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.

Estimating large covariance matrices and their inverses

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 Σ

B. Estimating Σ^{-1}

Estimating the covariance matrix Σ

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).
- Σ with reduced effective rank (Bunea & Xiao, 2012).
- Approximate factor model with sparse error covariance (Fan, Liao & Minchev, 2013).

Estimating the inverse covariance matrix Σ^{-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 Σ

- 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 Σ^{-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 Σ^{-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 Σ^{-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).
- Simultaneous estimation and selection (Yuan & Lin, 2007; Yuan, 2010; Cai, Liu, & Luo, 2011; Ren, Sun, Zhang, & Zhou, 2013).
- 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 Σ^{-1}

Unpenalized Gaussian likelihood estimation of Σ^{-1}

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

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

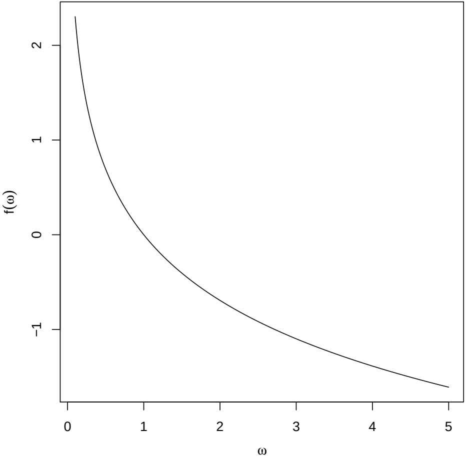
Set the gradient at $\hat{\Omega}$ to zero:

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

- 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 Σ^{-1}

We will study

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

- $q = 1$ 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_{all}, M_{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 Σ^{-1}

The case when $q = 1$ is

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

- $\hat{\Omega}_{\lambda,1}(M_{\text{off}})$ 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).

Review of work on solution existence

- Banerjee et al. (2008) showed that $\hat{\Omega}_{\lambda,1}(M_{\text{all}})$ exists if $\lambda > 0$.
- Ravikumar et al. (2008) showed that $\hat{\Omega}_{\lambda,1}(M_{\text{off}})$ exists if $\lambda > 0$ and $S \circ I \in \mathbb{S}^p_+$.
- Lu (2008) showed that $\hat{\Omega}_{\lambda,1}(M)$ exists if $S + \lambda M \circ I \in \mathbb{S}^p_+$.

Lasso-penalized likelihood solution existence

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

Theorem. The solution $\hat{\Omega}_{\lambda,1}(M)$ exists if and only if $A_{1,\lambda}(M) = \{\Sigma \in \mathbb{S}_+^p : |\sigma_{ij} - s_{ij}| \le m_{ij}\lambda\}$ 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. $\lambda > 0$, $S \circ I \in \mathbb{S}_+^p$ and $\min_{i \neq j} m_{ij} > 0$;
3. $S \in \mathbb{S}_+^p$;
4. $\mathrm{soft}(S, \lambda M) \in \mathbb{S}_+^p$.

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 Σ^{-1}

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

- 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

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

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

Example. $m_{ij} = 1(|i-j| > k)$. Then $\mathcal{U}$ 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 $\mathcal{U}$ 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 $\mathcal{U}$ 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 $\bar{\lambda}$ sufficiently large so that $\hat{\Omega}_{\bar{\lambda},1}(M)$ 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

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

- Each iteration minimizes

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

  - 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,

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

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

Majorizing f at Ω_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 Ω_k to get the majorizer.

Majorizing f at Ω_k part 2

- The minimizer of the majorizer to f at Ω_k is

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

  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).

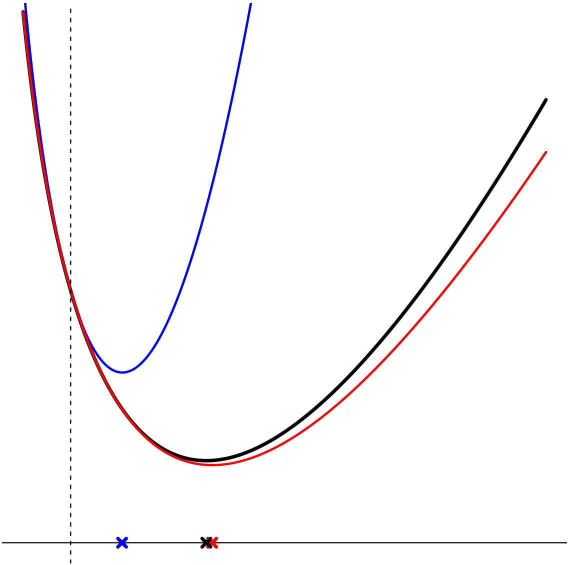
Acceleration by minorizing f at Ω_k

- Get the minorizer by replacing the entire penalty $\sum_{i,j} m_{ij}\omega_{ij}^2$ with a linear approximation at our current iterate Ω_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 $\Omega_0 \in \mathbb{S}^p_+$. 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

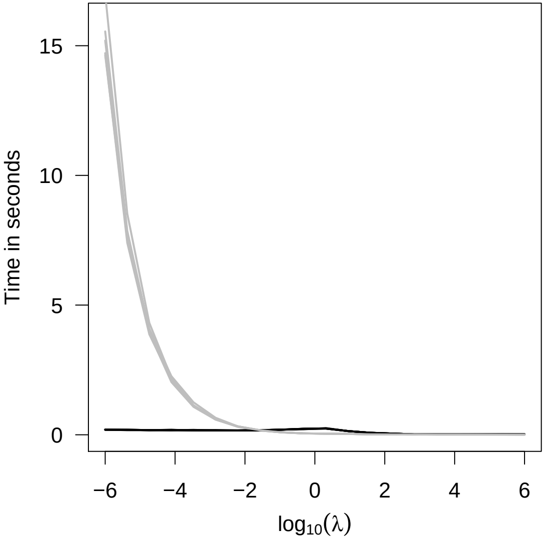
In each replication,

1. randomly generated Σ_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 $\hat{\Omega}_{\lambda,2}(M_{\text{off}})$.

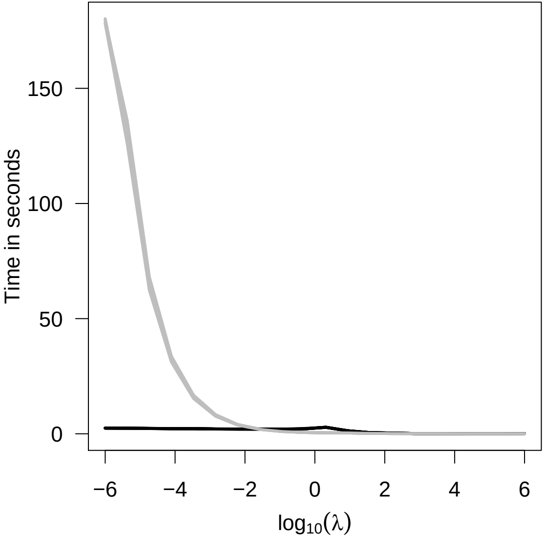
Results for $n = 50$ & $p = 100$

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



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

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

  - $S^{(j)}$ is computed from observations inside the jth subset (centered by training sample means)
  - $\hat{\Omega}_{\lambda}^{(-j)}$ is the inverse covariance estimate computed from the observations outside the jth 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.

	M_{off}	M_{all}
L_1 standardized	33	34
L_1	33	35
ridge standardized	33	37
ridge	31	42

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:

Rothman, A. J. and Forzani, L. (2013) Properties of optimizations used in penalized Gaussian likelihood inverse covariance matrix estimation. *Submitted*

An R package will be available soon