracy-Widom density evaluated at \(\hat{r} + 1\) eigenvalue is less than \(\delta_0\) then stop and return the number of components as \(\hat{r}\). Otherwise, go to Step 6.
6: Increase \(\hat{r}\) by one, i.e., \(\hat{r} = \hat{r} + 1\) and go to Step 5.

Theorem 2.1 Assume that the correlation matrix \(\Sigma\) of data matrix \(X\) generated from the model in (2) has exactly \(r\) spiked eigenvalues that are greater than \((1 + \sqrt{\gamma})\), where \(r\) is an unknown positive integer and the aspect ratio \(\gamma\) is the ratio of the number of columns to the number of rows. Moreover, assume that the data matrix \(X\) satisfy assumptions (A.1)-(A.6). Then, we show that the estimate of the number of components in the Algorithm 1 is consistent, as \(n \to \infty\), i.e.
\[
P(\hat{r} = r) \to 1, \text{ as } n \to \infty.
\]

Proof See the Appendix.

The likelihood-based estimator in Algorithm 1 in comparison to the other methods, such as PA, is more sensitive to the normality assumption in (A.4)-(A.5). Moreover, the likelihood-based estimator assumes that the spiked eigenvalues to be large, see assumption (A.6). As we discuss, the usefulness of the likelihood-based estimator lies in correctly pegging (or centering) our proposed
confidence intervals for the number of components around a consistent estimator for the number of components.

2.3 Subsampling algorithm

We propose a subsampling-based approach for estimating confidence intervals for the number of components. Our algorithm is described as follows. Consider a data matrix $X$ generated from the factor model in (2). We partition the data matrix $X$ into a lone submatrix and a set of $(b - 1)$ submatrices, i.e., \( \{X_\star, \{X_{\pi_i}\}_{i=1}^{b-1}\} \) such that all $b$ submatrices are conditionally independent given $X$ and are of same dimensions with the common aspect ratio as that of $X$, i.e., $\gamma_n = p/n$. The rationale for choosing the submatrices of the same dimensions is to make the singular values of all the partitions comparable. Since we know from Theorem 11.11 of [31] (pg 234-235, Chapter 11) that the distribution of eigenvalue of any sample covariance matrix is parametrized in its aspect ratio, therefore we fix the aspect ratio of the above submatrices as that of the aspect ratio of $X$. We use eigenvalues of $(b - 1)$ subsampled covariance matrices, i.e., \( \{\frac{X_{\pi_i}X_{\pi_i}^\top}{(n/b)}\}_{i=1}^{b-1} \) to construct empirical confidence intervals for eigenvalues of the unknown population covariance submatrix corresponding to the subsampled covariance matrices at the confidence level $\beta$, where $0 < \beta < 1$. Then, using the eigenvalues of the lone subsampled covariance matrix $\frac{X_\star X_\star^\top}{(n/b)}$, we obtain our preliminary point estimate as one less than the first index of the empirical confidence intervals that does not contain the corresponding eigenvalues of $\frac{X_\star X_\star^\top}{(n/b)}$, see Figure 3. This approach can be likened to the third approach in the existing literature (Section 1.2). Recall that the third approach entails the step of comparing eigenvalues of the sample covariance matrix against an empirical threshold that can be interpreted as testing whether eigenvalues lie in a one-sided confidence interval. In comparison, our approach entails testing whether eigenvalues of the sample covariance matrix of lone submatrix lie in a two-sided confidence interval.

We trim the confidence intervals by $\epsilon_0/[n/b]$ on both ends. For the fixed $\beta$, the trimming of the confidence interval would tend to decrease the preliminary estimate. The trimming constant is scaled by $[n/b]$ for keeping the trimming constant comparable with the eigenvalues of the subsampled covariance matrix. The default choice of $\epsilon_0$ is 0.02 is rather arbitrary and one could select any arbitrarily small positive number. However, choosing $\epsilon_0$ as a large number is not desirable as it might significantly reduce the preliminary estimate to possibly zero. The trimming of the confidence interval does not affect the theory of our approach because it is equivalent to selecting a lower value of confidence level $\beta$. However, in practice, trimming gives a slightly improved performance.
by helping us effectively choose the optimum $\beta$ by refining the grid values of $\{\beta^{(i)}\}_{i=1}^g$ as a function of the size of the subsample matrix.

For further improving the preliminary point estimate, we generate $M$ random sets where each set consist of a lone submatrix and a set of $(b-1)$ submatrices of equal dimensions with the common aspect ratio $\gamma_n$ such that all $b$ submatrices are conditionally independent given $X$, i.e., $\{X_j^i, (X_j^i)_{i=1}^{b-1}\}_{j=1}^M$. Averaging the preliminary point estimate over $M$ sets gives us a much-improved point estimate, say $\hat{r}_1^\beta$. For estimating confidence intervals for the number of components, we sample $K$ sets of $(b-1)$ conditionally independent submatrices for every lone submatrix $X_j^i$ such that $K$ sets of $(b-1)$ subsampled matrices and the lone submatrix are conditionally independent given $X$, i.e., $\{X_j^i, (X_j^{ik})_{i=1}^{b-1}\}_{j=1,...,M,k=1,...,K}$. Averaging the preliminary point estimate across $M$ sets for $K$ sets of $(b-1)$ conditionally independent submatrices yield $\{\hat{r}_j^\beta\}_{j=1}^K$. By construction $\{\hat{r}_j^\beta\}_{j=1}^K$ are $K$ independent random variables conditional on $X$. Therefore, by applying the normal theory of confidence intervals on $\{\hat{r}_j^\beta\}_{j=1}^K$, we construct a two-sided confidence interval for the number of components at the confidence level $(1-\alpha)$, where $(1-\alpha)$ is the user-specified confidence level. The algorithm is summarised in algorithm 2.

It follows from the above discussion that our proposed confidence intervals depend on hyperparameters, namely: $b$, $\beta$, $K$, and $M$ besides the user-specified confidence level $(1-\alpha)$. For instance, a high value of $b$ means that we have smaller submatrices for accurately estimating the spiked eigenvalues and a low value of $b$ means that we have less number of submatrices for accurately estimating centering and scaling parameters of the normal distribution of the spiked eigenvalues. Similarly, a relatively high (low) value of $\beta$ could lead to an overestimation (underestimation) in the estimate of the number of components. As we discuss later, the choice of $M$ and $K$ also affects the performance of our proposed confidence interval. The hyperparameters in the above subsampling procedure need to be optimized for the optimum coverage probability of the confidence interval. This is typically the case in subsampling literature where hyperparameters are optimized for improving the performance of the subsampling algorithm, see [38], [39]. We discover that the optimum value of $b$ is $[n^{1/\beta}]$, but we defer that discussion until we develop the relevant theory, see Section 3. Likewise, the suitable choice of hyperparameters $K$ and $M$ is also deferred to Section 3.

2.4 Treating $\beta$ as an unknown hyperparameter

The difficulty with the above subsampling algorithm lies in interpreting $\beta$. We treat $\beta$ as an unknown fixed hyperparameter that should be optimally selected in a data-intensive manner to
improve the performance of our proposed confidence intervals. In particular, let \( \{\beta(i)\}^g_{i=1} \) vary over a grid of \( g \) values between 0.5 and 1. Moreover, let \( \{\{r_j^{(i)}\}_{i=1,\ldots,g}\}_{j=1,\ldots,K} \) denote \( K \) sets of conditionally independent random variables (conditional on \( X \)) corresponding to \( g \) grid values of \( \{\beta(i)\}^g_{i=1} \). Using the central limit theorem, for any fixed \( i \), the mean of \( \{r_j^{(i)}\}_{j=1}^K \) (conditional on \( X \)) would be approximately normal. We use this insight to find the optimum value of \( \beta \). Assume that \( M \) and \( K \) are moderately large and fixed. Then, the optimum \( \beta \) is the one that centers the realizations \( \{\hat{r}_j^{(i)}\}_{j=1}^K \) around one more than the estimate of the number of components, \( r_0 + 1 \). The rationale for centering \( \{\hat{r}_j^{(i)}\}_{j=1}^K \) around \( r_0 + 1 \) and not \( r_0 \) is to facilitate our algorithm for computing confidence intervals for all non-negative integer values of the number of components \( r \) including \( r=0 \). Let \( r_0 \) be the estimate of \( r \) from the likelihood approach or any other consistent estimator of \( r \). Then, we select the optimum \( \beta \) that centers the realizations \( \{r_j^{(i)}\}_{j=1}^K \) around \( r_0 + 1 \) while maximizing the following likelihood.

\[
t(t\left(\frac{\bar{r}(l) - r_0 - 1}{\omega(l)}; 1, 0\right), (5)
\]

where \( \bar{r}(l) = \sum_{j=1}^{K} r_j^{(l)} / K \), \( \omega(l) \) is the standard deviation of \( \{r_j^{(l)}\}_{j=1}^K \), and \( t(\cdot; 1, 0) \) denotes Student’s \( t \)-distribution with mean zero and one degree of freedom.

Using the optimum \( \beta^{(l)} \) and \( \{r_j^{(l)}\}_{j=1}^K \), we can construct a \((1 - \alpha)\%\) confidence interval for one more than the true number of components. Subtracting one from the lower and upper bound gives us the \((1 - \alpha)\%\) confidence interval for the true number of components, see algorithm 2.

### 3 Theoretical results

The performance of a confidence interval is evaluated by the closeness of the coverage probability (i.e., for a large number of independent experiments, the percentage of times the computed confidence interval covers the true parameter) of a confidence interval to its specified confidence level. The closer is the coverage probability to its specified confidence level, the better is the performance of the confidence interval at that specified confidence level. For providing theoretical guarantee for our proposed confidence intervals, we derive a non-asymptotic upper bound for the absolute deviation of the coverage probability from the specified confidence level. Using this bound we also establish that the coverage probability of our proposed confidence intervals is consistent. The above theoretical guarantee rely on deriving the first-order Edgeworth correction of spiked eigenvalues of the sample covariance matrix when the underlying data was generated from a factor model in (2).
Algorithm 2 Subsampling Algorithm

1: Input: A matrix $X$ with $n$ rows and $p$ columns, and user-specified significance level $\alpha > 0$.
2: Let the default value of $\epsilon_0 = 0.02$.
3: Compute $r_0$ using algorithm 1 or using the deterministic parallel algorithm proposed by [27].
4: Consider a grid of confidence levels in $[0.5, 1]$ as $\{\beta(i)\}_{i=1}^q$.
5: Let $b = \lceil n^{1/3} \rceil$, and then compute $p_* = \lfloor p/b \rfloor$, $n_* = \lfloor n/b \rfloor$.
6: Randomly select a submatrix $X_*$ of $X$ with dimension $n_*$ rows and $p_*$ columns.
7: Compute the SVD of sample covariance matrix $X_*/n_* = UD_*V^\top$.
8: Store sample singular values of $D_*$ in $l_1^n \geq \cdots \geq l_{p_*}$.
9: Compute $b - 1$ conditionally independent submatrices of equal dimensions shown as follows.
   i. Denote $(b - 1)$ independent subsetted data matrix by $\{X_{n_1}\}_{i=1}^{b-1}$, which are also independent
      of $X_*$. Let the corresponding $(b - 1)$ sample covariance matrices be given by $\{X_{n_1}/n_*\}_{i=1}^{b-1}$,
   ii. For each $i = 1, \cdots, b - 1$, compute the SVD of $X_{n_1}/n_* = R_i Q_i S_i^\top$,
   iii. Store singular values of $Q_i$ in $l_i^{n_1} \geq \cdots \geq l_i^{p_*}$, where $i = 1, \cdots, b - 1$.
10: Compute $\mu_j = \sum_{i=1}^{b-1} l_i^j / (b-1)$ and $\sigma_j = \sqrt{\sum_{i=1}^{b-1} (l_i^j - \mu_j)^2 / (b-1)}$.
11: For $i = 1: g$,
   i. At $\beta(i)$, define confidence interval $CI_j(i)$ as $[\mu_j + z_{\beta(i)}/2 \sigma_j + \epsilon_0/n_*, \mu_j + z_{1 - \beta(i)}/2 \sigma_j - \epsilon_0/n_*]$, and accept $r(i) = \max\{j: j \in \{1, \cdots, p_*\} \} I\{\{l_s^j \in CI_j(i) \text{ for all } s \in \{1, \cdots, j\}\} \cap \{l_{j+1}^i \notin CI_j(i)\}\}$.
12: Repeat Steps (2)-(12) $M$ times to get $M$ independent realizations of $\{r(i)\}$.
13: Repeat Steps (5)-(13) $K$ times and denote the estimate of the number of spikes by $\{r_{k,i}\}_{k=1, \cdots, K, i=1, \cdots, M}$.
14: Compute $\hat{r}_k = \frac{\sum_{j=1}^{K} r_{k,j}}{M}$, $\hat{r}(i) = \frac{\sum_{k=1}^{K} r_{k,i}}{K}$, and $\hat{\sigma}(r) = \sqrt{\frac{\sum_{k=1}^{K} (r_{k,i} - \hat{r}(i))^2}{K}}$.
15: Select $i^*$ as $i$ maximizing the following objective function

$$i^* \text{ as } \max_{i: i \in \{1, \cdots, g\}} t(\hat{r}(i) - r_0 - 1, \frac{\hat{\sigma}(r)}{\omega(i)}) \text{,}$$

where $\hat{r}(i) = \sum_{j=1}^{K} r_{j,i}^* / K$, $\omega(i)$ is the standard deviation of $\{r_{j,i}^*\}_{j=1}^{K}$, $t(\cdot; 1, 0)$ denotes Student’s t-distribution with one degree of freedom and mean zero.
16: Using the normal theory of confidence intervals and adjusting for a bias of one, the two sided

$(1 - \alpha)$ confidence interval for $r$ is given as $[\hat{r}(i^*) + z_{\alpha/2} \hat{\sigma}(r^*) - 1, \hat{r}(i^*) + z_{1 - \alpha/2} \hat{\sigma}(r^*) - 1]$, where $[\cdot]$ is the greatest integer function.
3.1 First-order Edgeworth correction of the spiked eigenvalues of substituted covariance matrix

Recently, Yang and Johnstone (2018) [40] proposed a first-order Edgeworth correction for the largest eigenvalue of the sample covariance matrix when the underlying data matrix $\mathbf{X}$ was generated under a principal component model. Unfortunately, their approach cannot be automatically generalized to the largest few eigenvalues of the sample covariance matrix generated under a factor model in (2) for the following reasons. First, their approach cannot be used for solving the determinant equation of eigenvalues of the sample covariance matrix generated under a factor model. Second, since the loadings in FA are distributed across $p$ factors, it is difficult to estimate the analytical form of the population mean and population standard deviation of spiked eigenvalues of the sample covariance matrix, see (3).

We overcome the above two problems as follows. For the first problem, we solve the determinant-based equation for a substitution covariance matrix which is positive semidefinite. Then, borrowing ideas from Yang and Johnstone (2018) [40], we derive a first-order Edgeworth correction for the spiked eigenvalues of the substitution covariance matrix. Subsequently, we use the Delta theorem and the upper bound of the spectral norm of the cross product of two random matrices to get a first-order Edgeworth correction for the spiked eigenvalues of the sample covariance matrix. For the second problem, we use a subsampling strategy for estimating the centering $\{\rho_i\}_{i=1}^r$ and scaling parameters $\{\sigma_i\}_{i=1}^r$ for top $r$ spiked eigenvalues of the sample covariance matrix. Essentially, we repeatedly subsample a submatrix with the same aspect ratio $\gamma_n$ (as that for data matrix $\mathbf{X}$) conditional on the data matrix $\mathbf{X}$ for empirically estimating the centering $\{\rho_i\}_{i=1}^r$ and the scaling $\{\sigma_i\}_{i=1}^r$ parameters for $r$ spiked eigenvalues. Theoretically speaking, the centering and the scaling parameter also depend on the empirical distribution of the $p$ sample eigenvalues of the residual sample covariance matrix $n^{-1}\mathbf{E}\mathbf{E}^\top$. Assume that the $F_n$ denotes the empirical eigenvalue distribution of the $p$ sample eigenvalues of $n^{-1}\mathbf{E}\mathbf{E}^\top$. As $n$ grows $F_n$ converges to the Marchenko-Pastur distribution $F_\gamma$ supported on $[a(\gamma), b(\gamma)]$ when $\gamma \leq 1$ and with a point mass of $(1 - \gamma^{-1})$ at zero when $\gamma > 1$, where $a(\gamma) = (1 - \sqrt{\gamma})^2, b(\gamma) = (1 + \sqrt{\gamma})^2$. The companion empirical distribution of the $n$ eigenvalues of $n^{-1}\mathbf{E}\mathbf{E}^\top$ converges to the companion MP law $F_\gamma = (1 - \gamma)I_{[0,\infty)} + \gamma F_\gamma$. In fact, as shown in [29] the skewness component is given in terms of the above-defined $F_\gamma(\cdot)$.

Lemma 3.1 Assume that the data matrix $\mathbf{X}$ generated under the factor model in (2) satisfy assumptions (A.1)-(A.6). Let the singular value decomposition of the population covariance matrix
\( \Sigma \) of the data matrix \( X \) be given by \( VMV^\top \), where the diagonal matrix \( M \) is given as below:

\[
M = \begin{bmatrix}
L & 0_{r \times n-r} \\
0_{r \times n-r} & I_{n-r \times n-r}
\end{bmatrix},
\]

with \( L = \text{diag}(l_1, \cdots , l_r) \), \( l_1 > \cdots > l_r > (1 + \sqrt{\gamma}) \), \( 0_{r \times n-r} \) denoting the matrix of dimension \( r \times (n-r) \) with all zero elements, \( V \) denoting a unitary matrix of dimension \( n \times n \), and \( \gamma_n = p/n \to \gamma \).

For \( H, \Theta, E \) defined in (2), define the substitution covariance matrix \( \Sigma_s \) as below:

\[
\Sigma_s = \frac{H\Theta H^\top}{n} + \frac{EE^\top}{n}.
\]

Let \( \hat{l}_i^s \) be the \( i \)th largest eigenvalue of the substitution covariance matrix \( \Sigma_s \) given in (8). Let \( \rho_i, \sigma_i \) be the centering and scaling parameter given in (4). Then, for any \( i \in \{1, \cdots , r\} \), the cumulative distribution function of \( T_{n,i}^s = n^{1/2}(\hat{l}_i^s - \rho_i)/\sigma_i \) has the following first-order Edgeworth expansion:

\[
P(T_{n,i}^s \leq x) = \Phi(x) + n^{-1/2}p_{1,n}(x)\phi(x) + o(n^{-1/2}), \text{ valid uniformly in } x,
\]

where \( Y_n = o(1) \) denotes that \( \lim_{n \to \infty} P(|Y_n| \geq \epsilon) = 0 \), and

\[
p_{1,n}(x) = \frac{1}{6} \kappa_{2,n}^{-3/2} \kappa_{3,n}(1 - x^2) - \kappa_{2,n}^{-1/2} \mu(g(n,j)),
\]

for \( g(n,j)(\lambda) = (\rho_j - \lambda)^{-1} \), \( \kappa_{2,n} = 2F_{\gamma_n}(g(n,j)^2) \), \( \kappa_{3,n} = 8F_{\gamma_n}(g(n,j)^3) \), \( \mu(\cdot) \) is the asymptotic mean in the central limit theorem of Bai-Silverstein limit [41].

The above lemma exploits the positive semidefinite structure of the substituted covariance matrix to obtain a first-order Edgeworth correction of spiked eigenvalues of the substituted covariance matrix. However, using the spiked eigenvalues of the substitution covariance matrix in Algorithm 2 would be computationally cumbersome as it would entail estimating \( H \) and \( E \) for every submatrix. Since Algorithm 2 is given in the terms of the sample covariance matrix, we need to extend the above lemma to the spiked eigenvalues of the sample covariance matrix. For extending the above Edgeworth correction result to the spiked eigenvalues of sample covariance matrix, we use an upper bound on the spectral norm of the cross product of two random matrices and the Delta theorem.

### 3.2 Spectral Norm of Cross Product of Two Random Matrices

The upper bound of the expectation of the spectral norm is known for random matrices with independent elements, see [42],[43], [44], and [45]. However, none of the existing results give an
upper bound for the expectation of the spectral norm of a cross product of two random matrices. To this end, we propose the following theorem.

**Proposition 3.2** Let $H, \Theta, \Lambda, E$ be as defined in (2) and assume that assumptions (A.1)-(A.6) hold, then we have the following bound

$$E(||Z\Theta^{1/2}A^T + EA\Theta^{1/2}Z^T||) \leq \left(8^{2/4}\exp(2)\log(p)\log(r) \max_{1 \leq l \leq r} \sqrt{\theta_l}\right)\sqrt{n\log(n)\log(p)\log(r)\max_{1 \leq l \leq r} \sqrt{\theta_l}}.$$  

**Proof** See the Appendix.

The proof of the above proposition uses the cancellation of terms in the expansion of trace to derive the above bound of the spectral norm, see [46], [47], [44] for reference. A comparable approach is to condition the cross product of two matrices on one of the two matrices and then repeatedly apply Theorem 1.1 of [48] to get the upper bound. Unfortunately, such an approach in our context yields an upper bound of $O(\max_{1 \leq l \leq r} \sqrt{\theta_l}n)$ which is not sharp compared to Proposition 3.2. The above spectral upper bound of the cross product of two random matrices along with the Delta theorem allows us to extend the Edgeworth correction result for the spiked eigenvalues of the substituted covariance matrix to the spiked eigenvalues of the sample covariance matrix.

**Theorem 3.3** Assume the data matrix $X$, generated under the factor model in (2), satisfy assumptions (A.1)-(A.6). Let the singular value decomposition of the population covariance matrix $\Sigma$ be given by $VMV^T$, where the diagonal matrix $M$ is given as follows

$$M = \begin{bmatrix} L & \theta_l^{T}r \times n-r \\ \theta_l r \times n-r & I_{n-r \times n-r} \end{bmatrix}$$

(11)

with $L = \text{diag}(l_1, \cdots, l_r)$, $l_1 > \cdots > l_r > (1 + \sqrt{\gamma})$, $\theta_l r \times n-r$ denoting the matrix of dimension $r \times n - r$ with all zero elements, and $V$ denoting a unitary matrix of dimension $n \times n$.

Let $\tilde{l}_i$ be the $i$th largest eigenvalue of the sample covariance matrix. Assume that the centering and scaling parameters $\rho_i$ and $\sigma_i$ are given in (4). Then, we show that the cumulative distribution function of $T_{n,i} = n^{1/2}(\tilde{l}_i - \rho_i)/\sigma_i$ has a first-order Edgeworth expansion as follows

$$P(T_{n,i} \leq x) = \Phi(x) + n^{-1/2}p_1(x)\phi(x) + o(n^{-1/2}),$$

(12)

valid uniformly in $x \in \mathbb{R}$, and with

$$p_1(x) = \frac{1}{6}k_{2,n}^{-3/2}\kappa_{3,n}(1 - x^2) - \kappa_{2,n}^{-1/2}\mu(g(n,j)),$$

(13)

for $g(n,j)(\lambda) = (\rho_j - \lambda)^{-1}$, $\kappa_{2,n} = 2F_{\gamma}(g_{(n,j)}^2)$, $\kappa_{3,n} = 8F_{\gamma}(g_{(n,j)}^3)$, $\mu(\cdot)$ is the asymptotic mean in the central limit theorem of Bai-Silverstein limit, see Bai and Silverstein (2004) [41].
Proof See the Appendix.

Although, the above theorem is given for the spiked eigenvalues of the sample covariance matrix but in practice we can only compute the centering and scaling parameter for the spiked eigenvalues of the subsampled covariance matrices. Later in the paper, we use the above theorem to obtain a normal approximation of the spiked eigenvalues of the sample covariance matrix of the lone submatrix.

3.3 Comparison with the existing approaches

We numerically compare the above normal approximation with the approximation proposed by Larsen and Warne (2010) [11] and the first-order Edgeworth correction for spiked eigenvalues of PCA, see [29]. For finite sample, the mean of the above two approximation are far from the mean obtained using the subsampling approach. This is because the loadings in the FA are distributed across $p$ factors which may cause the population mean to become comparatively bigger or smaller. For a fair comparison, we center the two competing approximations the mean obtained using the subsampling approach. Figure 2 suggests that the two competing approximations overestimate the variance of the spiked eigenvalues.

Note that the assumption (A.6) for FA is far from benign. However, given that we lack an Edgeworth expansion result for the spiked eigenvalues of the sample covariance matrix, we believe that the above result could be useful. Also, recall that Yang and Johnstone (2018) [29] for the spiked eigenvalues of the sample covariance matrix for PCA under relatively simpler assumptions. Using these two results, we show that it is possible to gauge the coverage accuracy of our proposed confidence interval in algorithm 2.

3.4 Coverage Probability

At the heart of Algorithm 2 is the convolution of two approximately normal random variables, i.e.,

$$\sqrt{b-1} \left( \frac{\sum_{j=1}^{b-1} \tilde{l}_{ij}^2}{b-1} - \rho_i \right) / \hat{\sigma}_i$$

and $$(l_i^* - \rho_i)$$. Recall that the Theorem 3.1 states that $$(l_i^* - \rho_i)$$ has an Edgeworth expansion whereas Theorem 2.2 of Hall (1993) [32] implies that $$\sqrt{b-1} \left( \frac{\sum_{j=1}^{b-1} \tilde{l}_{ij}^2}{b-1} - \rho_i \right) / \hat{\sigma}_i$$ has an Edgeworth expansion. For the sake of completeness, we restate the above theorem in our setting.

Theorem 3.4 Assume that $X$ generated from (2). Let $\{X_{n_i}\}_{i=1}^{b-1} be conditionally independent (conditional on $X$) submatrices defined in algorithm 2. Let $\{l_{i}^*\}_{j=1}^{b-1}$ be $b-1$ $i^{th}$ largest eigenvalue of the
Figure 2: Approximation comparison. We generated 1000 data matrices under FA when $n = 1500$, $p = 600$, $r = 4$, and the scale factor, i.e. $(\theta_1, \theta_2, \theta_3, \theta_4) = (15, 15, 15, 15)$. We used 1000 data matrices to plot the histogram of top four spiked eigenvalues of the subsampled covariance matrices. Subsequently, we approximated the histogram of top four spiked eigenvalues using Larsen and Warne (2010)'s [11] approach (Low Asymptotics), first-order Edgeworth correction for PCA proposed by Yang and Johnstone (2018) [29] (Parametric), and the subsampling approach. The three approximations along with the histogram is plotted for first eigenvalue, second eigenvalue, fourth eigenvalue and third eigenvalue of the subsampled covariance matrices in clockwise manner. Vertical dark blue lines are drawn at $(1 + \sqrt{\gamma})^2$. 
sample covariance matrices of \( \{ \frac{X_i X_i^\top}{n/b} \}_{i=1}^{b-1} \). Let \( \rho_i \) and \( \sigma_i \) be the centering and the scaling parameter defined in (4). Then, we show that the cumulative distribution function of \( \sqrt{b - 1} \left( \frac{\sum_{i=1}^{b} \hat{\tau}_j^i}{b-1} - \rho_i \right) / \sigma_i \) has a first-order Edgeworth expansion as shown below

\[
P(\sqrt{b - 1} \left( \frac{\sum_{j=1}^{b} \hat{\tau}_j^i}{b-1} - \rho_i \right) / \sigma_i \leq x \mid X) = \Phi(x) + (b - 1)^{-1/2} p_1(x) \phi(x) + o((b - 1)^{-1}) \tag{14}
\]

valid uniformly in \( x \in \mathbb{R} \), and with

\[
p_1(x) = \frac{1}{6} \kappa_{2,n}^{-3/2} \kappa_{3,n}(1 - x^2) - \kappa_{2,n}^{-1/2} \mu(g_{n,j}), \tag{15}
\]

for \( g_{n,j}(\lambda) = (\rho_j - \lambda)^{-1} \), \( \kappa_{2,n} = 2F_{\gamma_n}(g_{n,j}^2) \), \( \kappa_{3,n} = 8F_{\gamma_n}(g_{n,j}^3), \) \( \mu(\cdot) \) is the asymptotic mean in the central limit theorem of Bai-Silverstein limit, see Bai and Silverstein (2004) [41].

We use the above two Edgeworth expansions to get a normal approximation of the weighted difference of the two random variables. Moreover, since the proposed confidence interval in algorithm 2 is constructed using a set of conditionally independent random variables therefore we use Berry-Esseen inequality to quantify the accuracy of the proposed confidence interval.

**Theorem 3.5 (Coverage Accuracy)** The absolute deviation between the coverage probability of the confidence interval in Algorithm 2 and the confidence level \( 1 - \alpha \) has the following upper bound.

\[
|P(r \in [\hat{\mu} + z_{\alpha/2} \hat{\sigma}, \hat{\mu} + z_{1-\alpha/2} \hat{\sigma}]) - (1 - \alpha)| \leq \rho \left( 2x^2 + 1 \right) \phi(x) / 6 \sigma^3 \sqrt{K} + o \left( \max \left\{ \frac{1}{K}, r \sqrt{\frac{b}{n}}, \frac{r}{b-1} \right\} \right), \tag{16}
\]

where \( \sigma \) is the unknown population standard deviation of \( \{ \hat{\tau}_\beta \}'s \) in algorithm 2.

The above theorem bounds the departure of the coverage probability of our proposed confidence interval from the expected confidence level. Clearly, minimizing this bound would improve the performance of the confidence interval. It is easy to see the error bound is minimized as a function of \( b \) when \( b = \lfloor n^{1/3} \rfloor \). Moreover, the above error bound will be minimized by selecting a high value of \( K \) while minimizing the skewness \( \rho \).

**Remark 3.6** The choice of \( b = \lfloor n^{1/3} \rfloor \) minimizes the coverage probability in the Theorem 3.5

**Remark 3.7** Note that the R.H.S. of (16) decreases to zero as long as \( r n^{-1/3} \) goes to zero. Therefore for higher value of \( r \) the performance of our proposed algorithm is worse. Moreover, we see that the first term in R.H.S. of (16) depends on the normal density evaluated at \( z_\alpha \), i.e. \( \phi(z_\alpha) \). It is easy to see the performance of our proposed interval is better when \( \phi(z_\alpha) \) is considerably smaller.
3.5 Justification of optimum $\beta$

Recall from algorithm 2 that $\{\beta_l\}_{l=1}^q$ consist of a grid of values ranging from 50% to 100%. From the definition of skewness $\rho$, in the R.H.S. of (16), is $E(\hat{r}_\beta - r - 1)^3$. Let $l(r \mid \{\hat{r}_\beta\}, X)$ denote the conditional log likelihood given $X$. Let $\bar{l}(r \mid \{\hat{r}_\beta\}, X), \bar{\bar{l}}(r \mid \{\hat{r}_\beta\}, X)$, and $\bar{\bar{\bar{l}}}(r \mid \{\hat{r}_\beta\}, X)$ denote the first, second and third derivative of the conditional log likelihood, where the derivative taken with respect to $r_\beta$. Then, applying Taylor series expansion for a fixed $\hat{r}_\beta$, we get

$$\bar{l}(r + 1 \mid \{\hat{r}_\beta\}, X) = \bar{l}(\hat{r}_\beta \mid \{\hat{r}_\beta\}, X) + (r + 1 - \hat{r}_\beta)\bar{\bar{l}}(\hat{r}_\beta \mid \{\hat{r}_\beta\}, X) + \frac{(r + 1 - \hat{r}_\beta)^2}{2} \bar{\bar{\bar{l}}}(\hat{r}_\beta \mid \{\hat{r}_\beta\}, X).$$

Recall by definition, for optimum $\beta^*$, we have $\bar{l}(\hat{r}_\beta^* \mid \{\hat{r}_\beta^*\}, X) = 0$. Then, we have

$$r + 1 - \hat{r}_\beta^* = \frac{\bar{l}(r + 1 \mid \{\hat{r}_\beta^*\}, X)}{\bar{l}(\hat{r}_\beta^* \mid \{\hat{r}_\beta^*\}, X) + 0.5(r + 1 - \hat{r}_\beta^*) \bar{\bar{l}}(\hat{r}_\beta^* \mid \{\hat{r}_\beta^*\}, X).}$$

(17)

Then, using the Central Limit Theorem, the boundedness of the third derivative of the conditional likelihood in (17) to show that $|r + 1 - \hat{r}_\beta^*|$ is upper bounded by a constant. This can be shown by verifying the Cramer-Rao conditions, see [49].

For bounding the coverage accuracy in the R.H.S. of (16), we show that the two terms in the R.H.S. of (16) can be minimized. Consider the first term in the R.H.S. of (16) that is given in terms of $\rho, \sigma, K$, and $\phi(z_{\alpha/2})$, where $\phi(\cdot)$ is the normal density and $z_{\alpha/2}$ is the normal density quantile evaluated at $\alpha/2$. From the preceding discussion in this section, $\rho$ is bounded when $\beta$ is selected as described in the algorithm 2. Suppose for fixed large $K, M, \epsilon_0$, we have $\sigma > \sigma_0 > 0$. Then, the first term becomes small for large quantiles $z_{\alpha/2}$ and large $K$. From Remark 3.6 and constant $r$, the second term in the R.H.S. of (16) is $o(n^{-1/3})$. For non-asymptotic case, the performance of proposed confidence intervals in the algorithm 2 is maximized by selecting $b = \lfloor n^{1/3} \rfloor$, $\beta$ the maximum likelihood estimate described in the algorithm 2, a large enough $K, M$, and a large confidence interval $(1 - \alpha)$. The consistency of the coverage accuracy follows from letting $K$ and $n$ increase.

4 Numerical Experiments

We evaluated the performance of Algorithm 2 (SS) by computing coverage probability for various simulation scenarios that varied with the true number of components $r$, the aspect ratio $\gamma_n$, and the scale of the components $\{\theta_i\}_{i=1}^r$. In particular, we vary the true number of factors $r$ over $\{0, 1, 2, 3, 4, 5\}$, the aspect ratio $\gamma_n$ over $\{0.2, 0.5\}$. We choose the scale of components in an increasing manner, as shown in Table 1. The rationale for choosing the scale of components $\{\theta_i\}_{i=1}^r$
Figure 3: Visual representation of the scheme to obtain the preliminary point estimate of the number of components. The depicted confidence interval is constructed using $b - 1$ eigenvalues of subsampled covariance matrices whereas square dots denote the eigenvalues of the sample covariance matrix of the lone subsampled matrix. The preliminary point estimate is one less than the first time when the square dots are not in the confidence interval.

in Table 1 is to avoid any multiplicity of spiked eigenvalues while keeping the spiked eigenvalues moderately large. We use the settings in Table 1 to test our method when the underlying data matrix was generated under a factor model and a principal component model.

Table 1: Choice of Scaling Factor.

| True Number of Components | Scale Factor |
|---------------------------|--------------|
| 0                         | NA           |
| 1                         | {10}         |
| 2                         | {10, 15}     |
| 3                         | {10, 15, 20} |
| 4                         | {10, 15, 20, 25} |
| 5                         | {10, 15, 20, 25, 30} |

Tables 2 - 3 compile the coverage probability for our proposed confidence intervals at range of confidence levels over {5%, 10%, 20%, 40%, 60%, 80%, 90%, 95%} for the simulation scenarios in Table 1. For computing the coverage probability, we generated the data matrix 100 times using the factor
model in (2) with the parameter settings in Table 1. Then, for each of the 100 simulations we used Algorithm 2

As discussed in Section 3, Tables 2-3 confirm that the performance of our proposed confidence interval is better for smaller and larger confidence levels, i.e., \{0.05, 0.1\} or \{0.9, 0.95\} confidence levels. Adding to this observation, Tables 2 clearly underlines that the performance of our confidence interval for middling confidence levels is highly inaccurate at larger number of components. This effect is somewhat mitigated for larger value of \(\gamma_n\), i.e., for \(\gamma_n = 0.5\), see Table 3. This holds because for larger \(\gamma_n\), the standard deviation in Theorem 3.5 is larger. Moreover as discussed, there is a trend that the performance of our proposed confidence intervals worsen with increasing number of components.

4.1 Comparison

In the previous subsection, we studied the performance of Algorithm 2 when the data matrix \(X\) satisfies the assumptions A.1-A.6. However in practice, it is important to evaluate the performance of Algorithm 2 under some stress scenarios. Motivated by Fan, Guo, and Zheng (2020)[12], we consider the following stress-testing scenarios.

1. Scenario a) \((r = 3), (\theta_1, \theta_2, \theta_3) = (1, 1, 10), \text{the noise factor} = (1, 1, 1), \gamma = (0.2),\)
2. Scenario b) \((r = 3), (\theta_1, \theta_2, \theta_3) = (10, 10, 1), \text{the noise factor} = (1, 1, 1), \gamma = (0.2),\)
3. Scenario c) \((r = 3), (\theta_1, \theta_2, \theta_3) = (1, 1, 1), \text{the noise factor} = (6, 6, 6), \gamma = (0.2),\)
4. Scenario d) \((r = 3), (\theta_1, \theta_2, \theta_3) = (1, 1, 10), \text{the noise factor} = (1, 1, 1), \gamma = (0.5),\)
5. Scenario e) \((r = 3), (\theta_1, \theta_2, \theta_3) = (10, 10, 1), \text{the noise factor} = (1, 1, 1), \gamma = (0.5),\)
6. Scenario f) \((r = 3), (\theta_1, \theta_2, \theta_3) = (1, 1, 1), \text{the noise factor} = (6, 6, 6), \gamma = (0.5).\)

Scenarios (1)-(6) is used for stress testing our method and provides a good yardstick for comparing competing methods. Scenarios (1), (4) consists of two low strength components and one high strength factor for different value of \(\gamma\). Scenarios (2), (5) consists of two high strength factors and one low strength factor for \(\gamma\) varying over \((0.2, 0.5)\). Scenarios (3), (6) consists of three low strength factors in presence of elevated level of random noise.

For evaluating the performance of Algorithm 2 (SS) under the stress-scenarios, we compare the performance of Algorithm 2 against a couple of existing methods. In particular, we compare
Table 2: Estimated coverage probability of confidence interval for the number of components when the number of rows and columns of the data matrix was (1500, 300).

| Model | True r | 5% CI | 10% CI | 20% CI | 40% CI | 60% CI | 80% CI | 90% CI | 95% CI |
|-------|--------|-------|-------|--------|--------|--------|--------|--------|--------|
| FA    | 0      | 0.03  | 0.05  | 0.09   | 0.32   | 0.51   | 0.70   | 0.85   | 0.94   |
| FA    | 1      | 0.05  | 0.07  | 0.16   | 0.30   | 0.54   | 0.77   | 0.86   | 0.93   |
| FA    | 2      | 0.02  | 0.04  | 0.18   | 0.43   | 0.59   | 0.83   | 0.93   | 0.96   |
| FA    | 3      | 0.07  | 0.13  | 0.21   | 0.40   | 0.66   | 0.90   | 0.95   | 0.98   |
| FA    | 4      | 0.02  | 0.03  | 0.05   | 0.17   | 0.31   | 0.56   | 0.8    | 0.88   |
| FA    | 5      | 0.03  | 0.07  | 0.12   | 0.28   | 0.55   | 0.75   | 0.85   | 0.92   |
| PCA   | 0      | 0.05  | 0.1   | 0.18   | 0.38   | 0.62   | 0.91   | 0.91   | 0.94   |
| PCA   | 1      | 0.05  | 0.08  | 0.14   | 0.21   | 0.4    | 0.68   | 0.78   | 0.9    |
| PCA   | 2      | 0.07  | 0.15  | 0.31   | 0.56   | 0.79   | 0.94   | 0.99   | 1      |
| PCA   | 3      | 0.04  | 0.09  | 0.17   | 0.47   | 0.74   | 0.90   | 0.94   | 0.97   |
| PCA   | 4      | 0.06  | 0.07  | 0.17   | 0.41   | 0.58   | 0.76   | 0.86   | 0.93   |
| PCA   | 5      | 0.01  | 0.04  | 0.07   | 0.21   | 0.39   | 0.68   | 0.81   | 0.89   |

Algorithm 2 (SS) against BEMA, a method for computing confidence interval proposed by Ke, Ma, and Lin (2020) [22] and a non-parametric bootstrap method (NB). Recall that BEMA relies on approximating the bulk eigenvalue using the weighted quantile of the Marchenko-Pastur distribution. Therefore in practice, we find that the confidence intervals obtained by BEMA can be rather narrow. For NB method, we sample rows from the data matrix with replacement $M$ times to get $M$ estimates of the number of components. Averaging over $M$ times gives us a point estimate of the number of components. Repeating the above process $M$ times gives us $M$ realizations of the point estimate which we use to estimate standard deviation of the point estimate. Then, we use the normal theory of confidence intervals to get a confidence interval for the number of components.

Table 6 compiles coverage probability of Algorithm 2 (SS), NB, and BEMA for scenarios (1)-(6). In Scenarios (1)-(2), (4)-(5) the performance of Algorithm 2 remains stable whereas the performance of NB and BEMA is bad. The bad performance of NB and BEMA can be attributed to the lower strength of signals. For scenarios (3), (6), the performance of Algorithm 2 worsens but fare better in comparison to the performance of NB and BEMA. In these scenario, NB performs overestimates the coverage probability whereas BEMA overestimates. The problem with BEMA is that it relies on approximating the bulk eigenvalues and therefore are susceptible.
Figure 4: Visual representation of the performance of the proposed confidence interval at 95% confidence level. We plot hundred 95% confidence intervals (of the number of components) for dataset of dimension $1500 \times 750$ generated using FA for the true number of components $r$ varying over $\{0, 1, 2, 3, 4, 5\}$. Each confidence is color coded with green (red) denoting that the confidence interval covers (doesn’t cover) the true number of components. Every scenario has different number of the true number of components with vertical bar indicating the true number of components.
Figure 5: Visual representation of the performance of the proposed confidence interval at 95% confidence level. We plot hundred 95% confidence intervals (of the number of components) for dataset of dimension $1500 \times 750$ generated using PCA for the true number of components $r$ varying over $\{0, 1, 2, 3, 4, 5\}$. Each confidence is color coded with green (red) denoting that the confidence interval covers (doesn’t cover) the true number of components. Every scenario has different number of the true number of components with vertical bar indicating the true number of components.
Table 3: Estimated coverage probability of confidence interval for the number of components when the number of rows and columns of the data matrix was (1500, 750).

| Model | True r | 5 % CI | 10 % CI | 20 % CI | 40 % CI | 60 % CI | 80 % CI | 90 % CI | 95 % CI |
|-------|--------|--------|---------|---------|---------|---------|---------|---------|---------|
| FA    | 0      | 0.06   | 0.11    | 0.23    | 0.43    | 0.66    | 0.91    | 0.98    | 0.99    |
| FA    | 1      | 0.08   | 0.09    | 0.12    | 0.37    | 0.56    | 0.81    | 0.97    | 0.99    |
| FA    | 2      | 0.06   | 0.11    | 0.2     | 0.45    | 0.67    | 0.86    | 0.95    | 0.99    |
| FA    | 3      | 0.04   | 0.07    | 0.17    | 0.41    | 0.60    | 0.75    | 0.86    | 0.96    |
| FA    | 4      | 0.06   | 0.11    | 0.30    | 0.54    | 0.76    | 0.94    | 0.97    | 0.97    |
| FA    | 5      | 0.03   | 0.07    | 0.16    | 0.36    | 0.53    | 0.7     | 0.84    | 0.93    |
| PCA   | 0      | 0.02   | 0.06    | 0.12    | 0.42    | 0.62    | 0.89    | 0.96    | 0.98    |
| PCA   | 1      | 0.04   | 0.10    | 0.2     | 0.35    | 0.57    | 0.81    | 0.92    | 0.96    |
| PCA   | 2      | 0.02   | 0.06    | 0.14    | 0.34    | 0.62    | 0.9    | 0.97    | 0.99    |
| PCA   | 3      | 0.02   | 0.07    | 0.11    | 0.22    | 0.4    | 0.74    | 0.88    | 0.95    |
| PCA   | 4      | 0.03   | 0.06    | 0.11    | 0.29    | 0.54    | 0.74    | 0.85    | 0.92    |
| PCA   | 5      | 0.04   | 0.09    | 0.18    | 0.36    | 0.58    | 0.77    | 0.85    | 0.94    |

5 Real Data Analysis

For real data analysis, we consider the single nucleotide polymorphism (SNP) genotyping dataset from the Human Genome Diversity Project (HGDP) dataset ([50],[51]). The dataset was collected for studying the genetic variation across the human populations around the world. The SNP genotyping dataset is collected for 1043 samples from 51 representing populations from Africa, Europe, Asia, Oceania, and the Americas. The dataset can be downloaded from https://hagsc.org/hgdp/files.html.

Following [27], we study the SNP genotyping data for one of the smallest human chromosome 22. The SNP genotyping dataset on chromosome 22 comprises of 1043 samples and 9743 SNPs. Since we did not have access to the reference allele, we used the allele frequency across 1043 samples to determine the minor allele at every RSid site of the chromosome. Using the minor allele determination, we converted the SNP genotyping dataset into a numerical matrix of dimension $n \times p$, where $X_{ij} \in \{0, 1, 2\}$ is the number of minor allele of SNP $j$ (at a particular RSid location on the chromosome 22) in the $i^{th}$ individual. For analyzing the dataset, we replaced any missing values with 0. Moreover, we centered and scale the remaining dataset SNP-wise. As we discuss, we notice that some results are somewhat different from [27]. This is because they had access to
Table 4: Estimated coverage probability of confidence interval for the number of components.

| Method | Sc | 5 % CI | 10 % CI | 20 % CI | 40 % CI | 60 % CI | 80 % CI | 90 % CI | 95 % CI |
|--------|----|--------|---------|---------|---------|---------|---------|---------|---------|
| SS     | a  | 0.05   | 0.11    | 0.22    | 0.38    | 0.63    | 0.78    | 0.86    | 0.92    |
| NB     | a  | 0      | 0       | 0       | 0       | 0       | 0       | 0       | 0       |
| BEMA   | a  | 0      | 0       | 0       | 0       | 0       | 0       | 0       | 0       |
| SS     | b  | 0.05   | 0.14    | 0.22    | 0.50    | 0.71    | 0.92    | 0.98    | 0.99    |
| NB     | b  | 0      | 0       | 0       | 0       | 0       | 0       | 0       | 0       |
| BEMA   | b  | 0      | 0       | 0       | 0       | 0       | 0       | 0       | 0       |
| SS     | c  | 0.06   | 0.16    | 0.28    | 0.53    | 0.76    | 0.96    | 0.98    | 1       |
| NB     | c  | 0.5    | 0.73    | 0.93    | 1       | 1       | 1       | 1       | 1       |
| BEMA   | c  | 0      | 0       | 0       | 0       | 0       | 0       | 0       | 0       |
| SS     | d  | 0.06   | 0.18    | 0.31    | 0.50    | 0.77    | 0.92    | 1       | 1       |
| NB     | d  | 0      | 0       | 0       | 0       | 0       | 0       | 0       | 0       |
| BEMA   | d  | 0      | 0       | 0       | 0       | 0       | 0       | 0       | 0       |
| SS     | e  | 0.05   | 0.17    | 0.29    | 0.61    | 0.79    | 0.93    | 0.98    | 0.99    |
| NB     | e  | 0      | 0       | 0       | 0       | 0       | 0       | 0       | 0       |
| BEMA   | e  | 0      | 0       | 0       | 0       | 0       | 0       | 0       | 0       |
| SS     | f  | 0.07   | 0.13    | 0.28    | 0.56    | 0.78    | 0.89    | 0.96    | 1       |
| NB     | f  | 0      | 0.02    | 0.09    | 0.56    | 0.93    | 1       | 1       | 1       |
| BEMA   | f  | 0      | 0       | 0       | 0       | 0       | 0       | 0       | 0       |
Table 5: 99 % Confidence Interval for the Number of Components of SNP genotyping dataset with different estimate of the number of components.

| Estimate | Likelihood-Based | DPA | DDPA+ | BEMA |
|----------|------------------|-----|-------|------|
|          | Lower  | Upper  | Lower | Upper | Lower  | Upper  | Lower  | Upper  |
| 99 % CI  | 9      | 14     | 24    | 30    | 8      | 15     | 117    | 122    |

Table 6: 99 % Confidence Interval for the Number of Components of SNP genotyping dataset with different estimate of the number of components.

| Likelihood-Based | DPA | DDPA+ | BEMA |
|------------------|-----|-------|------|
| 178              | 212 | 13    | 120  |

the reference allele or a different method for determining minor allele.

We used Likelihood-based method, DPA, and DDPA+ for estimating the number of components. Then, for each of these estimate of the number of components, we estimate a 99% confidence interval for the number of components. Surprisingly, we notice that the 99% confidence interval for Likelihood-based method and DPA does not contain the respective estimated number of components. This phenomena can be explained as follows. In particular, this is because both Likelihood-based method and DPA estimated

Recall that the algorithm 2 is constructed using the eigenvalues of the subsampled covariance matrices that have relatively weaker signal strength compared to the original data matrix. Moreover, the empirical histogram of the number of components in algorithm 2 is obtained after averaging over conditionally independent subsamples that also brings down the empirical histogram of the number of components. However, when the estimated number of components is not large, as in the case of DDPA+. Based on the above discussion, it is fair to conclude that the estimated confidence interval tend to be more robust whereas individual methods for estimating the number of components.

Since the truth about the true number of components is not known about this dataset, we cannot simply validate our 99% confidence interval estimate of the number of components. Nonetheless, it is prudent to provide some heuristic validation for our estimated 99% confidence interval. Motivated by [52] and [27], we provide graphical validation for our estimated 99% confidence interval. Figures show
Figure 6: Visual representation of the left singular vectors 1 – 8 of HGDP data
Figure 7: Visual representation of the left singular vectors 9 – 16 of HGDP data
6 Discussion

We proposed a subsampling algorithm for obtaining confidence intervals for the number of components in FA and PCA. We also showed that the coverage accuracy of the proposed confidence interval is good when the confidence level is high. The above theoretical result is based on obtaining the Edgeworth expansion of the spiked eigenvalues of the sample covariance matrix. Although Yang and Johnstone (2018) [29] obtained the Edgeworth expansion for the spiked eigenvalues of the sample covariance matrix under benign conditions for PCA but our assumptions in the case of FA is comparatively demanding. Therefore, we believe that it may be possible to improve upon these conditions.

References

[1] Anderson, T. W. (2003) An Introduction to Multivariate Statistical Analysis. Wiley New York.

[2] Bai, J. and Ng, S. (2008) Large dimensional factor analysis. Foundations and Trends in Econometrics, 3, 89–163.

[3] Jolliffe, I. T. and Cadima, J. (2016) Principal component analysis : A review and recent developments. Philosophical Transactions of the Royal Society A, 374.

[4] Abraham, G. and Inouye, M. (2014) Fast principal component analysis of large-scale genome-wide data. PLoS ONE, 9, e93766.

[5] Tsuyuzaki, K., Sato, H., and Nikaido, I. (2020) Benchmarking principal component analysis for large-scale single-cell rna-sequencing. Genome Biology, 13.

[6] Costello, A. B. and Osborne, J. (2005) Best practices in exploratory factor analysis : four recommendations for getting the most from your analysis. Practical Assessment, Research, and Evaluation, 10.

[7] Zwick, W. R. and Velicer, W. F. (1982) Factors influencing four rules of determining the number of components to retain. Multivariate Behavioral Research, 17, 253–269.

[8] Zwick, W. R. and Velicer, W. F. (1986) Comparison of five rules for determining the number of components to retain. Psychological Bulletin, 99, 432–442.
[9] O’Connor, B. P. (2000) Spss and sas programs for determining the number of components using parallel analysis and velicer’s map test. *Behavioral Research Methods, Instruments, & Computers*, **32**, 396–402.

[10] Thompson, B. (2004) Exploratory and confirmatory factor analysis: Understanding concepts and applications. *Washington DC: American Psychological Association*.

[11] Larsen, R. and Warne, R. T. (2010) Estimating confidence intervals for eigenvalues in exploratory factor analysis. *Behavior Research Methods*, **42**, 871–876.

[12] Fan, J., Guo, J., and Zheng, S. (2020) Estimating number of factors by adjusted eigenvalues thresholding. *Journal of the American Statistical Association*.

[13] Bai, J. and Ng, S. Determining the number of factors in approximate factor models. *Econometrica*, **70**, 191–221.

[14] Bai, Z., Choi, K. P., and Fujikoshi, Y. (2018) Consistency of aic and bic in estimating the number of significant components in high-dimensional principal component analysis. *The Annals of Statistics*, **46**, 1050–1076.

[15] Cattell, R. B. (1966) The scree test for the number of factors. *Multivariate Behavioral Research*, **1**.

[16] Onatski, A. Testing hypothesis about the number of factors in large factor models. *Econometrica*, **77**.

[17] Horn, J. L. (1965) A rationale and test for the number of factors in factor analysis. *Psychometrika*, **30**, 179–185.

[18] Buja, A. and Eyuboglu, N. (1992) Remarks on parallel analysis. *Multivariate behavioral research*, **27**, 509–540.

[19] Hong, D., Sheng, Y., and Dobriban, E. (2020) Selecting the number of components in pca via random signflips. *https://arxiv.org/pdf/2012.02985.pdf*.

[20] Dobriban, E. and Owen, A. B. (2019) Deterministic parallel analysis : An improved method for selecting factors and principal components. *Journal of the Royal Statistical Society Series B*, **81**.
[21] Cai, T., Han, X., and Pan, G. (2020+) Limiting laws for divergent spiked eigenvalues and largest non-spiked eigenvalue of sample covariance matrices. *The Annals of Statistics (to appear).*

[22] Ke, Z. T., Ma, Y., and Lin, X. (2020) Estimation of the number of spiked covariance matrix by bulk eigenvalue matching analysis. *preprint, https://arxiv.org/pdf/2006.00436.pdf.*

[23] Fan, J., Guo, J., and Zheng, S. Estimating number of factors by adjusted eigenvalues thresholding. *Journal of the American Statistical Association (to appear).*

[24] Anderson, T. W. (1963) Asymptotic theory for principal component analysis. *Annals of Mathematical Statistics,* pp. 122–148.

[25] Saccenti, E. and Timmerman, M. E. (2017) Considering horn’s parallel analysis from a random matrix theory point of view. *psychometrika,* 82, 186–209.

[26] Johnstone, I. M. (2001) On the distribution of the largest eigenvalue in principal components analysis. *Annals of Statistics,* 29, 295–327.

[27] Dobriban, E. and Owen, A. B. (2018) Deterministic parallel analysis: an improved method for selecting factors and principal components. *Journal of the Royal Statistical Society. Series B (Methodological),* 81, 163–183.

[28] Baik, J., Arous, G. B., and Pêché, S. (2005) Phase transition of the largest eigenvalue for nonnull complex sample covariance matrices. *Annals of Probability,* 33, 1643–1697.

[29] Johnstone, I. M. and Paul, D. (2018) Pca in high dimensions: An orientation. *Proceedings of the IEEE,* 106, 1277–1292.

[30] Paul, D. (2007) Asymptotics of sample eigenstructure for a large dimensional spiked covariance model. *Statistica Sinica,* 17, 1617–1642.

[31] Yao, J., Bai, Z., and Zheng, S. (2015) *Large Sample Covariance Matrices and High-Dimensional Data Analysis.* Cambridge University Press.

[32] Hall, P. (1993) *The Bootstrap and Edgeworth Expansion.* Springer Series in Statistics.

[33] Bai, J. and Li, K. (2012) Statistical analysis of factor models of high dimension. *Annals of Statistics,* 40, 436–465.
[34] Bai, J. and Ng, S. Determining the number of factors in approximate factor models. *Econometrica*, 70, 191–221.

[35] Fan, J., Liao, Y., and Mincheva, M. (2013) Large covariance estimation by thresholding principal components. *Journal of Royal Statistical Society Series B*, 75.

[36] Onatski, A. Testing hypotheses about the number of factor in large factor models. *Econometrica*, 77, 1447–1479.

[37] Lee, J. O. and Schnelli, K. (2016) Tracy-widom distribution for the largest eigenvalue of real sample covariance matrices with general population. *Annals of Applied Probability*, 26.

[38] Politis, D. N., Romano, J. P., and Wolf, M. (2001) On the asymptotic theory of subsampling. *Statistical Sinica*, 11.

[39] for Large Sample Logistic Regression, O. S. *Journal of the American Statistical Association*, 113, 829–844.

[40] Yang, J. and Johnstone, I. M. (2018) Edgeworth correction for the largest eigenvalue in a spiked pca model. *Statistical Sinica*, 28.

[41] Bai, Z. and Silverstein, J. W. (2004) CLT for linear spectral statistics of large-dimensional sample covariance matrices. *The Annals of Probability*, 32, 553–605.

[42] Bandeira, A. S. and Handel, V. R. (2016) Sharp nonasymptotic bounds on the norm of random matrices with independent entries. *Annals of Probability*, 44, 2479–2506.

[43] Handel, R. V. (2017) On the spectral norm of gaussian random matrices. *Transactions of the American Mathematical Society*, 369, 8161–8178.

[44] seginer, Y. (2000) The expected norm of random matrices. *Electronic Journal of Probability*, 9, 149–166.

[45] Latala, R. (2004) Some estimates of norms of random matrices. *Proceedings of the American Mathematical Society*, 133, 1273–1282.

[46] Füredi, Z. and Komlós, J. (1981) The eigenvalues of random symmetric matrices. *Combinatorica*, 1, 233–241.

[47] Vu, V. H. (2007) Spectral norm of random matrices. *Combinatorica*, 27, 721–736.
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