Properties of optimizations used in penalized Gaussian likelihood inverse covariance matrix estimation

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Estimating large covariance matrices and their inverses

- The covariance matrix is a fundamental quantity in multivariate analysis.
- In general, the sample covariance matrix $S$ performs poorly in high dimensions ($p \geq n$).
- Shrinkage or regularized estimators are used instead.
Desirable properties of the estimator

- low computational cost
- works well in applications, e.g. classification
- exploits variable ordering when appropriate

Two different problems:

A. Estimating $\Sigma$
B. Estimating $\Sigma^{-1}$
Estimating the covariance matrix $\Sigma$

General purpose methods

- Shrinking the eigenvalues of $S$ (Haff, 1980; Dey and Srinivasan, 1985; Ledoit and Wolf, 2003).
- Element-wise thresholding of $S$ (Bickel and Levina, 2008; El Karoui, 2008; Rothman, Levina, and Zhu, 2009; Cai & Zhou 2010; Cai & Liu, 2011).
- lasso-penalized Gaussian likelihood (Lam & Fan, 2009; Bien & Tibshirani, 2011).
- Other sparse and positive definite methods (Rothman, 2012; Xue, Ma, & Zou, 2012; Liu, Wang, & Zhao, 2013).
- $\Sigma$ with reduced effective rank (Bunea & Xiao, 2012).
- Approximate factor model with sparse error covariance (Fan, Liao & Minchev, 2013).
Estimating the inverse covariance matrix $\Sigma^{-1}$

General purpose methods
- Eigenvalue shrinkage (Ledoit and Wolf, 2003).
- Bayesian methods (Wong et al., 2003; Dobra et al, 2004).
- Penalized likelihood References given soon.
Exploiting variable ordering

when estimating the covariance matrix $\Sigma$

- Banding or tapering $S$ (Furrer & Bengtsson, 2007; Bickel & Levina, 2008; Cai, Zhang, and Zhou, 2010).
- Block thresholding (Cai & Yuan, 2012).
- Regularized estimation of the modified Cholesky factor of the covariance matrix (Rothman, Levina, & Zhu, 2010).

when estimating the inverse covariance matrix $\Sigma^{-1}$

- Regularized estimation of the modified Cholesky factor of the inverse covariance (Wu & Pourahmadi, 2003; Smith & Kohn, 2002; Bickel & Levina, 2008; Huang et al., 2006; Levina, Rothman, & Zhu, 2008).
Estimating $\Sigma^{-1}$ in applications

- Classification (Bickel & Levina, 2004)
- Regression (Witten & Tibshirani, 2009; Cook, Forzani, & Rothman, 2013)
- Multiple output regression (Rothman, Levina, & Zhu, 2010)
- Sufficient dimension reduction (Cook, Forzani, & Rothman, 2012)
Estimating $\Sigma^{-1}$ and Gaussian graphical models

- $(X_1, \ldots, X_p)' \sim N_p(0, \Sigma), \quad \Sigma \in \mathbb{S}^p_+.$
- The undirected graph $G = (V, E)$ has
  - vertex set $V = \{1, \ldots, p\}$ and
  - edge set $E = \{(i, j) : (\Sigma^{-1})_{ij} \neq 0\}.$

- Selection (Drton & Perlman, 2004; Kalisch & Bühlmann, 2007; Meinshausen and Bühlmann 2006).


- Estimation when $E$ is known Dempster, 1972; Buhl, 1993; Drton et al., 2009; Uhler, 2012).
Part I: On solution existence in penalized Gaussian likelihood estimation of $\Sigma^{-1}$
Unpenalized Gaussian likelihood estimation of $\Sigma^{-1}$

$S$ is from an iid sample of size $n$ from $N_p(\mu, \Sigma)$, where $\Sigma \in S^p_+$. The optimization for the MLE of $\Sigma^{-1}$ is

$$\hat{\Omega} = \arg \min_{\Omega \in S^p_+} \{ \text{tr}(\Omega S) - \log |\Omega| \}$$

Set the gradient at $\hat{\Omega}$ to zero:

$$S - \hat{\Omega}^{-1} = 0$$

- The solution, when it exists, is $\hat{\Omega} = S^{-1}$.
- $\hat{\Omega}$ exists (with probability one) if and only if $n > p$ (Dykstra, 1970).
Illustration – No solution when $n \leq p$

If $n = p = 1$, then $f(\omega) = 0 \omega - \log \omega$. 
Penalized Gaussian likelihood estimation of $\Sigma^{-1}$

We will study

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

- $q = 1$ is the lasso penalty, $q = 2$ is the ridge penalty
- $M$ is user-specified, symmetric with non-negative entries.
- The $m_{ij}$'s allow the user to incorporate prior information, e.g. it is known that $(\Sigma^{-1})_{21} = (\Sigma^{-1})_{12} \neq 0$ so set $m_{21} = m_{12} = 0$.
- Other examples $M_{\text{all}}, M_{\text{off}},$ and $m_{ij} = 1(|i - j| > k)$.
- We study when solutions exist and develop a new algorithm for the ridge penalty ($q = 2$).
Lasso penalized likelihood estimation of $\Sigma^{-1}$

The case when $q = 1$ is

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

- $\hat{\Omega}_{\lambda,1}(M_{\text{off}})$ Yuan & Lin (2007), Rothman et al. (2008), Lam & Fan (2009), and Ravikumar et al. (2008).
- $\hat{\Omega}_{\lambda,1}(M_{\text{all}})$ Banerjee et al. (2008), Friedman et al. (2008).
- Algorithms to compute $\hat{\Omega}_{\lambda,1}(M)$ for some $M$ Yuan (2008)/Friedman et al. (2008), Lu (2008), and Hsieh, Dhillon, Ravikumar, & A. Banerjee (2012).
Banerjee et al. (2008) showed that $\hat{\Omega}_{\lambda,1}(M_{all})$ exists if $\lambda > 0$.

Ravikumar et al. (2008) showed that $\hat{\Omega}_{\lambda,1}(M_{off})$ exists if $\lambda > 0$ and $S \circ I \in S_+^p$.

Lu (2008) showed that $\hat{\Omega}_{\lambda,1}(M)$ exists if $S + \lambda M \circ I \in S_+^p$. 


Theorem. The solution $\hat{\Omega}_{\lambda,1}(M)$ exists if and only if $A_{1,\lambda}(M) = \{\Sigma \in S^p_+ : |\sigma_{ij} - s_{ij}| \leq m_{ij}\lambda\}$ is not empty.

$A_{1,\lambda}(M)$ is the feasible set in the dual problem (Hsieh, Dhillon, Ravikumar, & A. Banerjee, 2012), but our proof technique is more general.

Corollary. $\hat{\Omega}_{\lambda,1}(M)$ exists if at least one of the following holds:

1. $\lambda > 0$ and $\min_j m_{jj} > 0$;
2. $\lambda > 0$, $S \circ I \in S^p_+$ and $\min_{i \neq j} m_{ij} > 0$;
3. $S \in S^p_+$;
4. $\text{soft}(S, \lambda M) \in S^p_+$. 

Lasso-penalized likelihood solution existence
Entry agreement between $\hat{\Omega}_{\lambda,1}(M)^{-1}$ and $S$

Define $\mathcal{U} = \{(i, j) : m_{ij} = 0\}$.

**Remark.** When $\hat{\Omega}_{\lambda,1}(M)$ exists,

$$\{\hat{\Omega}_{\lambda,1}(M)^{-1}\}_{ij} = s_{ij} \quad \text{for } (i, j) \in \mathcal{U}.$$

**Justification.** The zero subgradient equation is

$$S - \hat{\Omega}^{-1} + \lambda M \circ G = 0.$$
Ridge penalized likelihood estimation of $\Sigma^{-1}$

$$\hat{\Omega}_{\lambda,2}(M) = \arg \min_{\Omega \in S^p_+} \left\{ \operatorname{tr}(\Omega S) - \log |\Omega| + 0.5\lambda \sum_{i,j} m_{ij} \omega_{ij}^2 \right\}$$

- Why use the ridge penalty?
- Rothman et al. (2008) developed an algorithm to compute $\hat{\Omega}_{\lambda,2}(M_{\text{off}})$.
- Witten and Tibshirani (2009) developed a closed-form solution to compute $\hat{\Omega}_{\lambda,2}(M_{\text{all}})$.
Ridge-penalized likelihood solution existence

\[
\hat{\Omega}_{\lambda,2}(M) = \arg\min_{\Omega \in \mathbb{S}^p_+} \left\{ \text{tr}(\Omega S) - \log |\Omega| + 0.5 \lambda \sum_{i,j} m_{ij} \omega_{ij}^2 \right\}
\]

Recall that \( \mathcal{U} = \{(i, j) : m_{ij} = 0\} \).

**Theorem.** Suppose \( \lambda > 0 \). The solution \( \hat{\Omega}_{\lambda,2}(M) \) exists if and only if \( A_2(M) = \{\Sigma \in \mathbb{S}_+^p : \sigma_{ij} = s_{ij} \text{ when } (i, j) \in \mathcal{U}\} \) is not empty.

**Remark.** The MLE of the Gaussian graphical model with edge set \( \mathcal{U} \) exits if and only if \( A_2(M) \) is not empty (Buhl, 1993; Uhler, 2012)
Chordal graph example

From the theorem $\hat{\Omega}_{\lambda, 2}(M)$ exists if and only if the MLE of the Gaussian graphical model with edge set $U = \{(i, j) : m_{ij} = 0\}$ exists.

**Example.** $m_{ij} = 1(|i - j| > k)$. Then $U$ is an edge-set for a Chordal graph with maximum clique size $k + 1$. So $\hat{\Omega}_{\lambda, 2}(M)$ exists if and only if $n \geq k + 2$.

This follows from

**Theorem**[Buhl, 1993; Uhler, 2012]. Suppose that $U$ is the edge set for a Chordal graph with maximum clique size $q$. The MLE of the zero mean Gaussian graphical model with edge set $U$ exists if and only if $n \geq q$. 
Entry agreement between $\hat{\Omega}_{\lambda,2}(M)^{-1}$ and $S$

Recall $\mathcal{U} = \{(i, j) : m_{ij} = 0\}$.

**Remark.** When $\hat{\Omega}_{\lambda,2}(M)$ exists,

$$\{\hat{\Omega}_{\lambda,2}(M)^{-1}\}_{ij} = s_{ij} \quad \text{for (i, j) } \in \mathcal{U}.$$ 

**Justification.** The zero gradient equation is

$$S - \tilde{\Omega}^{-1} + \lambda M \circ \tilde{\Omega} = 0.$$
Ridge and lasso connections

Recall that $\mathcal{U} = \{(i,j) : m_{ij} = 0\}$

$$A_{1,\lambda}(M) = \{\Sigma \in \mathbb{S}^p_+ : |\sigma_{ij} - s_{ij}| \leq m_{ij}\lambda\}$$

$$A_2(M) = \{\Sigma \in \mathbb{S}^p_+ : \sigma_{ij} = s_{ij} \text{ when } (i,j) \in \mathcal{U}\}$$

- $A_{1,\lambda}(M) \subset A_2(M)$.
- If $\hat{\Omega}_{\lambda,1}(M)$ exists, then $\hat{\Omega}_{\tilde{\lambda},2}(M)$ exists for all $\tilde{\lambda} > 0$.
- If $\hat{\Omega}_{\lambda,2}(M)$ exists for some $\lambda > 0$, then it exists for all $\lambda > 0$, and there exists a $\tilde{\lambda}$ sufficiently large so that $\hat{\Omega}_{\tilde{\lambda},1}(M)$ exists.
Part II: new algorithm for the ridge penalty
The SPICE algorithm to compute the Ridge solution

Rothman, Bickel, Levina, & Zhu (2008)’s iterative algorithm to minimize

$$\text{tr}(\Omega S) - \log |\Omega| + \frac{\lambda}{q} \sum_{i \neq j} |\omega_{ij}|^q$$

- Each iteration minimizes

$$\text{tr}(\Omega S) - \log |\Omega| + \frac{\lambda}{2} \sum_{i \neq j} m_{ij} \omega_{ij}^2.$$ 

- Re-parameterize using Cholesky factorization: $\Omega = T'T$.
- Minimize with cyclical coordinate descent.
- Computational complexity $O(p^3)$. 
Accelerated MM algorithm to compute the Ridge solution (our proposal)

Minimizes the objective function $f$,

$$f(\Omega) = \text{tr}(\Omega S) - \log |\Omega| + 0.5\lambda \sum_{i,j} m_{i,j} \omega_{i,j}^2.$$  

- At the $k$th iteration, the next iterate $\Omega_{k+1}$ is the minimizer of a majorizing function to $f$ at $\Omega_k$.
- Every few iterations a minorizing function to $f$ at $\Omega_k$ is minimized. This minimizer is accepted if it improves objective function value.
- Computational complexity $O(p^3)$.  

Majorizing $f$ at $\Omega_k$ part 1

Decompose the penalty:

$$\sum_{i,j} m_{ij} \omega_{ij}^2 = \max_{i,j} m_{ij} \sum_{i,j} \omega_{ij}^2 - \sum_{i,j} (\max_{i,j} m_{ij} - m_{ij}) \omega_{ij}^2.$$ 

Replace the second term with a linear approximation at our current iterate $\Omega_k$ to get the majorizer.
Majorizing $f$ at $\Omega_k$ part 2

- The minimizer of the majorizer to $f$ at $\Omega_k$ is

$$\Omega_{k+1} = \arg \min_{\Omega \in S^p_+} \left\{ \text{tr}(\Omega\tilde{S}) - \log |\Omega| + 0.5\tilde{\lambda} \sum_{i,j} \omega_{ij}^2 \right\},$$

where $\tilde{S} = S - \lambda \Omega_k \circ [\max_{i,j} m_{ij} - m_{ij}]$ and $\tilde{\lambda} = \lambda \max_{i,j} m_{ij}$.

- Closed-form solution derived by Witten and Tibshirani (2009).
Acceleration by minorizing $f$ at $\Omega_k$

- Get the minorizer by replacing the entire penalty $\sum_{i,j} m_{ij} \omega_{ij}^2$ with a linear approximation at our current iterate $\Omega_k$.
- The minimizer of the minorizer (when it exists) is
  \[
  \tilde{\Omega}_{k+1} = (S + \lambda \Omega_k \circ M)^{-1}
  \]
- Accept $\tilde{\Omega}_{k+1}$ if $f(\tilde{\Omega}_{k+1}) < f(\Omega_k)$. 

Illustration
Algorithm convergence

**Theorem.** Suppose that acceleration attempts are stopped after a finite number of iterations and the algorithm is initialized at $\Omega_0 \in S^p_+$. If the global minimizer $\hat{\Omega}_{\lambda,2}(M)$ exits, then

$$\lim_{k \to \infty} \| \Omega_k - \hat{\Omega}_{\lambda,2}(M) \| = 0.$$ 

Also, if the algorithm converges, then it converges to the global minimizer.
Simulation: our algorithm vs the SPICE algorithm

In each replication,

1. randomly generated $\Sigma_0$:
   - eigenvectors were the right singular vectors of $Z \in \mathbb{R}^{p \times p}$, where the $z_{ij}$ were drawn independently from $N(0, 1)$;
   - eigenvalues drawn independently from the uniform distribution on $(1, 100)$.

2. generated $S$ from an iid sample of size $n = 50$ from $N_p(0, \Sigma_0)$

Compared our MM algorithm to SPICE when computing $\hat{\Omega}_{\lambda,2}(M_{\text{off}})$. 
Results for $n = 50 \& p = 100$

$\hat{\Omega}_{\lambda,2}(M_{\text{off}})$
Results for $n = 50 \& p = 200$

$\hat{\Omega}_{\lambda,2}(M_{\text{off}})$
Tuning parameter selection

*J*-fold cross validation maximizing validation likelihood

- Randomly partition the *n* observations into *J* subsets of equal size.
- Compute

\[
\hat{\lambda} = \arg \min_{\lambda \in \mathcal{L}} \sum_{j=1}^{J} \left\{ \text{tr} \left( \hat{\Omega}_\lambda^{(-j)} S^{(j)} \right) - \log \left| \hat{\Omega}_\lambda^{(-j)} \right| \right\},
\]

- *S*(*)j*) is computed from observations inside the *j*th subset (centered by training sample means)
- \( \hat{\Omega}_\lambda^{(-j)} \) is the inverse covariance estimate computed from the observations outside the *j*th subset
- \( \mathcal{L} \) is some user defined finite subset of \( \mathbb{R}_+ \), e.g. \{10^{-8}, 10^{-7.5}, \ldots, 10^8\}.
Classification example

Task: discriminate between metal and rocks using sonar data.
- The data were taken from the UCI machine learning data repository.
- Sonar was used to produce energy measurements at $p = 60$ frequency bands for rock and metal cylinder examples.
- There were 111 metal cases and 97 rock cases.
- Quadratic discriminant analysis, with regularized covariance estimators was applied.
- Performed leave-one-out cross validation to compare classification performance.
Results: QDA on the sonar data

The number of classification errors made in leave-one-out cross validation on 208 examples.

<table>
<thead>
<tr>
<th>Method</th>
<th>$M_{\text{off}}$</th>
<th>$M_{\text{all}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_1$ standardized</td>
<td>33</td>
<td>34</td>
</tr>
<tr>
<td>$L_1$</td>
<td>33</td>
<td>35</td>
</tr>
<tr>
<td>ridge standardized</td>
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<td>37</td>
</tr>
<tr>
<td>ridge</td>
<td>31</td>
<td>42</td>
</tr>
</tbody>
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These methods outperform using $S^{-1}$, which had 50 errors, and using $(S \circ I)^{-1}$, which had 68 errors.
Thank you

This talk is based on:


An R package will be available soon