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On the existence of the weighted bridge penalized Gaussian likelihood precision matrix estimator

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Abstract: We establish a necessary and sufficient condition for the existence of the precision matrix estimator obtained by minimizing the negative Gaussian log-likelihood plus a weighted bridge penalty. This condition enables us to connect the literature on Gaussian graphical models to the literature on penalized Gaussian likelihood.

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1. Introduction

Let \mathbb{R} , \mathbb{R}_+ , \mathbb{R}^p , and $\mathbb{R}^{p \times q}$ denote the sets of real numbers, positive real numbers, real valued p -dimensional vectors, and real valued p by q matrices, respectively. When $A, B \in \mathbb{R}^{p \times q}$, let A' be the transpose of A and let $A \circ B = [a_{ij}b_{ij}] \in \mathbb{R}^{p \times q}$ be the Hadamard product of A and B . When $A \in \mathbb{R}^{p \times p}$, let $\text{tr}(A)$ denote the trace of A , let $|A|$ denote the determinant of A , and define $\mathbb{S}^p = \{A \in \mathbb{R}^{p \times p} : A = A'\}$. When $A \in \mathbb{S}^p$, let $\varphi_j(A)$, $\varphi_{\min}(A)$, and $\varphi_{\max}(A)$ denote the j th largest eigenvalue, minimum eigenvalue, and maximum eigenvalue of A , respectively. Define $\mathbb{S}_0^p = \{A \in \mathbb{S}^p : \varphi_{\min}(A) \geq 0\}$ and $\mathbb{S}_+^p = \{A \in \mathbb{S}^p : \varphi_{\min}(A) > 0\}$.

Since the sample covariance matrix S is singular with probability one when the number of variables p is greater than the sample size n , regularization is required to estimate an inverse covariance matrix. There are many types of regularization that could be applied, e.g. a Moore–Penrose generalized inverse of S or the inverse of a linear combination of S and the identity matrix (Ledoit and Wolf, 2003). Pourahmadi (2011) reviews several approaches.

We study regularized inverse covariance estimators obtained by weighted bridge penalized Gaussian likelihood. The inverse covariance matrix estimator is

$$\hat{\Omega}_{\lambda,q}(M) = \arg \min_{\Omega \in \mathbb{S}_+^p} \left\{ \text{tr}(\Omega S) - \log |\Omega| + \frac{\lambda}{q} \sum_{i,j} m_{ij} |\omega_{ij}|^q \right\}, \quad (1)$$

where $M \in \mathbb{S}^p$ is a known weight matrix with non-negative entries, λ is a non-negative tuning parameter, and $q \in [1, 2]$ is the bridge parameter. The weight matrix M allows the user to incorporate prior information in the penalty, e.g. if it were known that the (i, j) th entry of the population inverse covariance matrix were non-zero or large, then one could set $m_{ij} = 0$. Without prior information on the location of small entries, one could set $M = M_{\text{all}}$ or $M = M_{\text{off}}$, where M_{all} is the weight matrix of ones and M_{off} is the weight matrix with ones on its off-diagonal and zeros on its diagonal.

The inverse covariance estimator obtained through (1) with $q = 1$ has been studied extensively. Yuan and Lin (2007) proposed and analyzed $\hat{\Omega}_{\lambda,1}(M_{\text{off}})$ and Rothman et al. (2008), Lam and Fan (2009), and Ravikumar et al. (2011) established theoretical properties when $p > n$. Banerjee, El Ghaoui and d'Aspremont (2008) proposed and studied the optimization to compute $\hat{\Omega}_{\lambda,1}(M_{\text{all}})$. The general weighted penalty in (1) with $q = 1$ was considered by Friedman, Hastie and Tibshirani (2008), Lu (2010), and Hsieh et al. (2012). The solution to (1) with $q = 1$, when it exists, could be computed with the graphical lasso algorithm (Yuan, 2008; Friedman, Hastie and Tibshirani, 2008) or the QUIC algorithm (Hsieh et al., 2011). Speed improvements to compute $\hat{\Omega}_{\lambda,1}(M_{\text{all}})$ for large values of λ were proposed by Witten, Friedman and Simon (2011) and Mazumder and Hastie (2012). A benefit of using $q = 1$ is that for λ sufficiently large, a subset of the off-diagonal entries in $\hat{\Omega}_{\lambda,1}(M)$ are zero and when S is computed from n independent copies of a p -variate Normal random vector, the locations of non-zero entries in $\hat{\Omega}_{\lambda,1}(M)$ could be used to estimate the edges in a Gaussian graphical model (Yuan and Lin, 2007).

The use of the bridge penalty in (1) was proposed by Rothman et al. (2008) in the special case when $M = M_{\text{off}}$. They proposed an algorithm to compute $\hat{\Omega}_{\lambda,q}(M_{\text{off}})$ for $q \in [1, 2]$, but they only explored its use when $q = 1$. Witten and Tibshirani (2009) derived a closed-form solution to compute $\hat{\Omega}_{\lambda,2}(M_{\text{all}})$.

The inverse covariance estimator $\hat{\Omega}_{\lambda,q}(M)$ could be used within methods for supervised learning, e.g. discriminant analysis (Rothman et al., 2008), covariance regularized regression (Witten and Tibshirani, 2009), and multivariate regression with covariance estimation (Rothman, Levina and Zhu, 2010b). When the population inverse covariance matrix is sparse or approximately sparse, there are theoretical advantages to set $q = 1$, but in general settings $q \in (1, 2]$ may be useful.

There has been some study of sufficient conditions for the solution to (1) to exist: Banerjee, El Ghaoui and d'Aspremont (2008) showed that the solution to (1) exists with probability one if $q = 1$, $M = M_{\text{all}}$, and $\lambda > 0$; Ravikumar et al. (2011) showed that the solution to (1) exists if $q = 1$, $M = M_{\text{off}}$, $\lambda > 0$,

and $S \circ I \in \mathbb{S}_+^p$; and Lu (2010) showed that the solution to (1) exists if $q = 1$ and $S + \lambda M \circ I \in \mathbb{S}_+^p$. Necessary and sufficient conditions for there to exist a solution to (1) are still unknown, and we establish these in this article.

2. Properties of the optimization

2.1. Solution existence

The optimization in (1) is strictly convex. When an optimal solution exists, this solution is the unique global minimizer. Let $\mathcal{U} = \{(i, j) : m_{ij} = 0\}$ be the set of unpenalized indices.

Theorem 1. *Suppose that $\lambda \in \mathbb{R}_+$ and $q \in (1, 2]$. An optimal solution to (1) exists if and only if the set $\mathcal{A}(M) = \{\Sigma \in \mathbb{S}_+^p : \sigma_{ij} = s_{ij} \text{ when } (i, j) \in \mathcal{U}\}$ is not empty.*

Theorem 2. *Suppose that $q = 1$. An optimal solution to (1) exists if and only if the set $\mathcal{A}_1(\lambda, M) = \{\Sigma \in \mathbb{S}_+^p : |\sigma_{ij} - s_{ij}| \leq \lambda m_{ij} \text{ for all } i, j\}$ is not empty.*

We prove Theorems 1 and 2 in Appendix A. Hsieh et al. (2012) stated a dual problem to (1) with $q = 1$ for which $\mathcal{A}_1(\lambda, M)$ is the feasible set; however, we do not use this duality to prove Theorem 2. Our proof technique is also used to prove Theorem 1.

When the diagonal entries are unpenalized, i.e. $\max_j m_{jj} = 0$, the condition that $\mathcal{A}(M)$ is not empty is necessary and sufficient for the maximum likelihood estimator of the inverse covariance matrix to exist in the Gaussian graphical model with edge set \mathcal{U} ; see, for example, Theorem 2.1 of Uhler (2012). As a consequence, we have the following example.

Example 1. Suppose that S is computed from an iid sample of size n from a p -variate normal distribution with positive definite covariance matrix and $m_{ij} = 1(|i - j| > k)$, where $k \in \{0, \dots, p - 1\}$. Then the set of unpenalized indices \mathcal{U} is the edge set of a Chordal graph with maximum clique size $k + 1$. From Corollary 2.3 of Uhler (2012), the MLE of the Gaussian graphical model with edge set \mathcal{U} exists with probability one if and only if $k < n - 1$. This result is also in Buhl (1993) and the MLE in this case can be computed by inverse Cholesky banding (Rothman, Levina and Zhu, 2010a). Thus, by Theorem 1, the solution to (1) with $q \in (1, 2]$ exists with probability one if and only if $k < n - 1$.

Define the weighted soft-thresholded sample covariance matrix by $\text{soft}(S, \lambda M) = [\text{sign}(s_{ij})(|s_{ij}| - \lambda m_{ij})_+]$, where $(y)_+ = y1(y > 0)$.

Corollary 1. *An optimal solution to (1) exists if at least one of the following conditions is true: (i) $\lambda \in \mathbb{R}_+$ and $\min_j m_{jj} > 0$; (ii) $S \circ I \in \mathbb{S}_+^p$, $\lambda \in \mathbb{R}_+$, and $\min_{i \neq j} m_{ij} > 0$; (iii) $S \in \mathbb{S}_+^p$; (iv) $\text{soft}(S, \lambda M) \in \mathbb{S}_+^p$.*

We prove Corollary 1 in Appendix A. In particular, if all diagonal entries are penalized in (1), then a solution exists for any choice of the off-diagonal of M . Also, if all off-diagonal entries are penalized and the diagonal entries of

S are positive, then a solution exists for any choice of the diagonal of M , e.g. the diagonal of zeros. One could check if $\text{soft}(S, \lambda M)$ is positive definite, which guarantees an optimal solution to (1) exists, but we have encountered several examples where the realization of $\text{soft}(S, \lambda M)$ was indefinite and an optimal solution to (1) with $q = 1$ existed.

Since $\mathcal{A}_1(\lambda, M) \subset \mathcal{A}(M)$ for all $\lambda \geq 0$, we see that if $\hat{\Omega}_{\lambda,1}(M)$ exists for some $\lambda \in \mathbb{R}_+$, then $\hat{\Omega}_{\hat{\lambda},q}(M)$ exists for all $(\hat{\lambda}, q) \in \mathbb{R}_+ \times (1, 2]$. Also, if there exists a $\bar{\Sigma} \in \mathcal{A}(M)$, then there exists a $\bar{\lambda} \in \mathbb{R}_+$ sufficiently large such that $\bar{\Sigma} \in \mathcal{A}_1(\bar{\lambda}, M)$. From this and the definition of $\mathcal{A}(M)$ we have that if $\hat{\Omega}_{\lambda,q}(M)$ exists for some $(\lambda, q) \in \mathbb{R}_+ \times (1, 2]$, then $\hat{\Omega}_{\tilde{\lambda},\tilde{q}}(M)$ exists for all $(\tilde{\lambda}, \tilde{q}) \in \mathbb{R}_+ \times (1, 2]$ and there exists a $\bar{\lambda} \in \mathbb{R}_+$ sufficiently large such that $\hat{\Omega}_{\bar{\lambda},1}(M)$ exists.

2.2. The effect of unpenalized entries

From first-order conditions and convexity, a feasible point $\hat{\Omega} \in \mathbb{S}_+^p$ is optimal for (1) if and only if it solves the zero gradient equation when $q \in (1, 2]$ or the zero subgradient equation when $q = 1$. In both cases, this equation can be written as

$$0 = S - \hat{\Omega}^{-1} + \lambda M \circ G, \quad (2)$$

where the (i, j) th entry of G is a function evaluated at the (i, j) th entry of $\hat{\Omega}$, e.g. Meinshausen (2008) gave an expression for (2) when $q = 1$ and $M = M_{\text{off}}$. We see that if $\hat{\Omega}$ is optimal for (1) then $(\hat{\Omega}^{-1})_{ij} = s_{ij}$ when $(i, j) \in \mathcal{U}$.

3. Discussion

In an earlier submission of this work, we proposed an accelerated majorize minimize algorithm to solve (1) with $q = 2$ and any weight matrix M . This special case can be used to iteratively solve (1) with $q \in [1, 2)$ (Rothman et al., 2008). In our numerical experiments, our algorithm was competitive for all values of the tuning parameter when $M = M_{\text{off}}$, but it was uncompetitive for mid-range values of the tuning parameter when $m_{ij} = 1(|i - j| > k)$ with $k \geq 1$. We are currently addressing this problem.

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Appendix A: Proofs

For $c, d \in \mathbb{R}_+$, define the set $\mathcal{G}_{c,d} = \{\Omega \in \mathbb{S}_+^p : c \leq \varphi_{\min}(\Omega) \leq \varphi_{\max}(\Omega) \leq d\}$.

To prove Theorems 1 and 2 we will use the following Lemma, which is a modification of an argument made by Bien and Tibshirani (2011).

Lemma 1. *Suppose that a function $v : \mathbb{S}_+^p \rightarrow \mathbb{R}$ satisfies $v(\Omega) \geq a + b \operatorname{tr}(\Omega) - \log |\Omega|$ for all $\Omega \in \mathbb{S}_+^p$, where $a \in \mathbb{R}$ and $b \in \mathbb{R}_+$. If $\Omega_0 \in \mathbb{S}_+^p$, then there exist $c, d \in \mathbb{R}_+$ such that $\{\Omega \in \mathbb{S}_+^p : v(\Omega) \leq v(\Omega_0)\} \subset \mathcal{G}_{c,d}$.*

Proof of Lemma 1. Our proof modifies an argument of Bien and Tibshirani (2011). We have that

$$v(\Omega) \geq a + \sum_{j=1}^p \{b\varphi_j(\Omega) - \log \varphi_j(\Omega)\}. \tag{3}$$

Define $r(\cdot; b) : \mathbb{R}_+ \rightarrow \mathbb{R}$ by $r(x; b) = xb - \log x$. Then $\nabla_x r(x; b) = b - 1/x$, so $\hat{x} = 1/b$ minimizes $r(\cdot; b)$ and $r(x; b) \geq r(\hat{x}; b) = 1 + \log b$. From (3),

$$\begin{aligned} v(\Omega) &\geq a + \sum_{j=1}^p r\{\varphi_j(\Omega); b\} \\ &= a + r\{\varphi_j(\Omega); b\} + \sum_{k=1, k \neq j}^p r\{\varphi_k(\Omega); b\} \\ &\geq a + r\{\varphi_j(\Omega); b\} + (p - 1)(1 + \log b), \end{aligned}$$

for $j \in \{1, \dots, p\}$. Given any $\Omega_0 \in \mathbb{S}_+^p$ define $\mathcal{R}(\Omega_0) = \{\Omega \in \mathbb{S}_+^p : v(\Omega) \leq v(\Omega_0)\}$. For all $\bar{\Omega} \in \mathcal{R}(\Omega_0)$, $v(\Omega_0) \geq v(\bar{\Omega}) \geq a + r\{\varphi_j(\bar{\Omega}); b\} + (p - 1)(1 + \log b)$ and so for all $\bar{\Omega} \in \mathcal{R}(\Omega_0)$,

$$\varphi_j(\bar{\Omega}) \in \{\phi \in \mathbb{R}_+ : r(\phi; b) \leq \delta_0\}, \quad j = 1, \dots, p,$$

where $\delta_0 = v(\Omega_0) - (p - 1)(1 + \log b) - a$. Since $r(\cdot; b)$ is decreasing on $(0, \hat{x})$, increasing on (\hat{x}, ∞) , $\lim_{x \rightarrow 0^+} r(x; b) = \infty$, and $\lim_{x \rightarrow \infty} r(x; b) = \infty$, there exist $c, d \in \mathbb{R}_+$ such that $c \leq \varphi_{\min}(\bar{\Omega}) \leq \varphi_{\max}(\bar{\Omega}) \leq d$ for all $\bar{\Omega} \in \mathcal{R}(\Omega_0)$. \square

Proof of Theorem 1. Let f be the objective function in (1). Suppose that $\mathcal{A}(M)$ is not empty and that $\bar{\Sigma} \in \mathcal{A}(M)$. Then

$$\begin{aligned} f(\Omega) + \log |\Omega| &= \operatorname{tr}\{\Omega \bar{\Sigma}\} + \operatorname{tr}\{\Omega(S - \bar{\Sigma})\} + \frac{\lambda}{q} \sum_{i,j} m_{ij} |\omega_{ij}|^q \\ &= a_1 + a_2 + a_3. \end{aligned}$$

We have that $a_1 \geq \varphi_{\min}(\bar{\Sigma}) \sum_{j=1}^p \varphi_j(\Omega)$. Also,

$$a_2 + a_3 = \sum_{i,j} \{\omega_{ij}(s_{ij} - \bar{\sigma}_{ij}) + \lambda m_{ij} |\omega_{ij}|^q / q\}.$$

If $m_{ij} = 0$ then $s_{ij} = \bar{\sigma}_{ij}$ so the (i, j) th entry in this sum is zero. The non-zero entries in this sum are also bounded from below because $\lambda m_{ij} |\omega_{ij}|^q / q > |\omega_{ij}(s_{ij} - \bar{\sigma}_{ij})|$ if $|\omega_{ij}|$ is sufficiently large. Thus there exists an $a \in \mathbb{R}$ for which $a_2 + a_3 \geq a$. We have shown that $f(\Omega) \geq a + b \operatorname{tr}(\Omega) - \log |\Omega|$, where $b = \varphi_{\min}(\bar{\Sigma}) \in \mathbb{R}_+$. So for any $\Omega_0 \in \mathbb{S}_+^p$, Lemma 1 implies that there exists $c, d \in \mathbb{R}_+$ such that $\{\Omega \in \mathbb{S}_+^p : f(\Omega) \leq f(\Omega_0)\} \subset \mathcal{G}_{c,d}$. Given $\Omega_0 \in \mathbb{S}_+^p$, we can shrink the

feasible set in (1) to the compact subset $\mathcal{G}_{c,d}$ and since f is convex, a global minimizer exists in $\mathcal{G}_{c,d}$.

Now suppose that a global minimizer $\hat{\Sigma}^{-1} \in \mathbb{S}_+^p$ of (1) exists. Then $\hat{\Sigma} \in \mathbb{S}_+^p$ and since $\nabla f(\hat{\Sigma}^{-1}) = 0$, we have that $S - \hat{\Sigma} + \lambda M \circ G = 0$, where the (i, j) th entry of G is determined by the (i, j) th entry of $\hat{\Sigma}^{-1}$, so $s_{ij} = \hat{\sigma}_{ij}$ when $(i, j) \in \mathcal{U}$. Thus $\hat{\Sigma} \in \mathcal{A}(M)$, so $\mathcal{A}(M)$ is not empty. \square

Proof of Theorem 2. Let u be the objective function in (1) with $q = 1$. Suppose that $\mathcal{A}_1(\lambda, M)$ is not empty and take $\bar{\Sigma} \in \mathcal{A}_1(\lambda, M)$. Then

$$\begin{aligned} u(\Omega) + \log |\Omega| &= \text{tr}\{\Omega \bar{\Sigma}\} + \text{tr}\{\Omega(S - \bar{\Sigma})\} + \lambda \sum_{i,j} m_{ij} |\omega_{ij}| \\ &= a_1 + a_2 + a_3. \end{aligned}$$

We have that $a_1 \geq \varphi_{\min}(\bar{\Sigma}) \sum_{j=1}^p \varphi_j(\Omega)$. Also,

$$a_2 + a_3 = \sum_{i,j} \{\omega_{ij}(s_{ij} - \bar{\sigma}_{ij}) + \lambda m_{ij} |\omega_{ij}|\}.$$

Since $\bar{\Sigma} \in \mathcal{A}_1(\lambda, M)$, $|s_{ij} - \bar{\sigma}_{ij}| \leq \lambda m_{ij}$ for all i, j , so $a_2 + a_3 \geq 0$. Therefore, $u(\Omega) \geq a + b \text{tr}(\Omega) - \log |\Omega|$ for all $\Omega \in \mathbb{S}_+^p$, where $a = 0$ and $b = \varphi_{\min}(\bar{\Sigma})$. Thus, for any $\Omega_0 \in \mathbb{S}_+^p$, Lemma 1 implies that there exists $c, d \in \mathbb{R}_+$ such that $\{\Omega \in \mathbb{S}_+^p : u(\Omega) \leq u(\Omega_0)\} \subset \mathcal{G}_{c,d}$. Given $\Omega_0 \in \mathbb{S}_+^p$, we can shrink the feasible set in (1) to the compact subset $\mathcal{G}_{c,d}$ and since u is convex, a global minimizer exists in $\mathcal{G}_{c,d}$.

Now suppose that a global minimizer $\hat{\Sigma}^{-1} \in \mathbb{S}_+^p$ of (1) exists. From the discussion in Section 2.2, $S - \hat{\Sigma} + \lambda M \circ G = 0$, where, in this case, G has entries in $[-1, 1]$. So $\hat{\Sigma} - S = \lambda M \circ G$, which implies that $|\hat{\sigma}_{ij} - s_{ij}| = \lambda m_{ij} |g_{ij}| \leq \lambda m_{ij}$ for all i, j . Thus $\hat{\Sigma} \in \mathcal{A}_1(\lambda, M)$. \square

Proof of Corollary 1. Since $\mathcal{A}_1(\lambda, M) \subset \mathcal{A}(M)$ for all $\lambda \geq 0$, by Theorems 1 and 2, we only need to show that each of the four conditions imply that $\mathcal{A}_1(\lambda, M)$ is not empty.

For (i), take $\bar{\Sigma}_1 = S + \lambda \min_j m_{jj} I$. Then $\bar{\Sigma}_1 \in \mathcal{A}_1(\lambda, M)$. For (ii), pick an $\alpha \in \mathbb{R}_+$ sufficiently close to zero and let $\bar{\Sigma}_2 = (1 - \alpha)S + \alpha S \circ I$. Then $\bar{\Sigma}_2 \in \mathbb{S}_+^p$, $\bar{\sigma}_{2,jj} = s_{jj}$, and when $i \neq j$, $|\bar{\sigma}_{2,ij} - s_{ij}| = \alpha |s_{ij}| \leq \lambda m_{ij}$ provided that α is sufficiently close to zero. So $\bar{\Sigma}_2 \in \mathcal{A}_1(\lambda, M)$. For (iii), $S \in \mathcal{A}_1(\lambda, M)$. For (iv) take $\bar{\Sigma}_4 = \text{soft}(S, \lambda M)$. From Rothman, Levina and Zhu (2009), $|\bar{\sigma}_{4,ij} - s_{ij}| \leq \lambda m_{ij}$ so $\bar{\Sigma}_4 \in \mathcal{A}_1(\lambda, M)$. \square

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