Sparse Inverse Covariance Estimation Using Quadratic Approximation

Inderjit S. Dhillon
Dept of Computer Science
UT Austin

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Inverse Covariance Estimation

- Given: $n$ i.i.d. samples $\{y_1, \ldots, y_n\}$, $y_i \sim \mathcal{N}(\mu, \Sigma)$,
- Goal: Estimate the inverse covariance $\Theta = \Sigma^{-1}$.
- The sample mean and covariance are defined by

$$
\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} y_i \quad \text{and} \quad S = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{\mu})(y_i - \hat{\mu})^T.
$$

- Given the $n$ samples, the likelihood is

$$
P(y_1, \ldots, y_n; \hat{\mu}, \Theta) \propto \prod_{i=1}^{n} (\det \Theta)^{1/2} \exp \left( -\frac{1}{2} (y_i - \hat{\mu})^T \Theta (y_i - \hat{\mu}) \right)
= (\det \Theta)^{n/2} \exp \left( -\frac{1}{2} \sum_{i=1}^{n} (y_i - \hat{\mu})^T \Theta (y_i - \hat{\mu}) \right).
$$
Inverse Covariance Estimation

- The log likelihood can be written as
  \[
  \log(P(y_1, \ldots, y_n; \hat{\mu}, \Theta)) = \frac{n}{2} \log(\det \Theta) - \frac{n}{2} \text{tr}(\Theta S) + \text{constant}.
  \]

- The maximum likelihood estimator of \( \Theta \) is
  \[
  \Theta = \arg \min_{X \succ 0} \{- \log \det X + \text{tr}(SX)\}.
  \]

- In high-dimensions (\( p < n \)), the sample covariance matrix \( S \) is singular.
  - Want \( \Theta \) to be sparse.
Structure for Gaussian Markov Random Field

- The nonzero pattern of $\Theta$ is important:
- Each Gaussian distribution can be represented by a pairwise Gaussian Markov Random Field (GMRF)
- Conditional independence is reflected as zeros in $\Theta$:

$$\Theta_{ij} = 0 \iff y_i \text{ and } y_j \text{ are conditional independent given other variables.}$$

- In a GMRF $G = (V, E)$, each node corresponds to a variable, and each edge corresponds to a non-zero entry in $\Theta$. 
Examples

- An example – Chain graph: $y_j = \varphi y_{j-1} + \mathcal{N}(0, 1)$

$$
\Theta = \begin{pmatrix}
1 & -\varphi & & & \\
-\varphi & 1 + \varphi^2 & -\varphi & & \\
& \ddots & \ddots & \ddots & \\
-\varphi & 1 + \varphi^2 & -\varphi & 1
\end{pmatrix}
$$

- Real world example: graphical model which reveals the relationships between Senators: (Figure from Banerjee et al, 2008)
Prior Work

- **COVSEL**: Block coordinate descent method with interior point solver for each block (Banerjee et al, 2007).
- **Glasso**: Block coordinate descent method with coordinate descent solver for each block (Friedman et al, 2007).
- **VSM**: Nesterov’s algorithm (Lu, 2009).
- **PSM**: Projected Subgradient Method (Duchi et al, 2008).
- **SINCO**: Greedy coordinate descent method (Scheinberg and Rish, 2009).
- **ALM**: Alternating Linearization Method (Scheinberg et al, 2010).
- **IPM**: Inexact interior point method (Li and Toh, 2010).
- **PQN**: Projected Quasi-Newton method to solve the dual problem (Schmidt et al, 2009).
L1-regularized covariance selection

- A sparse inverse covariance matrix is preferred – add $\ell_1$ regularization to promote sparsity.
- The resulting optimization problem:

  $$
  \Theta = \arg \min_{X \succ 0} \left\{ - \log \det X + \operatorname{tr}(SX) + \lambda \| X \|_1 \right\} = \arg \min_{X \succ 0} f(X),
  $$

  where $\| X \|_1 = \sum_{i,j=1}^n |X_{ij}|$.

- Regularization parameter $\lambda > 0$ controls the sparsity.
- Can be extended to a more general regularization term:

  $$
  \| \Lambda \circ X \|_1 = \sum_{i,j=1}^n \lambda_{ij} |X_{ij}|
  $$
Second Order Method

- Newton method for twice differentiable function:

  \[ \mathbf{x} \leftarrow \mathbf{x} - \eta (\nabla^2 f(\mathbf{x}))^{-1} \nabla f(\mathbf{x}) \]

- However, the sparse inverse covariance estimation objective

  \[ f(\mathbf{X}) = -\log \det \mathbf{X} + \text{tr}(\mathbf{S}\mathbf{X}) + \lambda \| \mathbf{X} \|_1 \]

  is not differentiable.

- Most current solvers are first-order methods:
  - Block Coordinate Descent (GLASSO), projected gradient descent (PSM), greedy coordinate descent (SINCO), alternating linearization method (ALM).
Quadratic Approximation

- Write objective as \( f(X) = g(X) + h(X) \), where

\[
g(X) = -\log \det X + \text{tr}(SX) \quad \text{and} \quad h(X) = \lambda \|X\|_1.
\]

- \( g(X) \) is twice differentiable while \( h(X) \) is convex but non-differentiable — we can only form quadratic approximation for \( g(X) \).

- The quadratic approximation of \( g(X_t + \Delta) \) is

\[
\bar{g}_{X_t}(\Delta) = \text{tr}((S - W_t)\Delta) + (1/2) \text{tr}(W_t\Delta W_t\Delta) - \log \det X_t + \text{tr}(SX_t),
\]

where \( W_t = (X_t)^{-1} \).

- Note that

\[
\text{tr}(W_t\Delta W_t\Delta) = \text{vec}(\Delta)^T(W_t \otimes W_t)\text{vec}(\Delta)
\]
Define the generalized Newton direction:

\[
D = \arg\min_{\Delta} \bar{g}_{X_t}(\Delta) + \lambda \|X + \Delta\|_1,
\]

where \(\bar{g}_{X_t}(\Delta) \equiv g(X_t + \Delta) = \text{tr}((S - W_t)\Delta) + \frac{1}{2} \text{tr}(W_t\Delta W_t\Delta)\).

Can be rewritten as a Lasso type problem with \(p(p + 1)/2\) variables:

\[
\frac{1}{2} \text{vec}(\Delta)^T(W_t \otimes W_t)\text{vec}(\Delta) + \text{vec}(S - W_t)^T\text{vec}(\Delta) + \lambda \|\text{vec}(\Delta)\|_1.
\]

Coordinate descent method is efficient at solving Lasso type problems.
Coordinate Descent Updates

- Can use cyclic coordinate descent to solve $\arg \min_{\Delta} \{ \bar{g}_{X_t}(\Delta) + \lambda \| \Delta \|_1 \}$:
  - Generate a sequence $D_1, D_2..., $ where $D_i$ is updated from $D_{i-1}$ by only changing one variable.
  - Variables are selected by cyclic order.

- Naive approach has an update cost of $O(p^2)$ because
  \[ \nabla_i \bar{g}(\Delta) = ((W_t \otimes W_t) \text{vec}(\Delta) + \text{vec}(S - W_t))_i \]

- Next we show how to reduce the cost from $O(p^2)$ to $O(p)$. 
Coordinate Descent Updates

- Each coordinate descent update:

\[ \bar{\mu} = \arg\min_{\mu} g(D + \mu(e_ie_j^T + e_je_i^T)) + 2\lambda|X_{ij} + D_{ij} + \mu| \]

\[ D_{ij} \leftarrow D_{ij} + \bar{\mu} \]

- The one-variable problem can be simplified as

\[ \frac{1}{2}(W_{ij}^2 + W_{ii}W_{jj})\mu^2 + (S_{ij} - W_{ij} + w_i^T D w_j)\mu + \lambda|X_{ij} + D_{ij} + \mu| \]

- Quadratic form with L1 regularization — soft thresholding gives the exact solution.
Efficient solution of one-variable problem

If we introduce $a = W_{ij}^2 + W_{ii}W_{jj}$, $b = S_{ij} - W_{ij} + w_i^T D w_j$, and $c = X_{ij} + D_{ij}$, then the minimum is achieved for:

$$
\mu = -c + S(c - b/a, \lambda/a),
$$

where $S(z, r) = \text{sign}(z) \max\{|z| - r, 0\}$ is the soft-thresholding function.

The main cost arises while computing $w_i^T D w_j$: direct computation requires $O(p^2)$ flops.

Instead, we maintain $U = D W$ after each coordinate updates, and then compute $w_i^T u_j$ — only $O(p)$ flops per updates.
Adopt Armijo’s rule — try step-sizes $\alpha \in \{\beta^0, \beta^1, \beta^2, \ldots \}$ until $X_t + \alpha D_t$:

1. is positive definite
2. satisfies a sufficient decrease condition

$$f(X_t + \alpha D_t) \leq f(X_t) + \alpha \sigma \Delta_t$$

where $\Delta_t = \text{tr}(\nabla g(X_t)D_t) + \lambda \|X_t + D_t\|_1 - \lambda \|X_t\|_1$.

Both conditions can be checked by performing Cholesky factorization — $O(p^3)$ flops per line search iteration.

Can possibly do better by using Lanczos [K.C.Toh]
Recall the time cost for finding descent direction:

\[ O(p^2) \text{ variables, each update needs } O(p) \text{ flops } \rightarrow \text{ total } O(p^3) \text{ flops per sweep.} \]

Our goal: Reduce the number of variables from \( O(p^2) \) to \( \|X_t\|_0 \).

\( \|X_t\|_0 \) can be much smaller than \( O(p^2) \) as the suitable \( \lambda \) should give a sparse solution.

Our strategy: before solving the Newton direction, make a guess on which variables to update.
Free and Fixed Sets

- \((X_t)_{ij}\) belongs to \textit{fixed} set if and only if

\[ |\nabla_{ij} g(X_t)| < \lambda, \text{ and } (X_t)_{ij} = 0. \]

- The remaining variables constitute the \textit{free} set.

- We then perform the coordinate descent updates only on \textit{free} set.
In practice, the size of free set is small.

Take Hereditary dataset as an example:

\[ p = 1869, \text{ number of variables} = p^2 = 3.49 \text{ million}. \] The size of free set drops to 20,000 at the end.
Recently, (Mazumder and Hastie, 2012) and (Witten et al, 2011) proposed a block decomposition approach.

Consider the thresholded covariance matrix $E_{ij} = \max(|S_{ij}| - \lambda, 0)$.

When $E$ is block-diagonal, the solution is also block-diagonal:

$$E = \begin{bmatrix} E_1 & 0 & \ldots & 0 \\ 0 & E_2 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & E_n \end{bmatrix}, \quad \Theta^* = \begin{bmatrix} \Theta_1^* & 0 & \ldots & 0 \\ 0 & \Theta_2^* & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \Theta_n^* \end{bmatrix}$$

Based on this approach, the original problem can be decomposed into $n$ sub-problems.
Our method automatically discovers the block-diagonal structure too.

Key observation: off-diagonal blocks are always in the fixed set.

Recall the definition of fixed set: $|\nabla_{ij} g(X_t)| < \lambda$ and $(X_t)_{ij} = 0$.

For $(i, j)$ in off-diagonal blocks:

1. Initialize from the identity matrix, so $(X_0)_{ij} = 0$.
2. $\nabla_{ij} g(X_t) = S_{ij} - (X_t)^{-1}_{ij} = S_{ij}$.
3. $E_{ij} = \max( |S_{ij}| - \lambda, 0 ) = 0$ implies $|\nabla_{ij} g(X_t)| < \lambda$. So $(i, j)$ is always in the fixed set.

Off-diagonal blocks are always 0, so QUIC gets the speedup for free.
Final Algorithm

**QUIC: QUadratic approximation for sparse Inverse Covariance estimation**

**Input**: Empirical covariance matrix $S$, scalar $\lambda$, initial $X_0$.

For $t = 0, 1, \ldots$

1. Compute $W_t = X_t^{-1}$.
2. Form the second order approximation $\bar{g}_{X_t}(X)$ to $g(X)$ around $X_t$.
3. Partition variables into free and fixed sets
4. Use coordinate descent to find descent direction:
   \[ D_t = \arg \min_{\Delta} \bar{f}_{X_t}(X_t + \Delta) \]
   over the free variable set, (A Lasso problem.)
5. Use an Armijo-rule based step-size selection to get $\alpha$ s.t.
   \[ X_{t+1} = X_t + \alpha D_t \]
   is positive definite and objective sufficiently decreases.
Methods included in our comparisons

- **QUIC**: Proposed method.
- **ALM**: Alternating Linearization Method (Scheinberg et al, 2010).
- **Glasso**: Block coordinate descent method (Friedman et al, 2007).
- **PSM**: Projected Subgradient Method (Duchi et al, 2008).
- **SINCO**: Greedy coordinate descent method (Scheinberg and Rish, 2009).
- **IPM**: Inexact interior point method (Li and Toh, 2010).
Senate dataset

- 100 Senators ($p = 100$) and 542 bill votes (either $+1$ or $-1$).
- Solve the sparse inverse covariance problem.

Figure from Banerjee et al, 2008
Synthetic datasets

We generate the two following types of graph structures for GMRF:

- **Chain graphs**: The ground truth inverse covariance matrix $\Sigma^{-1}$ is set to be $\Sigma_{i,i-1} = -0.5$ and $\Sigma_{i,i} = 1.25$.

- **Graphs with Random Sparsity Structures**: First, generate a sparse matrix $U$ with nonzero elements equal to $\pm 1$. Set $\Sigma^{-1}$ to be $U^T U$. Add a diagonal term to ensure $\Sigma^{-1}$ is positive definite.

Control the number of nonzeros in $U$ so that the resulting $\Sigma^{-1}$ has approximately $10p$ nonzero elements.
Experimental settings

- Test under two values of $\lambda$: one discovers correct number of nonzeros, and one discovers 5 times the number of nonzeros.
- For each distribution we draw $n = p/2$ i.i.d. samples as input.
- We report the time for each algorithm to achieve $\epsilon$-accurate solution: $f(X_t) - f(X^*) < \epsilon f(X^*)$.
- * indicates the run time exceeded 30,000 seconds (8.3 hours).
### Results for Synthetic datasets

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<th>Dataset setting</th>
<th>Time (in seconds)</th>
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Real datasets

(a) Time for Estrogen, $p = 692$
(b) Time for hereditarybc, $p = 1,869$

**Figure:** Comparison of algorithms on real datasets. The results show QUIC converges faster than other methods.
Conclusions

- Proposed a quadratic approximation method for sparse inverse covariance learning (QUIC).
- Three key ingredients:
  - Exploit structure of Hessian
    - we have done this in the context of coordinate descent
    - Nocedal & colleagues (2012) have recently developed other methods to exploit structure of Hessian, e.g., Newton-CG
  - Armijo-type stepsize rule
  - Division into free and fixed sets
- Initial paper published in NIPS 2011:
- Journal version coming soon......
- Question: How can we solve problems with 100,000 variables?
  Answer: QUIC-2
References


