A generalized information criterion for high-dimensional PCA rank selection

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Abstract

Principal component analysis (PCA) is the most commonly used statistical procedure for dimension reduction. An important issue for applying PCA is to determine the rank, which is the number of dominant eigenvalues of the covariance matrix. The Akaike information criterion (AIC) and Bayesian information criterion (BIC) are among the most widely used rank selection methods. Both use the number of free parameters for assessing model complexity. In this work, we adopt the generalized information criterion (GIC) to propose a new method for PCA rank selection under the high-dimensional framework. The GIC model complexity takes into account the sizes of covariance eigenvalues and can be better adaptive to practical applications. Asymptotic properties of GIC are derived and the selection consistency is established under the generalized spiked covariance model. The proposed GIC is shown to be an intermediate method between AIC and BIC. On one hand, GIC is more capable than AIC in excluding noise eigenvalues. On the other hand, it is more sensitive than BIC in detecting signal eigenvalues. Our result also extends the selection consistency of AIC and BIC under the simple spiked covariance model (Bai, Choi and Fujikoshi; 2018) to the case of generalized spiked covariance model.

Key Words: AIC, BIC, GIC, high dimensionality, model selection, PCA.
1 Introduction

Principal component analysis (PCA) is the most widely used statistical procedure for dimension reduction. Let \( X \in \mathbb{R}^p \) be a random vector distributed from an arbitrary cumulative distribution function \( G \) with mean \( \mu \) and covariance \( \Sigma \). Consider the spectral decomposition \( \Sigma = \Gamma \Lambda \Gamma^\top \), where \( \Gamma = [\gamma_1, \ldots, \gamma_p] \in \mathbb{R}^{p \times p} \) satisfies \( \Gamma^\top \Gamma = I_p \), and \( \Lambda \in \mathbb{R}^{p \times p} \) is a diagonal matrix with positive diagonal entries arranged in descending order

\[
\lambda_1 > \lambda_2 > \cdots > \lambda_{r_0} \gg \lambda_{r_0+1} > \cdots > \lambda_p. \tag{1}
\]

Here we assume the existence of a sufficient gap between \( \lambda_{r_0} \) and \( \lambda_{r_0+1} \) so that \( r_0 \) can be treated as the target rank of \( \Sigma \). With a rigorous definition of \( r_0 \), which will be given in Section 3.1, model (1) is called the generalized spiked covariance model. Then, the leading eigenvectors \( [\gamma_1, \ldots, \gamma_{r_0}] \) are the target of PCA for dimension reduction. In the sample level, let \( \{X_i\}_{i=1}^n \) be a random sample with size \( n \), and let \( S_n = \frac{1}{n} \sum_{i=1}^n (X_i - \bar{X})(X_i - \bar{X})^\top \) with \( \bar{X} = \frac{1}{n} \sum_{i=1}^n X_i \) be the sample covariance matrix. Consider the spectral decomposition

\[
S_n = \sum_{j=1}^p \hat{\lambda}_j \hat{\gamma}_j \hat{\gamma}_j^\top. \tag{2}
\]

If \( r_0 \) is known, then PCA suggests to map the data \( \{X_i\}_{i=1}^n \) onto the space spanned by the leading eigenvectors \( [\hat{\gamma}_1, \ldots, \hat{\gamma}_{r_0}] \) for the subsequent analysis. Since \( r_0 \) is usually unknown, an important issue of PCA is the determination of the target rank \( r_0 \) in (1). Two commonly used information criteria for PCA rank selection are the Akaike information criterion (AIC) and the Bayesian information criterion (BIC). These methods adopt the number of free parameters as the penalty to prevent the selection of a saturated model. The difference between the two criteria is that AIC uses a constant 2 to weight the model penalty, while BIC uses \( \ln n \). Recently, statistical properties of AIC and BIC for PCA rank selection under the high-dimensional setting have been studied by Bai, Choi and Fujikoshi (2018), wherein the authors worked on the simple spiked covariance model, which assumes (1) but with \( \lambda_{r_0+1} = \cdots = \lambda_p \).

Due to its sparseness when \( r_0 \ll p \), the simple spiked covariance model provides a feasible alternative to its generalized counterpart (1). However, choosing \( r_0 \) via the model selection
criteria, such as AIC and BIC, derived under the assumption that the simple spiked covariance model is true may no longer be suitable, provided all or some of the tail eigenvalues in (1) are distinct from each other. This leads to the problem of PCA rank selection under model misspecification. There is a rich literature on model selection under misspecification; see Konishi and Kitagawa (1996), Lv and Liu (2014), Hsu, Ing and Tong (2019) and the references therein. Lv and Liu (2014) have introduced the generalized BIC (GBIC) and generalized AIC (GAIC) based on rigorous asymptotic expressions of the Bayesian and KL divergence principles in misspecified generalized linear models. Hsu, Ing and Tong (2019) have proposed the misspecification-resistant information criterion (MRIC) via an asymptotic expression for the mean squared prediction error of a misspecified time series model. These criteria, however, focusing on regression-type models, are not directly applicable to PCA rank selection. Konishi and Kitagawa (1996), on the other hand, have established an asymptotic expression of the KL divergence principle in a general misspecification framework, leading to their celebrated generalized information criterion (GIC). Although the framework considered in Konishi and Kitagawa (1996) is quite general, their derivation of GIC is reliant on some high-level assumptions, which may fail to hold for (misspecified) PCA models; see Section 2.2 for details.

In this paper, we derive an asymptotic bias correction to the KL divergence for the PCA rank selection problem, when a misspecified simple spiked covariance model is postulated. While our bias correction, $\hat{b}_{\text{GIC}}$, resembles the one given in Theorem 2.1 of Konishi and Kitagawa (1996), it is obtained under mild moment and distributional assumptions, thereby alleviating the difficulty mentioned in the previous paragraph. Moreover, we show that $\hat{b}_{\text{GIC}}$ has an elegant expression in terms of the sizes of covariance eigenvalues when Gaussianity is assumed. This expression not only provides a deeper understanding of the KL divergence principle in misspecified PCA models, but it also leads to a model selection criterion with a penalty term more adaptive to various spiked covariance structures than those of AIC and BIC, which simply depend on the number of free parameters. In particular, the proposed GIC is shown to be an intermediate method between AIC and BIC. On one hand, GIC is more capable than AIC in excluding noise eigenvalues. On the other hand, it is more sensitive than BIC in detecting signal eigenvalues.
The rest of this article is organized as follows. Our GIC-based selection criterion is derived in Section 2. Its asymptotic properties and selection consistency are investigated in Section 3. Numerical studies and a real data application are provided in Section 4. This article ends with a discussion in Section 5. All proofs are placed in the Appendix.

2 GIC for PCA Rank Selection

2.1 Review of AIC and BIC

The AIC for PCA rank selection starts from fitting \( \{X_i\}_{i=1}^n \) with the \textit{rank-}r \textit{simple spiked covariance model} as the working model:

\[
\Sigma_r = \Gamma_r \Lambda_r \Gamma_r^\top + \sigma_r^2 Q_r, \tag{3}
\]

where \( \Gamma_r = [\gamma_1, \ldots, \gamma_r] \), \( \Lambda_r = \text{diag}(\lambda_1, \ldots, \lambda_r) \) with \( \lambda_1 > \cdots > \lambda_r > \sigma_r^2 > 0 \), and \( Q_r = I - \Gamma_r \Gamma_r^\top \). The benefit of model (3) is that \( r \) can be directly explained as the target rank of interest, and a certain information criterion can be straightforwardly applied to determine a suitable value of \( r \). Assume the Gaussian distribution assumption \( X \sim N(\mu, \Sigma_r) \), and let

\[
\theta_r = (\text{vec}(\Gamma_r)^\top, \lambda_1, \ldots, \lambda_r, \sigma_r^2, \mu^\top)^\top. \tag{4}
\]

The log-likelihood of \( \theta_r \) (up to a constant term) is given by

\[
\ell_n(\theta_r) = \int \ell(x|\theta_r) dG_n(x) \quad \text{with} \quad \ell(x|\theta_r) = -\frac{1}{2} \ln |\Sigma_r| - \frac{1}{2} \text{tr} \left\{ (x - \mu)(x - \mu)^\top \Sigma_r^{-1} \right\},
\]

where \( G_n \) is the empirical distribution of \( \{X_i\}_{i=1}^n \). Straightforward calculation shows that the MLE of \( \theta_r \), i.e., \( \hat{\theta}_r = \arg\max_{\theta_r} \ell_n(\theta_r) \), consists of

\[
\hat{\Gamma}_r = [\hat{\gamma}_1, \ldots, \hat{\gamma}_r], \quad \hat{\Lambda}_r = \text{diag}(\hat{\lambda}_1, \ldots, \hat{\lambda}_r), \quad \hat{\sigma}_r^2 = \frac{1}{p - r} \sum_{j>r} \hat{\lambda}_j, \quad \hat{\mu} = \bar{X}, \tag{5}
\]

where \( \hat{\gamma}_j \)'s and \( \hat{\lambda}_j \)'s are defined in (2). Since \( \text{tr}(S_n \hat{\Sigma}_r^{-1}) = p \),

\[
\ell_n(\hat{\theta}_r) = -\frac{1}{2} \ln |\hat{\Sigma}_r| - \frac{p}{2} \quad \text{with} \quad \hat{\Sigma}_r = \hat{\Gamma}_r \hat{\Lambda}_r \hat{\Gamma}_r^\top + \hat{\sigma}_r^2 \hat{Q}_r, \tag{6}
\]

where \( \hat{Q}_r = I - \hat{\Gamma}_r \hat{\Gamma}_r^\top \). Then, AIC estimates \( r_0 \) by

\[
\hat{r}_{\text{AIC}} = \arg\max_{r \leq q} \left\{ \ell_n(\hat{\theta}_r) - \frac{1}{n} b_r \right\} = \arg\min_{r \leq q} \left\{ \ln |\hat{\Sigma}_r| + \frac{2}{n} b_r \right\}, \tag{7}
\]
where $q$ is a pre-determined upper bound of the model rank, and

$$b_r = \left\{ pr - \frac{r(r + 1)}{2} \right\} + r + 1 + p$$

is the number of free parameters in $\theta_r$. BIC estimates $r_0$ in a similar manner with AIC, except that BIC uses $\ln n$ as the weight for $b_r/n$:

$$\hat{r}_{BIC} = \arg\min_{r \leq q} \left\{ \ln |\hat{\Sigma}_r| + \frac{\ln n}{n} b_r \right\}.$$

(9)

Bai, Choi and Fujikoshi (2018) have studied the statistical properties of $\hat{r}_{AIC}$ and $\hat{r}_{BIC}$ under the simple spiked covariance model and $p/n \to c > 0$. We remind the reader that the true model considered in this paper is the generalized spiked covariance model (1), while the rank-$r$ simple spiked covariance model (3) is only a working model for rank selection.

Let $\theta_r^*$ be the population version of MLE from fitting the rank-$r$ simple spiked covariance model (3). By (5), we have that $\theta_r^*$ consists of

$$\Gamma_r^* = [\gamma_1, \ldots, \gamma_r], \quad \Lambda_r^* = \text{diag}(\lambda_1, \ldots, \lambda_r), \quad \sigma_r^{*2} = \frac{1}{p - r} \sum_{j > r} \lambda_j, \quad \mu^* = \mu,$$

(10)

and the rank-$r$ simple spiked covariance matrix induced by $\theta_r^*$ is given by

$$\Sigma_r^* = \Gamma_r^* \Lambda_r^* \Gamma_r^{*\top} + \sigma_r^{*2} Q_r^*,$$

where $Q_r^* = I - \Gamma_r^* \Gamma_r^{*\top}$. The notation $\theta_r^*$ and $\Sigma_r^*$ will be used in the subsequent discussion.

**Remark 1.** Note that $\hat{\Sigma}_r$ from maximizing $\ell_n(\theta_r)$ also minimizes the matrix log-determinant divergence between $S_n$ and $\Sigma_r$: $D_{\text{log, det}}(S_n, \Sigma_r) = -\frac{1}{2} \ln |S_n \Sigma_r^{-1}| + \frac{1}{2} \text{tr} (S_n \Sigma_r^{-1}) - \frac{p}{2}$. Thus, if the Gaussian assumption is not valid, the MLE $\hat{\Sigma}_r$ discussed above can still have the nice property of being the minimum log-determinant divergence estimator.

### 2.2 GIC for model complexity measure

AIC, penalizing model complexity based on the number of free parameters, is obtained under the crucial assumption that model (3) is the true data generating distribution. However, this simple spiked model assumption can be easily violated in practical applications of high dimensional data. When (3) is used as a working model but the true model is (1), the
GIC of Konishi and Kitagawa (1996), taking model misspecification into account, appears to be a more appealing alternative. To derive GIC in this case, one must first establish an asymptotic expression for the bias incurred by using the within-sample prediction error to approximate the likelihood-based prediction error,

\[ E \left\{ \int \ell(x|\hat{\theta}_r)dG_n(x) - \int \ell(x|\hat{\theta}_r)dG(x) \right\}, \tag{11} \]

which is suggested by the KL divergence principle, and then provide a reliable estimate of this expression provided it depends on unknown parameters. Here, the expectation is taken with respect to \(X_1, \ldots, X_n \text{i.i.d.} G\). Note that the true distribution \(G\) need not be Gaussian.

Theorem 2.1 in Konishi and Kitagawa (1996) suggests that (11) can be expressed as \(n^{-1}\mathcal{b}_{\text{GIC}} + o(n^{-1})\), where

\[ \mathcal{b}_{\text{GIC}} = E \left\{ \left[ \frac{\partial \ell(X|\theta^*_r)}{\partial \theta_r} \right]^\top \text{IF}_T_r(X; G) \right\} \tag{12} \]

with the expectation being taken with respect to \(X \sim G\). Here \(\text{IF}_T_r(x; G)\) is the influence function of the MLE functional \(T_r\) from fitting the rank-\(r\) simple spiked model (3), i.e., \(\theta^*_r = T_r(G)\) and \(\hat{\theta}_r = T_r(G_n)\). The derivation of Konishi and Kitagawa (Theorem 2.1, 1996), however, is based on the functional Taylor series expansion of \(T_r\) around \(G\) under the assumption that \(T_r\) is second-order compact differentiable at \(G\). The second-order compact differentiability is difficult to check and can be violated for eigenvalues and eigenvectors as functionals of \(G\). It is known that even the sample mean is not compact differentiable (Beutner and Zähle, 2010).

Furthermore, the proof of their Theorem 2.1 involves interchanging expectations and probability limits, such as \(\lim_{n \to \infty} E \{o_p(1)\} = 0\), which is in general not true without imposing some smoothness conditions on \(G\). In Theorem 1 we give a rigorous derivation for prediction error bias correction for PCA rank selection and show that the asymptotic expression given in Konishi and Kitagawa (1996) is still valid.

**Theorem 1.** Assume the following two conditions:

(i) \(X\) has finite \(4q\)th moments for some \(q > 1\).

(ii) The distribution of \(X\) satisfies the Lipschitz condition: there exist \(c_\alpha > 0\), \(0 < \nu \leq 1\), \(0 < \delta \leq 1\) such that \(\sup_{v \in \mathbb{R}^p, \|v\|=1} P (-\omega \leq v^\top X \leq \omega) \leq c_\alpha (2\omega)^\nu\) for all \(0 < \omega \leq \delta/2\).
Then, \( \lim_{n \to \infty} nE \left\{ \int \ell(x|\hat{\theta}_r)dG_n(x) - \int \ell(x|\hat{\theta}_r)dG(x) \right\} = b_r^{\text{GIC}} \) for any fixed \( r \) and \( p \).

Whereas (i) imposes a mild moment restriction, assumptions like (ii) have been frequently used to derive information criteria in a rigorous manner. For example, under correct specification of the model and an assumption slightly stronger than (ii), Findley and Wei (2002) have presented the first mathematically complete derivation of AIC for vector autoregressions. As shown in Section 4 of Findley and Wei (2002), their stronger assumption is fulfilled by a rich class of multivariate distributions, including the normal, \( t \), and \( \varepsilon \)-contaminated normal. Note that we assume in Theorem 1 the finiteness of \( p \) for mathematical tractability. We are not able to extend the result to the case of diverging \( p \). Nevertheless, to the best of our knowledge there is no existent study for GIC-based PCA rank selection even for the fixed \( p \) case. The finiteness of \( p \), however, is merely to establish Theorem 1. In the rest of the article, this assumption is no longer required in the development of our method nor for the selection consistency theorem.

It is worth emphasizing that \( b_r^{\text{GIC}} \) consists of two parts: the differential of log-likelihood \( \partial \ell(x|\theta)/\partial \theta \) under the working model \( N(\mu, \Sigma_r) \), and the influence function \( \text{IF}_{T_r}(x; G) \) of MLE under the true \( G \) with the generalized spiked covariance matrix (1). Intuitively, \( b_r^{\text{GIC}} \) can be estimated by \( \frac{1}{n} \sum_{i=1}^{n} \left\{ \frac{\partial \ell(X_i|\hat{\theta}_r)}{\partial \theta} \right\}^\top \text{IF}_{T_r}(X_i; G_n) \) using empirical data. However, a closer look at the calculation of \( b_r^{\text{GIC}} \) reveals that its estimation under the PCA rank selection problem involves the fourth moments of \( X \), which can be unstable in practice. Fortunately, a neat expression of \( b_r^{\text{GIC}} \) that avoids calculating higher-order moments of \( X \) can be derived under the working assumption of Gaussianity on \( X \).

**Theorem 2.** Assume \( X \sim N(\mu, \Sigma) \) with the generalized spiked covariance matrix (1). Then, \( b_r^{\text{GIC}} \) can be expressed as

\[
\begin{align*}
  b_r^{\text{GIC}} &= b_{\Gamma_r}^{\text{GIC}} + b_{\Lambda_r}^{\text{GIC}} + b_{\sigma^2}^{\text{GIC}} + b_{\mu}^{\text{GIC}},
\end{align*}
\]

where

\[
\begin{align*}
  b_{\Gamma_r}^{\text{GIC}} &= \binom{r}{2} + \sum_{j \leq r} \sum_{f > r} \frac{\lambda_f (\lambda_j - \sigma^2_r)}{\sigma^2_r (\lambda_j - \lambda_f)}, \\
  b_{\Lambda_r}^{\text{GIC}} &= r, \\
  b_{\sigma^2}^{\text{GIC}} &= \frac{1}{p-r} \sum_{j > r} \lambda_j^2 \left( \frac{1}{p-r} \sum_{j > r} \lambda_j \right)^{-2}, \\
  b_{\mu}^{\text{GIC}} &= p.
\end{align*}
\]
account for the model complexity corresponding to $\Gamma_r$, $\Lambda_r$, $\sigma_r^2$, and $\mu$. Here $\left(\frac{r}{2}\right) = 0$ if $r \leq 1$.

One can see from Theorem 2 that $b_r^{GIC}$ depends on the dispersion of $\lambda_j$’s, while the value of $b_r$ does not. More insights for terms making up $b_r^{GIC}$ are listed below:

- For $b_{\Gamma_r}^{GIC}$, first recall that $pr - \frac{r(r+1)}{2}$ is the number of free parameters in $\Gamma_r$. We have
  \[
  b_{\Gamma_r}^{GIC} - \left\{ pr - \frac{r(r+1)}{2} \right\} = \sum_{j \leq r} \xi_{j|r},
  \]
  where
  \[
  \xi_{j|r} = \sum_{\ell > r} \left\{ \frac{\lambda_{\ell}(\lambda_j - \sigma_r^2)}{\sigma_r^2(\lambda_j - \lambda_{\ell})} - 1 \right\} = \frac{\lambda_j}{\sigma_r^2} \sum_{\ell > r} \frac{\lambda_{\ell} - \sigma_r^2}{\lambda_j - \lambda_{\ell}}, \quad j \leq r.
  \]
  For given $r$, $\xi_{j|r}$ can be explained as the difference of model complexity for the $j$-th eigenvector between models without and with the requirement of correctly specifying the rank-$r$ simple spiked model (3). By the definition of $\sigma_r^2$ in (10), we have
  \[
  \xi_{j|r} \geq \frac{\lambda_j}{\sigma_r^2} \sum_{\ell > r} \frac{\lambda_{\ell} - \sigma_r^2}{\lambda_j - \sigma_r^2} = 0.
  \]
  This indicates that counting the number of free parameters generally underestimates the model complexity of $\Gamma_r$, especially when $\{\lambda_{\ell} : \ell > r\}$ deviates from their mean $\sigma_r^2$.

- For $b_{\sigma_r^2}^{GIC}$, we have
  \[
  b_{\sigma_r^2}^{GIC} = \left( \frac{\frac{1}{p-r} \sum_{j > r} \lambda_j^2}{\left( \frac{1}{p-r} \sum_{j > r} \lambda_j \right)^2} \right)^2 \geq 1,
  \]
  where the equality holds if and only if the elements of $\{\lambda_j : j > r\}$ are all equal. That is to say, except for the case $\Sigma = \Sigma_{r_0}$, where the population covariance exactly matches the simple spiked working covariance, counting the number of free parameters underestimates the model complexity for tail components. However, $b_{\sigma_r^2}^{GIC}$ can be more adaptive to the eigenvalue dispersion in assessing the complexity for tail components.

- For $b_{\Lambda_r}^{GIC}$ and $b_{\mu}^{GIC}$, GIC counts the number of free parameters in $\Lambda_r$ and $\mu$. It indicates that the misspecification of a generalized spiked model by a simple spiked model has no impact on the complexity of leading $r$ eigenvalues and mean vector.
From the observations above, we have

\[ \hat{b}_r^{\text{GIC}} \geq b_r \ \forall (r, \theta_r). \]  

(13)

Moreover, the equality in (13) holds (i.e., \( \hat{b}_r^{\text{GIC}} \) reduces to the number of free parameters) if and only if \( \Sigma = \Sigma_{r_0} \) and \( r \geq r_0 \) (see Remark 2 for details). As the simple spiked model (3) is rarely true, (13) implies that \( b_r \) generally underestimates the model complexity, in which situation model misspecification can be an issue.

With the expression of \( \hat{b}_r^{\text{GIC}} \), our GIC-based rank estimate is proposed to be

\[
\hat{r}_{\text{GIC}} = \arg\min_{r \leq q} \left\{ \ln |\hat{\Sigma}_r| + \frac{2}{n} \hat{c}_r^{\text{GIC}} \right\},
\]

(14)

where

\[
\hat{c}_r^{\text{GIC}} = \left\{ \binom{r}{2} + \sum_{j \leq r} \sum_{\ell > r} \hat{\lambda}_\ell (\hat{\lambda}_j - \hat{\sigma}_r^2) \right\} + r + \frac{1}{p-r} \sum_{j > r} \hat{\lambda}_j^2 \left( \frac{1}{p-r} \sum_{j > r} \hat{\lambda}_j \right)^2 + p
\]

(15)

is the sample version of \( c_r^{\text{GIC}} \) obtained by plugging in the sample eigenvalues, and \( q \) is a pre-determined upper bound of the model rank. Note that \( n^{-1}(b_{\hat{\lambda}_r} + b_{\hat{\sigma}_r^2}) = o(1) \), while \( n^{-1}b_{\hat{\mu}}^{\text{GIC}} = O(1) \), and that \( b_{\hat{\mu}}^{\text{GIC}} \) is independent of the model rank \( r \). This indicates that \( b_{\hat{\mu}}^{\text{GIC}} \) plays a dominant role in applying \( \hat{\tau}_{\text{GIC}} \). The form of \( b_{\hat{\tau}_r}^{\text{GIC}} \) also indicates that GIC will prevent the selection of a model rank with nearly multiple eigenvalues, in which situation a large value of \( \hat{b}_r^{\text{GIC}} \) is induced due to the division by \( (\hat{\lambda}_j - \hat{\lambda}_\ell) \). This scenario, however, cannot be reflected by \( b_r \) that simply counts the number of free parameters.

We close this section by noting that the Gaussian assumption in Theorem 2 is merely used to get an explicit neat expression for \( b_r^{\text{GIC}} \). This assumption is not critical in applying \( \hat{\tau}_{\text{GIC}} \). In Section 3, we will rigorously investigate the asymptotic properties of \( \hat{b}_r^{\text{GIC}} \) and \( \hat{\tau}_{\text{GIC}} \) under the high-dimensional setting and without requiring the Gaussian assumption.

**Remark 2.** The derivation of \( b_r^{\text{GIC}} \) in Theorem 2 is under the assumption of distinct eigenvalues (1). For \( \Sigma = \Sigma_{r_0} \), where the tail eigenvalues are equal, \( b_r^{\text{GIC}} \) can still be well-defined by setting \( 0/0 = 1 \) for these terms \( \frac{\lambda_j - \hat{\sigma}_r^2}{\lambda_j - \lambda_\ell} \). With this treatment, it is straightforward to show that \( b_r^{\text{GIC}} = b_r \) if and only if \( \Sigma = \Sigma_{r_0} \) and \( r \geq r_0 \).
3 Rank Selection Consistency

3.1 The target rank

The selection consistency is meaningful only when there is a precise definition of the target rank. The aim of this subsection is to provide a rigorous definition for the target rank $r_0$, which is identifiable under model (1).

We first review some basic results of random matrix theorem. Define the empirical spectral distribution (ESD) of $\Sigma$ to be

$$F_{\Sigma}(t) = \frac{1}{p} \sum_{j=1}^{p} I\{\lambda_j \leq t\},$$

where $I\{\cdot\}$ is the indicator function. Assume the following conditions (C1)–(C4), which are commonly used in random matrix theory (Bai and Yao, 2012).

(C1) For each $i$, $X_i$ takes the form $X_i = \Sigma^{1/2}Z_i$, where $Z_i \in \mathbb{R}^p$ consists of i.i.d. random variables with mean 0, variance 1, and finite fourth moment.

(C2) $p/n \to c \in (0, \infty)$.

(C3) $F_{\Sigma}$ converges weakly to $H$ as $p \to \infty$, where $H$ has bounded support.

(C4) The sequence of spectral norms of $\Sigma$ is bounded.

The distribution $H$ is called the limiting spectral distribution (LSD) of $\Sigma$. The LSD of the sample covariance matrix $S_n$ exists and is determined by $(c, H)$.

Theorem 3 (Yao, Zheng and Bai, 2015). Given $(c, H)$. Then, $F^{S_n}$ converges to the generalized Marčenko-Pastur distribution $F_{c,H}$ as $n \to \infty$. The Stieltjes transform of $F_{c,H}$, $s_{c,H}(z) = \int \frac{1}{1-z}dF_{c,H}(t)$, $z \in \mathbb{C}^+$, is implicitly determined via $s_{c,H}(z) = \int \frac{dH(t)}{i(1-c-zs_{c,H}(z))}$. Moreover, $F_{c,H}$ and $H$ share the same mean, i.e., $\int tdF_{c,H}(t) = \int tdH(t) = \mu_H$.

A major difficulty of random matrix theory is that $F_{c,H}$ has no explicit form for an arbitrary $H$. One known result for $F_{c,H}$ is under the simple spiked covariance model assumption:

(C5) $H(t) = I(t \geq \sigma^2)$ for some $\sigma^2 > 0$. 

Theorem 4 (Marčenko-Pastur Law). Assume further the simple spiked covariance model (C5); the distribution function of $F_{c,H}$ has a probability density function given by

$$f_{c,\sigma^2}(t) = \begin{cases} \frac{1}{2\pi c\sigma^2} \sqrt{(b-t)(t-a)}, & t \in [a, b] \\ 0, & t \notin [a, b] \end{cases}$$

with an additional point mass of value $1 - 1/c$ at the origin if $c > 1$, where $a = \sigma^2(1 - \sqrt{c})^2$ and $b = \sigma^2(1 + \sqrt{c})^2$. The mean under $F_{c,H}$ is $\mu_H = \sigma^2$.

An eigenvalue $\lambda_j$ is called a generalized spike eigenvalue if $\lambda_j$ does not belong to the support of $H$, denoted by $S(H)$. For the PCA rank selection problem, we assume in the rest of discussion that the generalized spike eigenvalues are larger than $\sup S(H)$, so that these spiked eigenvalues can be of the major interest. To study the asymptotic behavior of $\hat{\lambda}_j$, define

$$\psi(\lambda) = \lambda \left\{ 1 + c \int \frac{t}{\lambda - t} dH(t) \right\} \quad \text{and} \quad \psi'(\lambda) = \frac{\partial \psi(\lambda)}{\partial \lambda}, \quad \lambda \notin S(H).$$

Note that $\psi(\cdot)$ depends on $(c, H)$. The following results are modified from Bai, Chen and Yao (2010), Bai and Yao (2012), and Yao, Zheng and Bai (2015).

Theorem 5. Let $\lambda_j$ be a generalized spike eigenvalue with $\psi_j = \psi(\lambda_j)$, and let $b = \sup S(F_{c,H})$.

(i) $\psi_j \notin S(F_{c,H})$ (i.e., $\psi_j > b$) if and only if $\psi'(\lambda_j) > 0$.

(ii) If $\psi'(\lambda_j) > 0$, then $\hat{\lambda}_j \xrightarrow{a.s.} \psi_j$.

(iii) If $\psi'(\lambda_j) \leq 0$ and $j = o(p)$, then $\hat{\lambda}_j \xrightarrow{a.s.} b$.

(iv) For any $k = o(p)$, $\frac{1}{p-k} \sum_{\ell > k} \hat{\lambda}_\ell \xrightarrow{a.s.} \mu_H$.

These results show that a generalized spike eigenvalue $\lambda_j$ is not guaranteed to be identifiable in general. The identifiability of the $j$th spike further requires $\psi'(\lambda_j) > 0$ so that the corresponding limiting value $\psi_j$ can be separated from $S(F_{c,H})$. Thus, a generalized spike eigenvalue $\lambda_j$ is called a distant spike if $\psi'(\lambda_j) > 0$; otherwise, it is called a close spike. This definition also implies that for distant spikes $\lambda_j > \lambda_k$, one has $\psi_j > \psi_k > b$.

We are now in a position to define the target rank $r_0$ of a PCA model. Under the generalized spiked covariance model (1), we know from Theorem 5 that only distant spiked eigenvalues can be separated from $S(F_{c,H})$. This motivates the following definition of $r_0$. 

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Definition 1. Given \((c, H)\), define 
\[ r_0 = \sum_{j=1}^{p} I\{\psi'(\lambda_j) > 0\} \]
to be the number of distant spikes. We call \(r_0\) the target rank of a PCA rank selection problem calibrated by \((c, H)\).

The definition of \(r_0\) implies that \(\psi_{r_0} > b\); hence, the rank-\(r_0\) PCA subspace is identifiable under \((c, H)\). Consequently, for any given \((c, H)\), \(r_0\) is the well-defined target rank of (1), under which we can study the selection consistency of \(\hat{r}_{GIC}\).

3.2 Selection consistency of GIC

The asymptotic properties of \(\hat{r}_{GIC}\) heavily depend on the asymptotic increment of the GIC penalty when one increases the model rank from \((j-1)\) to \(j\):

\[
\kappa_j = \lim_{n \to \infty} \frac{1}{n} \left( \hat{b}_{j,GIC} - \hat{b}_{j-1,GIC} \right), \quad j \geq 1.
\]

Define the function

\[
\kappa(u) = c(u - 1)E\left\{ \frac{(T/\mu_H)}{u - (T/\mu_H)} \right\}, \quad u \in [b/\mu_H, \infty),
\]

where the expectation is taken with respect to \(T \sim F_{c,H}\). The function \(\kappa(u)\) is well defined for \(u > b/\mu_H\). As to the boundary point \(b/\mu_H\), it is defined by \(\kappa(b/\mu_H) = \lim_{u \to b/\mu_H} \kappa(u)\) and is assumed bounded. We have the following results for the asymptotic increment \(\kappa_j\).

Theorem 6. Assume conditions \((C1)-(C4)\).

(i) \(\kappa(u)\) is a strictly decreasing function. Moreover, \(\kappa(u) \geq c\) and \(\lim_{u \to \infty} \kappa(u) = c\).

(ii) For \(j = o(p)\), we have

\[
\kappa_j = \begin{cases} 
\kappa(\psi_j/\mu_H), & j \leq r_0, \\
\kappa(b/\mu_H), & j > r_0.
\end{cases}
\]

Note that the limiting value \(\kappa(b/\mu_H)\) is independent of \(j\).

The implications of Theorem 6 are threefold. First, we have

\[
\kappa_j \geq c \quad \text{for} \quad j = o(p).
\]
For the rank-0 PCA model, \( \lim_{n \to \infty} \frac{1}{n} b_0^{\text{GIC}} = \lim_{n \to \infty} \frac{1}{n} b_0 = 0 \). Since the asymptotic increment of \( \frac{1}{n} b_r \) is \( c \) (Bai, Choi and Fujikoshi, 2018), (18) implies that
\[
\lim_{n \to \infty} P(\hat{r}^{\text{GIC}} \leq \hat{r}^{\text{AIC}}) = 1.
\]
That is, GIC tends to select a smaller model than AIC. Second, for the model rank with a large eigenvalue, GIC tends to use the same penalty \( c \) as AIC does. Third, \( \kappa_j \) is an increasing function of \( j \) that attains the maximum value \( \kappa(b/\mu_H) \) when \( j > r_0 \). That is, GIC places a higher penalty on the model rank for a smaller eigenvalue, and places the maximum penalty \( \kappa(b/\mu_H) \) when the eigenvalue is smaller than the minimum distant spike \( \lambda_{r_0} \). This is reasonable since an eigenvector associated with a smaller eigenvalue is more difficult to estimate. Hence, one must pay a higher cost in its estimation. Consequently, when there exists a sufficiently large gap between \( \lambda_{r_0} \) and \( S(H) \) in the sense that \( \psi_{r_0} \) and \( b \) are well separated, the increment \( \kappa(b/\mu_H) \) for \( j > r_0 \) is expected to be sufficiently larger than \( \kappa(\psi_{r_0}/\mu_H) \). That is, one will undertake a large penalty when the model size goes beyond \( r_0 \), and this property will drive GIC to select the target rank \( r_0 \). Below we state the selection consistency of GIC.

**Theorem 7.** Assume conditions \( (C1)\)–\( (C4) \) and \( q = o(p) \). Then, \( \hat{r}^{\text{GIC}} \) achieves selection consistency if and only if the following conditions are satisfied:

\[
\begin{align*}
(G1) \quad & L_{\text{GIC}}(\psi_{r_0}/\mu_H) < 0, \\
(G2) \quad & L_{\text{GIC}}(b/\mu_H) > 0,
\end{align*}
\]

where \( L_{\text{GIC}}(u) = \ln u - (u - 1) + 2\kappa(u) \), and \( \kappa(u) \) is defined in (16).

Note that “\( \ln u - (u - 1) \)” in \( L_{\text{GIC}}(u) \) corresponds to a decrement in negative log-likelihood and “\( \kappa(u) \)” corresponds to an increment of model penalty, when the rank of model covariance increases. Following the terminology of Bai, Choi and Fujikoshi (2018), we call \( (G1)\)–\( (G2) \) the gap conditions of GIC. Condition \( (G1) \) gives the minimum size for the distant spiked eigenvalue \( \lambda_{r_0} \), while condition \( (G2) \) quantifies the maximum size for the upper bound \( b \) of \( S(F_{c,H}) \). Recall from Theorem 6 that \( \kappa(\cdot) \) achieves the maximum value at \( \kappa(b/\mu_H) \), which implies that \( (G2) \) is usually not as critical as \( (G1) \) to the selection consistency of GIC.
4 Data Analysis

We illustrate the proposed GIC rank selection by applying it to the dataset analyzed in Wu et al. (2011), which studies the habitual diet effect in the human gut microbiome. This dataset was also analyzed by Zheng, Lv and Lin (2020). It consists of \( n = 91 \) subjects, each with 301 measurements (214 for nutrient intake and 87 for gut microbiome composition). In our analysis, we first apply PCA to reduce the data dimension by preserving 99% of the variation. This leads to a resulting dimension \( p = 71 \) of principal components. We then apply GIC, AIC, and BIC (with \( q = 20 \)) on the \( 91 \times 71 \) data matrix (after componentwise standardization) to estimate the model rank.

The penalized log-likelihood of each method is presented in Figure 1 (a), which gives \( \hat{r}_{\text{GIC}} = 7 \), \( \hat{r}_{\text{AIC}} = 12 \), and \( \hat{r}_{\text{BIC}} = 4 \). The penalty functions \( \hat{b}_{r}^{\text{GIC}} \) and \( b_{r} \) are presented in Figure 1 (b), where \( b_{r} \) is a smooth curve, while \( \hat{b}_{r}^{\text{GIC}} \) is not a monotone function, indicating that \( \hat{b}_{r}^{\text{GIC}} \) is more adaptive to the underlying eigenvalue structures. Observe that \( \hat{b}_{r}^{\text{GIC}} \) has a peak at \( r = 10 \) that also results in a local minimum of the penalized log-likelihood of GIC at \( r = 10 \) (Figure 1 (a)). This sudden large value of \( \hat{b}_{10}^{\text{GIC}} \) indicates that the values of the 10th and 11th eigenvalues are very close (see the eigenvalues in Figure 1 (c), where \( \hat{\lambda}_{9} = 7.4073 \), \( \hat{\lambda}_{10} = 6.8382 \), \( \hat{\lambda}_{11} = 6.7148 \), and \( \hat{\lambda}_{12} = 6.0254 \)). By using \( \hat{b}_{r}^{\text{GIC}} \), the selection procedure tends to avoid an estimate of the model rank of 10. This scenario of nearly multiple eigenvalues for \( \{\hat{\lambda}_{10}, \hat{\lambda}_{11}\} \) (which usually results in unstable analysis results if the model rank is selected at 10), however, is not detected by \( b_{r} \), since it simply counts the number of free parameters without considering the eigenvalue dispersion. To evaluate the estimated model rank from different methods, one can see in Figure 1 (c) that an elbow cutoff looks around \( r = 8 \) or 9, which supports the result of \( \hat{r}_{\text{GIC}} = 7 \) better than \( \hat{r}_{\text{AIC}} = 12 \). The estimate \( \hat{r}_{\text{BIC}} = 4 \) is too small, and useful information can be lost. However, the scree plot method can be quite subjective and can depend on user bias. For a quantitative measure in evaluating the performance of different selection criteria, we also report in Figure 1 (d) the leave-one-out cross-validated (LOOCV) log-likelihood \( \text{CV}(r) = \frac{1}{n} \sum_{i=1}^{n} \ell(X_{i}|\hat{\theta}_{r}^{(i-1)}) \) at \( r \in \{1, 2, \ldots, 20\} \), where \( \hat{\theta}_{r}^{(i-1)} \) is the MLE of \( \theta_{r} \) without using \( X_{i} \). One can see that \( \text{CV}(r) \) achieves the maximum at \( r = 7 \), and the value \( \text{CV}(7) \) of GIC, is much larger than \( \text{CV}(12) \).
of AIC and CV(4) of BIC. All the findings above support the selection result \( \hat{r}_{\text{GIC}} = 7 \).

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Figure 1: Real data analysis. (a) Penalized log-likelihood from different criteria, where "∗" indicates the maximum value for each method. These maximum values correspond to \( \hat{r}_{\text{BIC}} = 4, \hat{r}_{\text{GIC}} = 7, \) and \( \hat{r}_{\text{AIC}} = 12. \) (b) Values of \( b_r^{\text{GIC}} \) and \( b_r \) for \( r = 1, \ldots, 20. \) (c) Eigenvalues of the sample covariance matrix, where \( \hat{\lambda}_4, \hat{\lambda}_7, \) and \( \hat{\lambda}_{12} \) corresponding to the BIC, GIC, and AIC are indicated on the plot. (d) The values of LOOCV log-likelihood \( CV(r) \), where "∗" indicates the maximum value. The values at the estimated model rank from each method are also indicated.