TUNING PARAMETER SELECTION FOR PENALIZED LIKELIHOOD
ESTIMATION OF INVERSE COVARIANCE MATRIX

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Abstract: In a Gaussian graphical model, the conditional independence between two variables are characterized by the corresponding zero entries in the inverse covariance matrix. Maximum likelihood method using the smoothly clipped absolute deviation (SCAD) penalty (Fan and Li, 2001) and the adaptive LASSO penalty (Zou, 2006) have been proposed in literature. In this article, we establish the result that using Bayesian information criterion (BIC) to select the tuning parameter in penalized likelihood estimation with both types of penalties can lead to consistent graphical model selection. We compare the empirical performance of BIC with cross validation method and demonstrate the advantageous performance of BIC criterion for tuning parameter selection through simulation studies.

Key words and phrases: BIC; Consistency; Cross validation; Gaussian graphical model; Model selection; Oracle property; Penalized likelihood

1. Introduction

A multivariate Gaussian graphical model is also known as a covariance selection model. The conditional independence relationships between the random variables are equivalent to the specified zeros among the inverse covariance matrix. More exactly, let $X = (X^{(1)}, ..., X^{(p)})$ be a $p$-dimensional random vector following a multivariate normal distribution $N_p(\mu, \Sigma)$ with $\mu$ denoting the unknown mean and $\Sigma$ denoting the nonsingular covariance matrix. Denote the inverse covariance matrix as $\Sigma^{-1} = C = (C_{ij})_{1 \leq i,j \leq p}$. The zero entries $C_{ij}$ in the inverse covariance matrix indicate the conditional independence between the two random variables $X^{(i)}$ and $X^{(j)}$ given all other variables (Dempster, 1972, Whitaker, 1990, Lauritzen, 1996). The Gaussian random vector $X$ can be represented by an undirected graph $G = (V, E)$, where $V$ contains $p$ vertices corresponding to the $p$ coordinates and the edges $E = (e_{ij})_{1 \leq i < j \leq p}$ represent the conditional dependency relationships between variables $X^{(i)}$ and $X^{(j)}$. It is of interest to
identify the correct set of edges, and estimate the parameters in the inverse covariance matrix simultaneously.

To address this problem, many methods have been developed up to date. In general, there would be no zero entries in the maximum likelihood estimate, which results in a full graphical structure. Dempster (1972) and Edwards (2000) proposed to use the penalized likelihood method with the $L_0$-type penalty

$$p_\lambda(|c_{ij}|_{i \neq j}) = \lambda I(|c_{ij}| \neq 0),$$

where $I(.)$ is the indicator function. Since the $L_0$ penalty is discontinuous, the resulting penalized likelihood estimator is unstable. Another standard approach to perform model selection in Gaussian graphical model is stepwise forward selection or backward elimination of the edges. However, this approach ignores the stochastic errors inherited in the multiple stages of the procedure (Edwards, 2000) and causes the statistical properties of the method hard to comprehend. Furthermore, the computational complexity of this greedy search algorithm increases exponentially with the number of vertices in the graph. Meinshausen and Bühlmann (2006) proposed a computationally attractive method for covariance selection. The proposed method performs the neighborhood selection for each node and combines the results to learn the overall graphical structure. It has been shown that this method is connected to the quadratic approximation of the loglikelihood with $L_1$ penalty (Yuan and Lin, 2007). Nevertheless this method performs the model selection and parameter estimation separately. Yuan and Lin (2007) proposed penalized likelihood methods for estimating the concentration matrix with $L_1$ penalty (LASSO) (Tibshirani, 1996). The method can be implemented through the maxdet algorithm in convex optimization. However, due to the inherent computational complexity, the maxdet algorithm can only handle matrices with small $p$.

Banerjee, Ghaoui and D'aspremont (2007) have proposed a block-wise updating algorithm for the estimation of inverse covariance matrix. For each block-wise update, the problem is a box-constrained quadratic program, which can be solved by an interior-point procedure. They further showed that the problem emerges from each step of block-wise update is equivalent to a linear regression under $L_1$ penalty. Further in this line, Friedman, Hastie and Tibshirani (2008) proposed the graphical LASSO algorithm to estimate the sparse inverse covariance matrix using the LASSO penalty through coordinate-wise updating scheme. It is the
fastest and most convenient algorithm to tackle this problem up to date. Fan, Feng and Wu (2009) proposed to estimate the inverse covariance matrix using adaptive LASSO and Smoothly Clipped Absolute Deviation (SCAD) penalty to attenuate the bias problem. They employed local linear approximation method (Zou and Li, 2008) to approximate the LASSO penalty as weighted $L_1$ penalty and the method is implemented through the graphical LASSO algorithm. The resulted methods with both SCAD and adaptive LASSO penalties are computationally convenient algorithms leading to asymptotically unbiased, sparse estimators which possess oracle property.

In practice, the performance of the penalized likelihood estimator depends on the proper choice of the regularization parameter. In this article, we focus on the tuning parameter selection in penalized likelihood estimation of the sparse inverse covariance matrix. Wang, Li and Tsai (2007) proposed to use the Bayesian information criterion (BIC) to select the tuning parameter for penalized likelihood method with SCAD penalty. They showed that BIC with SCAD penalty is able to identify the true model consistently in the setting of linear regression and partial linear model. Yuan and Lin (2007) used BIC to select the tuning parameter with the $L_1$ penalty in the estimation of inverse covariance matrix. But the consistency of BIC for Gaussian graphic model has not been investigated. In this article, we establish the consistency result of the BIC criterion with both SCAD and adaptive LASSO. We show that if SCAD or adaptive LASSO penalty is used, the optimum tuning parameter selected by BIC will yield the graphical structure identical to the true underlying graphical model with probability tending to one as $n \to \infty$. We also compare the performance of BIC with cross-validation method through extensive simulation studies. We demonstrate that in small sample size scenario, including the cases when the number of parameters greatly exceeds the sample size, BIC exhibits comparable performance as the computationally more intensive cross-validation method. However, when sample size increases, BIC consistently outperforms cross validation.

The rest of the article is organized as follows. In Section 2.1 we formulate the penalized likelihood function for inverse covariance matrix. In sections 2.2 and 2.3, we discuss the selection of tuning parameters through the BIC criterion and prove its consistency in graphical model selection with SCAD and adaptive
LASSO penalty. In section 3, simulation studies are presented to demonstrate the empirical performance of the tuning parameter selection with BIC compared with the cross validation method in small sample size and large sample size scenarios.

2.1 Penalized Likelihood Estimation of Inverse Covariance Matrix

Given a random sample $X_1, ..., X_n$ following a multivariate normal distribution $N_p(\mu, \Sigma)$, the loglikelihood for $\mu$ and $C = \Sigma^{-1}$ can be expressed as

$$\frac{n}{2} \log |C| - \frac{1}{2} \sum_{i=1}^{n} (X_i - \mu)' C (X_i - \mu),$$

up to a constant not depending on the parameters. The maximum likelihood estimator of $(\mu, \Sigma)$ is $(\bar{X}, \bar{A})$, where

$$\bar{A} = \frac{1}{n} \sum_{i=1}^{n} (X_i - \bar{X})(X_i - \bar{X})'.$$

Assume that the observations are properly centered, then the sample mean is zero. As $\hat{\mu}$ does not depend on $C$, we have $\hat{\mu} = 0$. To obtain the maximum likelihood estimator of the concentration matrix is equivalent to minimize

$$-\frac{2}{n} \ell(C) = -\log |C| + \text{tr}(C \bar{A}).$$

To achieve sparse graph structure, penalized likelihood methods have been proposed in literature and the resulting estimator $\hat{C}$ should minimize the following objective function:

$$Q(C) = -\log |C| + \text{tr}(C \bar{A}) + \sum_{i \neq j} p_\lambda(|c_{ij}|),$$

with $p_\lambda$ being some penalty function. Yuan and Lin (2007) have proposed to use LASSO penalty, $p_\lambda(|c_{ij}|) = \lambda |c_{ij}|$. Friedman, Hastie and Tibshirani (2008) proposed the graphical LASSO algorithm by using a coordinate descent procedure, which is computationally very fast and guarantees the positive definiteness of the resulting estimate. As the LASSO penalty increases linearly with the size of its argument, it leads to biases for the estimates of nonzero coefficients. To attenuate such estimation biases, Fan and Li (2001) proposed SCAD penalty. The penalty function satisfies $p_\lambda(0) = 0$, and its first-order derivative is

$$p_\lambda'(\theta) = \lambda I(\theta \leq \lambda) + \frac{(a \lambda - \theta)_+}{(a - 1) \lambda} I(\theta > \lambda),$$

for $\theta > 0$, where $I$ is the indicator function. In the following section, we will describe these methods in more detail.
where $a$ is some constant usually set to 3.7 (Fan and Li, 2001), and $(t)_+ = tI(t > 0)$ is the hinge loss function.

The SCAD penalty is a quadratic spline function with knots at $\lambda$ and $a\lambda$. It is singular at the origin which ensures the sparsity and continuity of the solution. The penalty function does not penalize as heavily as the $L_1$ penalty function on large parameters. More important advantage of the SCAD penalty is that the method not only selects the correct set of edges, but also produces parameter estimators as efficient as if we know the true underlying graphic structure. Namely, the estimators have the so called oracle property.

Zou (2006) proposed the adaptive LASSO penalty, which imposes a weight for each parameter and can be regarded as a weighted version of the LASSO penalty. In the current setting, the adaptive LASSO penalty takes the form of $p_\lambda(|c_{ij}|) = \lambda w_{ij}|c_{ij}|$, with $w_{ij} = 1/|\tilde{c}_{ij}|^\gamma$, for some consistent estimator $\tilde{C} = (\tilde{c}_{ij})_{1\leq i,j \leq p}$ and some $\gamma > 0$. As the empirical performance of the results does not differ much for different $\gamma$, we follow the conventional choice of $\gamma = 0.5$.

Both SCAD and adaptive LASSO can be efficiently implemented using the graphical LASSO algorithm. For SCAD penalty, Fan, Feng and Wu (2009) proposed to use local linear approximation (Zou and Li, 2008) to approximate the SCAD by a symmetric linear function. The proposed iterative re-weighted penalized likelihood method optimizes the objective function at step $(k + 1)$ as follows:

$$Q(C)^{(k+1)} = -\log |C| + \text{tr}(C\tilde{A}) + \sum_{i \neq j} w_{ij}|c_{ij}|,$$

(2.1.2)

with $w_{ij} = p'_\lambda(\hat{c}_{ij}^{(k)})$, and $\hat{c}_{ij}^{(k)}$ denoting the estimates obtained at previous step. The computation can be implemented by reiteratively using the graphical LASSO algorithm.

### 2.2. Consistency of BIC with SCAD

In literature, two approaches have been used for the selection of tuning parameters under the penalized likelihood framework, including the BIC criterion (Yuan and Lin, 2007) and cross validation (Friedman, Hastie and Tibshirani, 2008; Fan, Feng and Wu, 2009). The theoretical investigation of this paper will be focused on the consistency result regarding the model selection using BIC cri-
terion under the penalized likelihood framework with SCAD or adaptive LASSO penalty.

For the tuning parameter $\lambda$, it is desirable to have a data-driven method to make the selection automatically. Define the full graphical model $G_F$ with the full edge set $E_F = (e_{ij})_{1 \leq i < j \leq p}$. Define an arbitrary graphical model $G$ with the corresponding edge set $E \subseteq E_F$. Define a true model $G_T$, with the edge set $E_T = (e_{ij})_{(i,j): c_{ij,0} \neq 0, i < j}$, where $c_{ij,0}$ denotes the null value of the parameter. Define an over-fitted model $G$ if the corresponding edge set $E \supseteq E_T$ and $E \neq E_T$. Define an under-fitted model $G$ with the edge set $E \nsubseteq E_T$.

In practice, as $\lambda$ is unknown, we search for the optimal $\lambda$ from the bounded interval $\Omega = [0, \lambda_{\text{max}}]$, for some upper limit $\lambda_{\text{max}}$. We further assume that the upper limit $\lambda_{\text{max}} \to 0$, as $n \to \infty$. This implies that the search region shrinks to 0 as $n$ tends to infinity. Similar assumption can be found in Wang, Li and Tsai (2007). Given a tuning parameter $\lambda$, the penalized likelihood approach yields the estimated parameters $(\hat{c}_{ij,\lambda})_{1 \leq i < j \leq p}$. The resulting model is denoted as $G_\lambda$ with the edge set $E_\lambda = (e_{ij})_{(i,j): \hat{c}_{ij,\lambda} \neq 0}$. We define $\Omega_- = \{\lambda \in \Omega : E_\lambda \nsubseteq E_T\}$, $\Omega_0 = \{\lambda \in \Omega : E_\lambda = E_T\}$, and $\Omega_+ = \{\lambda \in \Omega : E_\lambda \supseteq E_T$ and $E_\lambda \neq E_T\}$. The three subsets of $\Omega_0$, $\Omega_-$, $\Omega_+$ lead to the true, under and over-fitted models, respectively.

Given a $\lambda$, the associated BIC criterion is defined as:

$$BIC_\lambda = -\log |\hat{C}_\lambda| + \text{tr}(\hat{C}_\lambda \tilde{A}) + \frac{\log(n)}{n} \sum_{1 \leq i < j \leq p} I(\hat{c}_{ij,\lambda} \neq 0).$$

On the other hand, suppose we know the correct model $G_T$ beforehand and perform the maximum likelihood estimation. Under $G_T$, the parameters can be partitioned into two sets: $C^{(1)} = \{c_{ij} : c_{ij} \neq 0\}$, and $C^{(2)} = \{c_{ij} : c_{ij} = 0\}$. The resulted maximum likelihood estimator is denoted as $\hat{C}_{G_T} = (\hat{C}_{G_T}^{(1)}, 0)$, with $C^{(2)}$ known to be 0. The associated BIC criterion is denoted as

$$BIC_{G_T} = -\log |\hat{C}_{G_T}| + \text{tr}(\hat{C}_{G_T} \tilde{A}) + \frac{\log(n)}{n} \sum_{1 \leq i < j \leq p} I(c_{ij,0} \neq 0).$$

In this subsection, we will focus on the discussion on SCAD penalty. We first construct a working sequence of reference tuning parameters $\lambda_n = \log(n)/\sqrt{n}$, which satisfies the requirement that as $\lambda_n \to 0$, $\sqrt{n}\lambda_n \to \infty$. Under such working sequence of tuning parameters, according to Theorem 5.2 in Fan, Feng and Wu
(2009), with probability tending to one, the resulted method will not only identify the correct set of true edges but also yield root-\(n\) consistent estimators for all the nonzero partial correlation coefficients. This guarantees the following result:

**Lemma 2.2.1.** For SCAD penalty, \(P_r(BIC_{\lambda_n} = BIC_{G_T}) \to 1\) as \(n \to \infty\).

**Proof.** According to Theorem 5.2 in Fan, Feng and Wu (2009), under the reference sequence of tuning parameters, we have \(\lim_{n \to \infty} P(\hat{c}_{ij,\lambda_n} = c_{ij,0}) = 1\). It follows that \(\lim_{n \to \infty} P(\sum_{i<j} I(\hat{c}_{ij,\lambda_n} \neq 0) = \sum_{i<j} I(c_{ij,0} \neq 0)) = 1\). Due to the oracle property, the proposed SCAD penalized likelihood approach estimates the parameter under the correct sub-model with probability tending to 1, namely, \(\lim_{n \to \infty} P(\hat{C}_{\lambda_n} = \hat{C}_{G_T}) = 1\). Then the result of the Lemma follows.

Next we will consider the under-fitted model, which is essentially a misspecified model with at least one of the nonzero parameters being mistakenly set to zero. Given \(\lambda \in \Omega_\ast\), let \(C^{(a)}\) denote \((c_{ij})_{(i,j) \in E_\lambda}\), and let \(C^{(b)}\) denote \((c_{ij})_{(i,j) \notin E_\lambda}\). The penalized likelihood \(\hat{C}_\lambda = (\hat{C}^{(a)}_\lambda, 0)\) is the local minimizer of

\[
Q_\lambda(C) = -\frac{2}{n} \ell(C^{(a)}, 0) + \sum_{(i,j) \in E_\lambda} p_\lambda(|c_{ij}|). \tag{2.2.1}
\]

Under the misspecified graphical model, the parameter space is denoted as \(C^\ast = \{C|c_{ij} = 0, for (i,j) \notin E_\lambda and c_{ij} \neq 0, for (i,j) \in E_\lambda\}\), which does not include the true value \(C_0\). According to the asymptotic theory for maximum likelihood estimation under misspecified model (White, 1982), the maximum likelihood estimates \(\hat{C}\) will converge to \(C^\ast\) almost surely where \(C^\ast\) is the unique parameter in the under-fitted model which minimizes the Kullback-Leibler distance to the true model, namely

\[
C^\ast = \arg\min_{C \in C^*} E\{\log f(X; C_0) - \log f(X, C)\}. \tag{2.2.2}
\]

For Gaussian graphical model, the \(C^\ast\) is uniquely defined as the \(-\log f(X; C)\) is strictly convex and so is the \(-E\{\log f(X; C)\}\). We further partition the pseudo null value \(C^\ast = (C^{(a)}\ast, C^{(b)}\ast)\), with \(C^{(a)}\ast = (c_{ij})_{(i,j) \in E_\lambda}\), and \(C^{(b)}\ast = (c_{ij})_{(i,j) \notin E_\lambda} = 0\). It remains to show that the penalized likelihood estimator \(\hat{C}_\lambda\) is also a root-\(n\) consistent estimator to such pseudo null value \(C^\ast\).
Lemma 2.2.2. Given $\lambda \in \Omega_-$, let $C^*$ be defined as in Equation (2.2.3). Let the objective function $Q_\lambda(C)$ be defined as in equation (2.2.1), with the penalty being the SCAD function. If $\lambda \to 0$, as $n \to \infty$, then there exists a local minimizer $\hat{C}_\lambda$ of $Q_\lambda(C)$, such that $\|\hat{C}_\lambda - C^*\| = O_p(n^{-\frac{1}{2}})$.

Proof. Consider a constant matrix $u$ with its vectorized form denoted as $\bar{u}$. Assume $u \in C^*$ and $||\bar{u}|| = M$. Let $\ell(C) = n/2(\log|C| - \text{tr}(CA))$. For $n$ large enough, we have

$$n(Q_\lambda(C^* + \frac{u}{\sqrt{n}}) - Q_\lambda(C^*)) \\
\geq -2\ell(C^* + \frac{u}{\sqrt{n}}) + 2\ell(C^*) + n \sum_{(i,j):c^*_{ij} \neq 0} \{p_\lambda(|c^*_{ij}|) + \frac{u_{ij}}{\sqrt{n}}\} - p_\lambda(|c^*_{ij}|)) \\
\geq -2\ell(C^*) - \bar{u} + \frac{1}{n}\bar{u}^T\ell''(C^*)\bar{u}(1 + o_p(1)) +$$

$$\sum_{(i,j):c^*_{ij} \neq 0} \{p_\lambda^1(|c^*_{ij}|)\frac{u_{ij}}{\sqrt{n}} + p_\lambda^2(|c^*_{ij}|)\frac{u_{ij}^2}{n}(1 + o(1))\},$$

with

$$\ell'(C^*) = \frac{\partial \ell(C^{(a)})}{\partial C^{(a)}}|_{(C^*^{(a)},0)},$$

and

$$\ell''(C^*) = \frac{\partial^2 \ell(C^{(a)})}{\partial^2 C^{(a)}}|_{(C^*^{(a)},0)}.$$

It is known that for $n$ large enough, and $c^*_{ij} \neq 0$, $p_\lambda^1(|c^*_{ij}|) = 0$ and $p_\lambda^2(|c^*_{ij}|) = 0$. Furthermore, $C^*$ satisfies $E\{(\frac{\partial \log f(X,C^*)}{\partial C^{(a)}})|_{(C^*^{(a)},0)}\} = 0$. This entails $\ell'(C^*) = O_p(\sqrt{n})$. By standard asymptotic theory, $\ell''(C^*) = O_p(n)$. By choosing $M$ large enough, the sign of Equation (2.2.3) is completely determined by the second term of its last line. This implies, for any given $\epsilon > 0$, by choosing a ball centered around $C^*$, with radius $M$ sufficiently large, we have

$$P\{\inf_{||u||=M} Q_\lambda(C^* + \frac{u}{\sqrt{n}}) - Q_\lambda(C^*) \geq 1 - \epsilon. \} \geq 1 - \epsilon. \quad \text{(2.2.4)}$$

This guarantees that the local minimizer $\hat{C}_\lambda$ is root-$n$ consistent for $C^*$. \qed

The result above is helpful to understand the asymptotic property of $BIC_\lambda$ under an under-fitted model. Concerning an over-fitted model, some zero-valued
parameters are included in the model to be estimated, which can be regarded as nuisance parameters. Under an over-fitted model, the parameter space contains the correct null value of the parameters. Thus the property of the resulting $BIC_\lambda$ can be derived under the standard likelihood theory under correct model assumption.

**Lemma 2.2.3.** If $\lambda_{\text{max}} \to 0$, and $\lambda_{\text{max}} > \log(n)/\sqrt{n}$ as $n \to \infty$, and the penalty is SCAD function, then $\Pr(\inf_{\lambda \in \Omega_- \cup \Omega_+} BIC_\lambda > BIC_{\lambda_n}) \to 1$.

**Proof.** First we consider $\lambda \in \Omega_-$. According to Lemma 2.2.2, $\hat{\lambda}$ is root-$n$ consistent to $C^*$. Furthermore, $\ell'(C^*) = O_p(\sqrt{n})$, and $\ell''(C^*) = O_p(n)$. We have

$$\frac{\ell(\hat{\lambda})}{n} = \ell(C^*) + \frac{\partial \ell}{\partial C}|_{C^*} (\hat{\lambda} - C^*) + \frac{n}{2} (\hat{\lambda} - C^*)^T \frac{\partial^2 \ell}{\partial^2 C}|_{C^*} (\hat{\lambda} - C^*) (1 + o_p(1))$$

$$= \ell(C^*) + O_p(1). \tag{2.2.5}$$

By similar argument, $\ell(\hat{\lambda}) = \ell(C_0) + O_p(1)$. By the weak Law of large numbers,

$$\frac{1}{n} \ell(C^*) \xrightarrow{p} E \log f(X; C^*);$$

$$\frac{1}{n} \ell(C_0) \xrightarrow{p} E \log f(X; C_0).$$

Furthermore, $E \log f(X; C^*) < E \log f(X; C_0)$ due to the Kullback-Leibler inequality. Thus,

$$\frac{1}{n} \ell(C_0) - \ell(C^*) = n[E \log f(X; C_0) - E \log f(X; C^*)] + o_p(n). \tag{2.2.6}$$

This entails

$$n(BIC_\lambda - BIC_{G_T}) = 2\ell(\hat{\lambda}) - 2\ell(\hat{\lambda}) + \log n(e_\lambda - e_T)$$

$$= 2\ell(C_0) - 2\ell(C^*) + \log n(e_\lambda - e_T) + O_p(1) > 0, \tag{2.2.7}$$

where $e_\lambda = \sum_{i<j} I(\tilde{c}_{ij, \lambda} \neq 0)$, and $e_T = \sum_{i<j} I(c_{ij, 0} \neq 0)$.

Next consider $\lambda \in \Omega_+$. Define the maximum likelihood estimator under the true model and under the over-fitted model as $\hat{\lambda}_{G_T}$ and $\hat{\lambda}_\lambda$. Note that $\hat{\lambda}_\lambda$ is different from $\hat{\lambda}$, as the former is the maximum likelihood estimate under the submodel $E_\lambda$, where the latter is the penalized likelihood estimate under the full model using $\lambda$ as the tuning parameter. According to the standard asymptotic
theory for the loglikelihood ratio statistic, we have $2(\ell(\hat{C}_\lambda) - \ell(\hat{C}_{G_T})) \sim \chi^2_{e_\lambda - e_T} = O_p(1)$. Furthermore, the penalized likelihood estimators under the over-fitted model are denoted as $\hat{C}_\lambda$. From Theorem 5.2 in Fan, Feng and Wu (2009), $|\hat{C}_\lambda - \tilde{C}_\lambda| = O_p(n^{-\frac{1}{2}})$. This entails $\ell(\hat{C}_\lambda) = \ell(\tilde{C}_\lambda) + O_p(1)$. Combining the results above, we have

$$n(BIC_\lambda - BIC_{G_T}) = -2\ell(\hat{C}_\lambda) + 2\ell(\hat{C}_{G_T}) + \log n(e_\lambda - e_T)$$

$$= -2\ell(\tilde{C}_\lambda) + 2\ell(\hat{C}_{G_T}) + \log n(e_\lambda - e_T) + O_p(1)$$

$$= \log n(e_\lambda - e_T) + O_p(1) > 0.$$  

This completes the proof.

This Lemma implies that the $\lambda$s that fail to identify the true model yield BIC always larger than $\lambda_n$. Consequently, the $\lambda$ value which minimizes the BIC criterion will identify the true model. Combining the two lemmas above, we establishes the consistency of the BIC criterion used under the penalized likelihood framework with the SCAD penalty.

**Theorem 2.2.4.** If $\lambda_{\max} \to 0$, and $\lambda_{\max} > \log(n)/\sqrt{n}$ as $n \to \infty$, then $Pr(G_{\hat{\lambda}_{BIC}} = G_T) \to 1$, where $\hat{\lambda}_{BIC}$ is the tuning parameter that minimizes the BIC criterion with the SCAD penalty.

**2.3. Consistency of BIC with adaptive LASSO**

In this section, we focus on the establishment of the consistency result of BIC with adaptive LASSO penalty. Given any $a_n$-consistent estimate $\tilde{C}$, namely, $a_n(\tilde{C} - C_0) = O_p(1)$, the weights of the adaptive LASSO are specified by $w_{ij} = 1/|\tilde{C}_{ij}|^\gamma$, for some $\gamma > 0$. We first construct a sequence of reference tuning parameters which satisfies the requirement that as $\lambda_n \to 0$, $\sqrt{n}\lambda_n = O_p(1)$, and $n^{\frac{1}{2}}\lambda_n a_n^\gamma \to \infty$. Under such working sequence of tuning parameters, according to Theorem 5.3 in Fan, Feng and Wu (2009), with probability tending to one, the resulting method will not only identify the correct set of true edges but also yield root-$n$ consistent estimators for all the nonzero partial correlation coefficients. This guarantees the following result:

**Lemma 2.3.5.** $Pr(BIC_{\lambda_n} = BIC_{G_T}) \to 1$ as $n \to \infty$. 

Next we will consider the under-fitted model in a similar manner as what we have derived for SCAD penalty.

**Lemma 2.3.6.** Given $\lambda \in \Omega_-$, the corresponding misspecified model is denoted as $G_\lambda$. Let $C^*$ be defined as in Equation (2.2.2). Let the objective function $Q_\lambda(C)$ defined as in equation (2.1.1) with adaptive LASSO penalty. If $\lambda_n \to 0$, $\sqrt{n} \lambda_n = O_p(1)$, and $n^{1/2} \lambda_n a_n^\gamma \to \infty$. Then there exists a local minimizer $\hat{C}_\lambda$ of $Q_\lambda(C)$, such that $\|\hat{C}_\lambda - C^*\| = O_p(n^{-1/2})$.

**Proof.** Consider a constant matrix $u$ with its vectorized form denoted as $\vec{u}$. Assume $u \in C^*$ and $||\vec{u}|| = M$. Let $\ell(C) = n/2(\log|C| - \text{tr}(CA))$. For $n$ large enough, we have

$$n(Q_\lambda(C^* + u\sqrt{n}) - Q_\lambda(C^*))$$
$$\geq -2\ell(C^* + u\sqrt{n}) + 2\ell(C^*) + n \sum_{(i,j): c_{ij}^{(a)}(a) \neq 0} \{p_\lambda(|c_{ij}^* + u_{ij}\sqrt{n}|) - p_\lambda(|c_{ij}^*|)\}$$
$$\geq -2\ell'(C^*) \frac{\vec{u}}{\sqrt{n}} + \frac{1}{n} \vec{u}^T \ell''(C^*) \vec{u}(1 + o_p(1)) + n \lambda_n \sum_{(i,j): c_{ij}^{(a)}(a) \neq 0} \{|c_{ij}^*|^{-\gamma} \frac{u_{ij}\sqrt{n}}{\sqrt{n}} \text{sign}(c_{ij}^*)\}.$$

(2.3.1)

Using similar arguments as in Lemma 2.2.2, we have $\ell'(C^*) = O_p(\sqrt{n})$, and $\ell''(C^*) = O_p(n)$. Furthermore, $|\tilde{c}_{ij}^*|^{-\gamma} = O_p(1)$, as $\tilde{c}_{ij}^*$ is a consistent estimator of $c_{ij}^* \neq 0$. Because $\sqrt{n} \lambda_n = O_p(1)$, the third term is also $O_p(1)$. By choosing $M$ large enough, the sign of Equation (2.2.3) is completely determined by the second term of its last line. This implies, for any given $\epsilon > 0$, by choosing a ball centered around $C^*$, with radius $M$ sufficiently large,

$$P\{\inf_{||u||=M} Q_\lambda(C^* + u\sqrt{n}) > Q_\lambda(C^*)\} \geq 1 - \epsilon.$$  

(2.3.2)

This guarantees that the local minimizer $\hat{C}_\lambda$ is root-$n$ consistent for $C^*$.

In light of the result above, we are able to study the asymptotic property of $BIC_\lambda$ under the under-fitted model and the over-fitted model. Let the working sequence of $\lambda_n$ be defined as above. Following the same argument as in Section 3.1, we have
Lemma 2.3.7. If $\lambda_{\text{max}} \to 0$, and $\lambda_{\text{max}} > \lambda_n$, as $n \to \infty$, then $Pr(\inf_{\lambda \in \Omega_- \cup \Omega_+} BIC_{\lambda} > BIC_{\lambda_n}) \to 1$.

Theorem 2.3.8. If $\lambda_{\text{max}} \to 0$, and $\lambda_{\text{max}} > \lambda_n$, as $n \to \infty$, then $Pr(G_{\hat{\lambda}_{\text{BIC}}} = G_T) \to 1$, where $\hat{\lambda}_{\text{BIC}}$ is the tuning parameter that minimizes the BIC criterion with adaptive LASSO penalty.

3. Simulation Studies

Next we conduct simulation studies to investigate the performance of BIC in penalized likelihood estimation of Gaussian graphical model. The main focus is to use empirical evidence to support the consistency result of BIC with SCAD penalty or Adaptive LASSO. We also compare its performance with cross validation, which is another commonly used tuning parameter selection method. The $K$-fold cross-validation method partitions all the samples into $K$ disjoint subsets and denote the indices of subjects in $k$-fold by $T_k$, $k = 1, \ldots, K$. The $K$-fold cross-validation score is defined as:

$$CV(\lambda) = \sum_{k=1}^{K} n_k(- \log |\hat{C}_{\lambda,-k}| + \text{tr}(\hat{C}_{\lambda,-k}A_k)),$$

where $n_k$ is the size of the subset $T_k$, $\hat{C}_{\lambda,-k}$ is the estimated concentration matrix based on the sample $\cup_{j \neq k} T_j$, and $A_k$ is the sample covariance matrix calculated on subset $T_k$. The optimum tuning parameter $\lambda$ is selected to minimize $CV$. In our simulation, $K$ is set to be 5.

We simulate three different graphical model structures.

- **Model 1.** An AR(1) model is considered with $c_{ii} = 1$, and $c_{i,i-1} = c_{i-1,i} = 0.5$.

- **Model 2.** An AR(2) model is considered with $c_{ii} = 1.5$, $c_{i,i-1} = c_{i-1,i} = 0.5$ and $c_{i,i-2} = c_{i-2,i} = 0.40$.

- **Model 3.** A general sparse graphical model is considered. We employed the data generating scheme of Li and Gui (2006). To be more specific, we generate $p$ nodes randomly on the unit and square and obtained their pairwise Euclidean distance. For each point, it is connected with an edge to the points
with the 3 smallest distances. For each edge, the corresponding entry in the inverse covariance matrix is generated uniformly over $[-1, -0.5] \cup [0.5, 1]$. In order to ensure the positive definiteness of the inverse covariance matrix, the magnitude of the $i$th diagonal entry is set as twice of the sum of the absolute values of all the off-diagonal entries on the $i$th row.

For each model, we use penalized likelihood methods with SCAD, adaptive LASSO and LASSO penalties. The tuning parameter for all three penalties are selected through either the BIC criterion or the cross-validation criterion. To assess the model selection performance, we evaluate the sensitivity, specificity, and Matthews correlation coefficient (MCC) which are defined as follows:

$$
specificity = \frac{TN}{TN + FP}, \quad sensitivity = \frac{TP}{TP + FN},
$$

$$
MCC = \frac{TP \times TN - FP \times FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}},
$$

where TP, TN, FP, FN are the numbers of true positives, true negatives, false positives, and false negatives. Taking both true and false positives and negatives into account, MCC has been widely used to measure the quality of binary classifiers. The larger the MCC is, the better the classifier performs. Means and standard deviations of the above measures are provided in Tables 1-3. Under each of the three models, we generated 100 simulated data sets with different combinations of $p$ and $n$. We considered three scenarios: $p = 35$, $n = 100$, and $p = 75$, $n = 100$. and $p = 35$, $n = 10000$. Specifically, when $p = 35$, and $n = 100$, the total number of parameters in the inverse covariance matrix to be estimated is 630, which is larger than the sample size $n = 100$. When $p = 75$, and $n = 100$, the corresponding number of parameters is 2850, which greatly exceeds $n$. Those settings can be useful to reveal the empirical performance of the different competing methods when the number of parameters is greater than the sample size. The settings with $p = 35$, and $n = 10000$ are used to assess the consistency of different methods in model selection when sample size tends to infinity.

The implementation is based on the GLASSO package in R (Friedman, Hastie and Tibshirani, 2008) and we apply the reiterative weighted LASSO (Fan, Feng and Wu, 2009) to obtain the estimates for SCAD method. For adaptive LASSO, we use the sample covariance as the initial estimate and obtain the
weights based on the sample covariance with the power $\gamma$ set to 0.5.

We examine the empirical performance of the three different penalty functions under the selection of optimal tuning parameter via BIC or cross-validation. Tables 1, 2 and 3 provide the average number of specificity, sensitivity and Matthew’s correlation coefficient over 100 simulated data sets. Standard errors are provided in the parenthesis. For the three cases of different sample and matrix sizes, across all three different graphical structures, the adaptive LASSO consistently yields better performance than the LASSO penalty. SCAD also outperforms the LASSO penalty except for a few cases with the sample size $n = 100$. When sample size increases, the advantages of adaptive LASSO and SCAD are more pronounced. Very interesting to note that when $n = 10000$, the SCAD and adaptive LASSO with BIC can yield sensitivity and specificity close to almost 1. For AR(1), the average specificity and sensitivity for SCAD is 0.981 and 1.000, and for adaptive LASSO are 0.965 and 1.000. For AR(2), the specificity and sensitivity for SCAD are 1.000 and 1.000, and for adaptive LASSO are 0.984, and 1.000. For sparse graph with three edges per node, the specificity and sensitivity for SCAD are 0.999 and 1.000, and for adaptive LASSO are 0.992, and 1.000. These results confirm with the theoretical results that when $n$ tends to infinity, penalized likelihood estimation with SCAD or adaptive LASSO is consistent and selects the true graphical model with probability tending to one. In comparison, the average specificity and sensitivity that the penalized likelihood estimation with LASSO under BIC selection are much lower. For instance, for AR(1) model, the sensitivity is only about 0.721; for AR(2) model, the sensitivity is only about 0.806. These results demonstrate that LASSO with BIC is not consistent in model selection across different underlying graphical structures.

We also compare the performance between BIC and 5-fold cross validation. When sample size $n = 100$, there is no complete dominance of one tuning method over the other. For instance, under the sparse graph with three edges per node, the relative performance of BIC versus cross validation depends on the penalty function. When $p = 35$ and $n = 100$, the overall MCC of BIC is higher than cross validation for penalty of LASSO but lower than cross validation for penalties of SCAD and ADAP. When $n = 10000$, BIC is more advantageous as it consistently yields higher specificity, sensitivity, and MCC than cross validation for all the
penalties and across all the graphical models in the simulation study. Overall, the BIC method exhibits comparable performance as cross validation in the small sample size scenario, but it outperforms cross validation when sample size gets large. Computationally, BIC is more convenient to use as cross validation is $K$ times more intensive to compute.

4. Conclusion

In this article, we investigate the tuning parameter selection for penalized likelihood estimation of the inverse covariance matrix in the Gaussian graphical model. We establish the consistency of the BIC criterion to select the true graphical model with the SCAD or adaptive LASSO penalty. Such consistency result of BIC can be extended to the general penalized likelihood estimation problems with these two penalties in other models satisfying mild regularity conditions.

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Table 4.1: Results for AR(1) Graphical Model. Averages and standard errors from 100 runs

| p   | n   | Tuning | LASSO SPEC | SENS | MCC | SCAD SPEC | SENS | MCC | ADAP SPEC | SENS | MCC |
|-----|-----|--------|------------|------|-----|-----------|------|-----|-----------|------|-----|
| 35  | 100 | BIC    | 0.695      | 1.000 | 0.402 | 0.710     | 1.000 | 0.413 | 0.849     | 1.000 | 0.568 |
|     |     |        | (0.032)    | (0.000) | (0.025) | (0.020)   | (0.000) | (0.017) | (0.021)   | (0.000) | (0.030) |
|     |     | CV     | 0.620      | 1.000 | 0.348 | 0.705     | 1.000 | 0.410 | 0.824     | 1.000 | 0.533 |
|     |     |        | (0.025)    | (0.000) | (0.016) | (0.016)   | (0.000) | (0.013) | (0.016)   | (0.000) | (0.021) |
| 75  | 100 | BIC    | 0.791      | 1.000 | 0.362 | 0.739     | 1.000 | 0.318 | 0.867     | 0.998 | 0.453 |
|     |     |        | (0.018)    | (0.000) | (0.017) | (0.015)   | (0.000) | (0.011) | (0.011)   | (0.005) | (0.016) |
|     |     | CV     | 0.712      | 1.000 | 0.299 | 0.749     | 1.000 | 0.325 | 0.901     | 0.997 | 0.515 |
|     |     |        | (0.017)    | (0.000) | (0.012) | (0.006)   | (0.000) | (0.005) | (0.007)   | (0.005) | (0.015) |
| 35  | 10000 | BIC | 0.721     | 1.000 | 0.424 | 0.981     | 1.000 | 0.902 | 0.965     | 1.000 | 0.839 |
|     |      |        | (0.025)    | (0.000) | (0.022) | (0.006)   | (0.000) | (0.028) | (0.008)   | (0.000) | (0.029) |
|     |      | CV     | 0.521      | 1.000 | 0.290 | 0.976     | 1.000 | 0.880 | 0.917     | 1.000 | 0.697 |
|     |      |        | (0.030)    | (0.000) | (0.016) | (0.007)   | (0.000) | (0.031) | (0.017)   | (0.000) | (0.040) |

SCAD: the SCAD penalty; LASSO: the $L_1$ penalty; ADAP: the adaptive LASSO penalty
| $p$ | $n$ | Tuning | SPEC | SENS | MCC | SPEC | SENS | MCC | SPEC | SENS | MCC |
|-----|-----|--------|------|------|-----|------|------|-----|------|------|-----|
| 35  | 100 | BIC    | 0.986| 0.459| 0.585| 0.982| 0.519| 0.616| 0.954| 0.754| 0.703|
|     |     | CV     | 0.657| 0.960| 0.432| 0.812| 0.905| 0.554| 0.865| 0.910| 0.627|
|     |     |        | (0.013)| (0.113)| (0.055)| (0.016)| (0.114)| (0.050)| (0.029)| (0.135)| (0.051)|
|     |     |        | (0.050)| (0.026)| (0.036)| (0.058)| (0.056)| (0.045)| (0.028)| (0.039)| (0.039)|
| 75  | 100 | BIC    | 0.996| 0.382| 0.563| 0.995| 0.420| 0.579| 0.992| 0.486| 0.610|
|     |     | CV     | 0.837| 0.887| 0.445| 0.895| 0.829| 0.503| 0.998| 0.362| 0.563|
|     |     |        | (0.003)| (0.065)| (0.035)| (0.003)| (0.065)| (0.032)| (0.005)| (0.091)| (0.041)|
|     |     |        | (0.043)| (0.031)| (0.036)| (0.024)| (0.045)| (0.027)| (0.002)| (0.058)| (0.039)|
| 35  | 10000 | BIC   | 0.806| 1.000| 0.606| 1.000| 1.000| 1.000| 0.984| 1.000| 0.954|
|     |     | CV     | 0.470| 1.000| 0.330| 0.997| 1.000| 0.991| 0.931| 1.000| 0.810|
|     |     |        | (0.031)| (0.000)| (0.038)| (0.000)| (0.000)| (0.000)| (0.006)| (0.000)| (0.020)|
|     |     |        | (0.032)| (0.000)| (0.019)| (0.007)| (0.000)| (0.023)| (0.020)| (0.000)| (0.045)|

SCAD: the SCAD penalty; LASSO: the $L_1$ penalty; ADAP: the adaptive LASSO penalty
Table 4.3: Results for a sparse Graphical Model with 3 edges per node. Averages and standard errors from 100 runs

| p   | n   | Tuning | SPEC  | SENS  | MCC   | SPEC  | SENS  | MCC   | SPEC  | SENS  | MCC   |
|-----|-----|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 35  | 100 | BIC    | 0.983 | 0.460 | 0.562 | 0.992 | 0.366 | 0.538 | 0.988 | 0.458 | 0.584 |
|     |     | CV     | 0.988 | 0.363 | 0.546 | 0.998 | 0.354 | 0.558 | 0.995 | 0.423 | 0.591 |
|     |     | CV     | 0.992 | 0.416 | 0.539 | 0.997 | 0.339 | 0.534 | 0.995 | 0.389 | 0.541 |
| 75  | 100 | BIC    | 0.998 | 0.353 | 0.555 | 0.998 | 0.353 | 0.549 | 1.000 | 0.303 | 0.536 |
|     |     | CV     | 0.998 | 0.353 | 0.555 | 0.998 | 0.353 | 0.549 | 1.000 | 0.303 | 0.536 |
| 35  | 10000 | BIC    | 0.932 | 1.000 | 0.769 | 0.999 | 1.000 | 0.996 | 0.992 | 1.000 | 0.966 |
|     |     | CV     | 0.657 | 1.000 | 0.407 | 0.997 | 1.000 | 0.991 | 0.959 | 1.000 | 0.851 |
|     |     | CV     | 0.657 | 1.000 | 0.407 | 0.997 | 1.000 | 0.991 | 0.959 | 1.000 | 0.851 |

SCAD: the SCAD penalty; LASSO: the $L_1$ penalty; ADAP: the adaptive LASSO penalty
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