

Topic 16: Graphical Network Inference

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Key points:

Disclaimer: The note is built on Prof. *Jinchi Lv's* lectures of the course at USC, DSO 607, High-Dimensional Statistics and Big Data Problems.

16.1 Motivation

Consider a classic question: For n observations of dimension p , how can we capture the statistical relationships between the variables of interest? Consider the example of the multivariate Gaussian distribution:

Example 16.1.1: Multivariate Gaussian Distribution

Suppose we have n observations of dimension p , $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$. let \mathbf{S} be the empirical covariance matrix. Then the probability density

$$f(\mathbf{x}) = \frac{1}{(2\pi)^{p/2} \det(\boldsymbol{\Sigma})^{1/2}} \exp \left\{ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right\}$$

define the **inverse covariance matrix** or **precision matrix** as $\boldsymbol{\Omega} = \boldsymbol{\Sigma}^{-1}$, then we have

$$f_{\boldsymbol{\mu}, \boldsymbol{\Omega}} = \exp \left\{ \boldsymbol{\mu}' \boldsymbol{\Omega} \mathbf{x} - \left\langle \boldsymbol{\Omega}, \frac{1}{2} \mathbf{x} \mathbf{x}' \right\rangle - \frac{p}{2} \log(2\pi) + \frac{1}{2} \log \det(\boldsymbol{\Omega}) - \frac{1}{2} \boldsymbol{\mu}' \boldsymbol{\Omega} \boldsymbol{\mu} \right\}$$

where $\langle \mathbf{A}, \mathbf{B} \rangle = \text{tr}(\mathbf{A}\mathbf{B})$.

In this example, we know that **every** multivariate Gaussian distribution can be represented by a pairwise **Gaussian Markov Random Field (GMRF)**, which an **undirected graph** $G = (V, E)$

- representing the collection of variables \mathbf{x} by a vertex set $\mathcal{V} = \{1, \dots, p\}$
- encoding correlations between variables by a set of edges $\mathcal{E} = \{(i, j) \in \mathcal{V} \mid i \neq j, \Omega_{ij} \neq 0\}$

For simplicity, we normalize $\boldsymbol{\mu} = \mathbf{0}$. If we draw n i.i.d. samples $\mathbf{x}_1, \dots, \mathbf{x}_n \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$, then the log-likelihood is

$$\begin{aligned} \mathcal{L}(\boldsymbol{\Omega}) &= \frac{1}{n} \sum_{i=1}^n \log f(\mathbf{x}_i) = \frac{1}{2} \log \det(\boldsymbol{\Omega}) - \frac{1}{2n} \sum_{i=1}^n \mathbf{x}_i' \boldsymbol{\Omega} \mathbf{x}_i \\ &= \frac{1}{2} \log \det(\boldsymbol{\Omega}) - \frac{1}{2} \left\langle \boldsymbol{\Omega}, \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i' \right\rangle \end{aligned}$$

What's the goal? We want to estimate a **sparse** graph structure given $n \ll p$ i.i.d. observations. But what does sparsity means in this context? A sparse graph is **equivalent** to a sparse precision matrix: the precision

matrix should have many 0s.

Sparse precision matrix for the Gaussian vector mentioned above $\mathbf{x} \sim \mathcal{N}(\mathbf{0}, \Sigma)$, we have $\forall u, v$

$$x_u \perp x_v \mid \mathbf{x}_{V \setminus \{u, v\}} \Leftrightarrow \Omega_{u, v} = 0$$

that is, sparsity of the precision matrix is equivalent to **conditional independence**¹. Consider a graph, where x_1 and x_4 are only connected through other nodes, that is x_1 and x_4 are conditional independent, then we can have the precision matrix be something like:

$$\Theta = \begin{bmatrix} * & * & 0 & 0 & * & 0 & 0 & 0 \\ * & * & 0 & 0 & 0 & * & * & 0 \\ 0 & 0 & * & 0 & * & 0 & 0 & * \\ 0 & 0 & 0 & * & 0 & 0 & * & 0 \\ * & 0 & * & 0 & * & 0 & 0 & * \\ 0 & * & 0 & 0 & 0 & * & 0 & 0 \\ 0 & * & 0 & * & 0 & 0 & * & 0 \\ 0 & 0 & * & 0 & * & 0 & 0 & * \end{bmatrix}$$

where 0 captures precisely the conditional independence.



x_1 and x_4 are connected



x_1 and x_4 are NOT connected, conditionally

Intuitively, a sparse graph is much simpler, which is why conditional independence is desired. So how to achieve sparsity? We can again use a L-1 regularization when maximizing the log-likelihood $\mathcal{L}(\Omega)$. Denote the sample covariance matrix as $\mathbf{S} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i'$, then the problem becomes the so-called **Graphical Lasso**

$$\max_{\Omega \geq 0} \log \det(\Omega) - \text{tr}(\mathbf{S}\Omega) - \rho \|\Omega\|_1$$

which is equivalent to

$$\min_{\Omega \geq 0} -\log \det(\Omega) + \text{tr}(\mathbf{S}\Omega) + \rho \|\Omega\|_1$$

16.2 Graphical Lasso

The graphical lasso method is developed by (Friedman et al., 2008). For the optimization problem

$$\min_{\Omega \geq 0} -\log \det(\Omega) + \text{tr}(\mathbf{S}\Omega) + \rho \|\Omega\|_1 \quad (16.1)$$

¹Meanwhile, for independence: $\Sigma_{u, v} = 0 \Leftrightarrow x_u \perp x_v$

The first-order optimality condition gives

$$\mathbf{0} \in \mathbf{\Omega}^{-1} - \mathbf{S} - \lambda \mathbf{\Gamma}$$

where $\mathbf{\Gamma}$ is a matrix of component-wise signs of $\mathbf{\Omega}$

$$\mathbf{\Gamma} = \partial \|\mathbf{\Omega}\|_1 \Rightarrow \gamma_{jk} \begin{cases} = \text{sign}(\omega_{jk}), & \omega_{jk} \neq 0 \\ \in [-1, 1], & \omega_{jk} = 0 \end{cases}$$

since in a graph, we always have that, following the global stationarity conditions, $\omega_{jj} > 0$, which implies that

$$w_{ii} = s_{ii} + \lambda \quad i = 1, \dots, p \quad (16.2)$$

where we denote a working version of $\mathbf{\Omega}^{-1}$ as \mathbf{W} .

The idea is to repeatedly cycle through all columns-rows and in each step optimize only a single column-row. Consider the following partition where all matrices are partitioned into one column/row versus the rest

$$\mathbf{\Omega} = \begin{pmatrix} \mathbf{\Omega}_{11} & \boldsymbol{\omega}_{12} \\ \boldsymbol{\omega}'_{12} & \omega_{22} \end{pmatrix} \quad \mathbf{S} = \begin{pmatrix} \mathbf{S}_{11} & \mathbf{s}_{12} \\ \mathbf{s}'_{12} & s_{22} \end{pmatrix} \quad \mathbf{W} = \begin{pmatrix} \mathbf{W}_{11} & \mathbf{w}_{12} \\ \mathbf{w}'_{12} & w_{22} \end{pmatrix} \quad \mathbf{\Gamma} = \begin{pmatrix} \mathbf{\Gamma}_{11} & \boldsymbol{\gamma}_{12} \\ \boldsymbol{\gamma}'_{12} & \gamma_{22} \end{pmatrix}$$

apply this partition to the optimality condition, get

$$\mathbf{\Omega}^{-1} = \mathbf{S} - \lambda \mathbf{\Gamma}$$

$$\begin{pmatrix} \mathbf{W}_{11} & \mathbf{w}_{12} \\ \mathbf{w}'_{12} & w_{22} \end{pmatrix} = \begin{pmatrix} \mathbf{S}_{11} & \mathbf{s}_{12} \\ \mathbf{s}'_{12} & s_{22} \end{pmatrix} + \lambda \begin{pmatrix} \mathbf{\Gamma}_{11} & \boldsymbol{\gamma}_{12} \\ \boldsymbol{\gamma}'_{12} & \gamma_{22} \end{pmatrix}$$

where $\mathbf{\Omega}_{11}$ is $(p-1) \times (p-1)$, $\boldsymbol{\omega}_{12}$ is $(p-1) \times 1$, ω_{22} is a scalar.

Consider a **blockwise** step: suppose we fix all but the last row/column, then using properties of inverses of block-partitioned matrices, we have

$$\begin{pmatrix} \mathbf{W}_{11} & \mathbf{w}_{12} \\ \mathbf{w}'_{12} & w_{22} \end{pmatrix} = \begin{pmatrix} \left(\mathbf{\Omega}_{11} - \frac{\boldsymbol{\omega}_{12} \boldsymbol{\omega}'_{12}}{\omega_{22}} \right)^{-1} & -\mathbf{W}_{11} \frac{\boldsymbol{\omega}_{12}}{\omega_{22}} \\ \frac{1}{\omega_{22}} - \frac{\boldsymbol{\omega}'_{12} \mathbf{W}_{11} \boldsymbol{\omega}_{12}}{\omega_{22}^2} & \end{pmatrix}$$

$$= \begin{pmatrix} \mathbf{\Omega}_{11}^{-1} + \frac{\mathbf{\Omega}_{11}^{-1} \boldsymbol{\omega}_{12} \boldsymbol{\omega}'_{12} \mathbf{\Omega}_{11}^{-1}}{\omega_{22} - \boldsymbol{\omega}'_{12} \mathbf{\Omega}_{11}^{-1} \boldsymbol{\omega}_{12}} & -\frac{\mathbf{\Omega}_{11}^{-1} \boldsymbol{\omega}_{12}}{\omega_{22} - \boldsymbol{\omega}'_{12} \mathbf{\Omega}_{11}^{-1} \boldsymbol{\omega}_{12}} \\ \frac{1}{\omega_{22} - \boldsymbol{\omega}'_{12} \mathbf{\Omega}_{11}^{-1} \boldsymbol{\omega}_{12}} & \end{pmatrix}$$

then, by the partitioned optimality condition, we have²:

$$\mathbf{0} = -\mathbf{w}_{12} + \mathbf{s}_{12} + \lambda \boldsymbol{\gamma}_{12} = \mathbf{W}_{11} \frac{\boldsymbol{\omega}_{12}}{\omega_{22}} + \mathbf{s}_{12} + \lambda \boldsymbol{\gamma}_{12} \quad (16.3)$$

$$\mathbf{0} = \frac{\mathbf{\Omega}_{11}^{-1} \boldsymbol{\omega}_{12}}{\omega_{22} - \boldsymbol{\omega}'_{12} \mathbf{\Omega}_{11}^{-1} \boldsymbol{\omega}_{12}} + \mathbf{s}_{12} + \lambda \boldsymbol{\gamma}_{12} = w_{22} \mathbf{\Omega}_{11}^{-1} \boldsymbol{\omega}_{12} + \mathbf{s}_{12} + \lambda \boldsymbol{\gamma}_{12} \quad (16.4)$$

The graphic Lasso algorithm then solves Eq.16.3 for $\boldsymbol{\beta} = \boldsymbol{\omega}_{12}/\omega_{12}$, that is

$$\mathbf{W}_{11} \boldsymbol{\beta} + \mathbf{s}_{12} + \lambda \boldsymbol{\gamma}_{12} = \mathbf{0}$$

²For Eq.16.4, by Eq.16.2, we know that $w_{22} = s_{22} + \lambda$, which is fixed.

where $\gamma_{12} \in \text{sign}(\beta)$ since $\omega_{22} > 0$, which is essentially solving:

$$\min_{\beta \in \mathbb{R}^{p-1}} \left\{ \frac{1}{2} \beta' \mathbf{W}_{11} \beta + \beta' \mathbf{s}_{12} + \lambda \|\beta\|_1 \right\}$$

and $\mathbf{W}_{11} > 0$ is assumed to be fixed.

This problem is analogous to a lasso regression problem of **the last variable on the rest**, but the cross-product matrix \mathbf{S}_{11} is replaced by its **current estimation** \mathbf{W}_{11} . It is relatively easier to solve using elementwise coordinate descent, then

$$\mathbf{w}_{12} = -\mathbf{W}_{11} \frac{\omega_{12}}{\omega_{22}} \quad \Rightarrow \quad \hat{\mathbf{w}}_{12} = -\mathbf{W}_{11} \hat{\beta} \quad \text{Step 1}$$

$$w_{22} = \frac{1}{\omega_{22}} - \frac{\omega'_{12} \mathbf{W}_{11} \omega_{12}}{\omega_{22}^2} \quad \Rightarrow \quad \frac{1}{\hat{\omega}_{22}} = w_{22} - \hat{\beta}' \hat{\mathbf{w}}_{12} \quad \text{Step 2}$$

$$\omega_{12} = -\mathbf{W}_{11}^{-1} \mathbf{w}_{12} \omega_{22} \quad \Rightarrow \quad \hat{\omega}_{12} = -\mathbf{W}_{11}^{-1} \hat{\mathbf{w}}_{12} \hat{\omega}_{22} \quad \text{Step 3}$$

notice that after solving for β and updating \mathbf{w}_{12} in Step 1, the graphic Lasso procedure can move onto the next block, that is, only Step 1 is used in the loop, Step 2 and 3 can be done at the end. The algorithm can be summarized as:

Algorithm 16.2.1: Graphical Lasso algorithm

- 1 Initialize $\mathbf{W} = \mathbf{S} + \lambda \mathbf{I}$
- Cycle around the columns repeatedly, performing the following steps till convergence:
 - a rearrange the rows/columns so that the target column is **the last** (implicitly)
 - b solve the lasso problem, starting the solution from the previous round for this column
 - c update the row/column (*off-diagonal*) of the covariance using $\hat{\mathbf{w}}_{12}$
 - d save $\hat{\beta}$ for this column in the matrix \mathbf{B}
- 3 after convergence, for every row/column, compute the diagonal entries $\hat{\omega}_{jj}$, and covert the \mathbf{B} matrix to $\hat{\Omega}$

16.3 What Is GLasso Solving?

Again, consider the optimization problem

$$\min_{\Omega \geq 0} -\log \det(\Omega) + \text{tr}(\mathbf{S}\Omega) + \rho \|\Omega\|_1$$

and its stationarity condition

$$\mathbf{0} = \Omega^{-1} - \mathbf{S} - \lambda \Gamma$$

rewrite the stationarity condition

$$\mathbf{0} = \Omega^{-1} - \mathbf{S} - \lambda \Gamma = \Omega^{-1} - (\mathbf{S} + \lambda \Gamma)$$

since $\Gamma = \text{sign}(\Omega)$, write $\tilde{\Gamma} = \lambda \Gamma$, then we have $\|\tilde{\Gamma}\|_\infty \leq \lambda$. Denote the element-wise absolute value matrix of Ω as $\text{abs}(\Omega)$, then

Issues of GLasso method :

- the non-monotonic behavior of GLasso in minimizing $f(\mathbf{\Omega})$
 - θ_{12} is entangled in \mathbf{W}_{11} , which is **incorrectly** treated as a constant
 - after updating θ_{12} , the entire (working) covariance matrix \mathbf{W} changes, but GLasso algorithm only updates \mathbf{w}_{12} and \mathbf{w}'_{12}
- high dimensionality problems
 - not computationally efficient when p is ultra-large
 - $\mathbf{\Sigma}^{-1}$ doesn't exist when $p > n$
 - method is not scalable

Next, we address these issues by introducing some modifications.

16.4 Graphical Lasso: Modifications

16.4.1 Primal GLasso

Consider the optimality condition in Eq.16.4:

$$0 = \frac{\mathbf{\Omega}_{11}^{-1} \omega_{12}}{\omega_{22} - \omega'_{12} \mathbf{\Omega}_{11}^{-1} \omega_{12}} + \mathbf{s}_{12} + \lambda \gamma_{12} = w_{22} \mathbf{\Omega}_{11}^{-1} \omega_{12} + \mathbf{s}_{12} + \lambda \gamma_{12}$$

Here, the dependence of the covariance submatrix \mathbf{W}_{11} on $\mathbf{\Omega}_{12}$ is **explicit**. Let $\alpha = \omega_{12} w_{22}$ with fixed $w_{22} \geq 0$ ³, then this optimality condition is essentially solving

$$\min_{\alpha \in \mathbb{R}^{p-1}} \left\{ \frac{1}{2} \alpha' \mathbf{\Omega}_{11}^{-1} \alpha + \alpha' \mathbf{s}_{12} + \lambda \|\alpha\|_1 \right\}$$

the minimizer of this problem $\hat{\alpha}$ can then be used to derive the estimation for ω_{12} :

$$\hat{\omega}_{12} = \frac{\hat{\alpha}}{w_{22}}$$

, then we can update ω_{22} as before via

$$\hat{\omega}_{22} = \frac{1}{w_{22}} + \hat{\omega}'_{12} \mathbf{\Theta}_{11}^{-1} \hat{\omega}_{12}$$

with $w_{22} = s_{22} + \lambda$. Another problem is how to obtain $\mathbf{\Omega}_{11}^{-1}$: as the iterations proceed, maintain $\mathbf{W} = \mathbf{\Omega}^{-1}$, and $\mathbf{\Omega}_{11}^{-1}$ can be derived from

$$\mathbf{\Omega}_{11}^{-1} = \mathbf{W}_{11} - \frac{\mathbf{w}_{12} \mathbf{w}'_{12}}{w_{22}}$$

once ω_{12} is updated, the **entire** working covariance matrix \mathbf{W} is updated using $\mathbf{\Omega}_{11}^{-1}$. This procedure, the so-called primal graphical lasso, can be represented in the following algorithm:

³ $w_{22} = 1/(\omega_{22} - \omega'_{12} \mathbf{\Omega}_{11}^{-1} \omega_{12})$

Algorithm 16.4.1: P-Glasso Algorithm

- 1 Initialize $\mathbf{W} = \text{diag}(\mathbf{S}) + \lambda \mathbf{I}$ and $\mathbf{\Omega} = \mathbf{W}^{-1}$
- 2 Cycle around the columns repeatedly, performing the following steps till convergence:
 - a rearrange the rows/columns so that the target column is the last (implicitly)
 - b compute $\mathbf{\Omega}_{11}^{-1}$ using $\mathbf{\Omega}_{11}^{-1} = \mathbf{W}_{11} - \frac{\mathbf{w}_{12}\mathbf{w}_{12}'}{w_{22}}$
 - c solve $\min_{\boldsymbol{\alpha} \in \mathbb{R}^{p-1}} \left\{ \frac{1}{2} \boldsymbol{\alpha}' \mathbf{\Omega}_{11}^{-1} \boldsymbol{\alpha} + \boldsymbol{\alpha}' \mathbf{s}_{12} + \lambda \|\boldsymbol{\alpha}\|_1 \right\}$ for $\boldsymbol{\alpha}$, using as warm starts the solution from the previous round of row/column updates. Then update $\hat{\omega}_{12} = \hat{\boldsymbol{\alpha}}/w_{22}$ and $\hat{\omega}_{22}$
 - d update $\mathbf{\Omega}$ and \mathbf{W} , ensuring that $\mathbf{\Omega}\mathbf{W} = \mathbf{I}_p$
- 3 output the solution: precision matrix $\mathbf{\Omega}$ and its exact inverse, covariance matrix \mathbf{W}

References

Jerome Friedman, Trevor Hastie, and Robert Tibshirani. Sparse inverse covariance estimation with the graphical lasso. *Biostatistics*, 9(3):432–441, 2008.