Sparse Inverse Covariance Estimation Using Quadratic Approximation

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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.
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:

\[
\Theta = \arg \min_{X > 0} \left\{ -\log \det X + \text{tr}(SX) + \lambda \|X\|_1 \right\} = \arg \min_{X > 0} f(X),
\]

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

  \[
  \text{tr}(W_t \Delta W_t \Delta) = \text{vec}(\Delta)^T (W_t \otimes W_t) \text{vec}(\Delta)
  \]
Descent Direction

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 \( \arg \min_\Delta \{ \bar{g}_{\mathbf{X}_t}(\Delta) + \lambda \| \Delta \|_1 \} \):

- Generate a sequence \( D_1, D_2, \ldots \), 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

\[
\nabla_i \bar{g}(\Delta) = \left( (W_t \otimes W_t) \text{vec}(\Delta) + \text{vec}(S - W_t) \right)_i
\]

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

Each coordinate descent update:

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

$$D_{ij} \leftarrow D_{ij} + \bar{\mu}$$

The one-variable problem can be simplified as

$$\frac{1}{2}(W_{ij}^2 + W_{ii}W_{jj})\mu^2 + (S_{ij} - W_{ij} + w_i^TD_{ij}w_j)\mu + \lambda|X_{ij} + D_{ij} + \mu|$$

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.
Line Search

- 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:

\( O(p^2) \) variables, each update needs \( O(p) \) flops → total \( O(p^3) \) 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: $p = 1869$, number of variables $= p^2 = 3.49$ 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. $\nabla_{ij} g(X_t) = S_{ij} - (X_t)_{ij}^{-1} = S_{ij}$.
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).
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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
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 $\Sigma_{i,i-1}^{-1} = -0.5$ and $\Sigma_{i,i}^{-1} = 1.25$.

- **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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Real datasets

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


