

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

$$\begin{aligned} \mathbf{0} &\in \mathbf{\Omega}^{-1} - \mathbf{S} - \lambda \partial \|\mathbf{\Omega}\|_1 \\ \Rightarrow \mathbf{\Omega}_{i,i}^{-1} &= \mathbf{S}_{i,i} + \lambda, \quad 1 \leq i \leq p \end{aligned} \quad \text{in diagonal entries (self-loop), } 1 \in \partial \|\mathbf{\Omega}_{i,i}\|_1$$

The idea is to repeatedly cycle through all columns-rows and in each step optimize only a single column-row. Denote a working version of $\mathbf{\Omega}^{-1}$ as \mathbf{W} , consider the following partition where all matrices are partitioned into one column/row versus the rest

$$\mathbf{\Omega} = \begin{pmatrix} \mathbf{\Omega}_{1,1} & \omega_{1,2} \\ \omega'_{1,2} & \omega_{2,2} \end{pmatrix} \quad \mathbf{S} = \begin{pmatrix} \mathbf{S}_{1,1} & \mathbf{s}_{1,2} \\ \mathbf{s}'_{1,2} & s_{2,2} \end{pmatrix} \quad = \begin{pmatrix} \mathbf{W}_{1,1} & \mathbf{w}_{1,2} \\ \mathbf{w}'_{1,2} & w_{2,2} \end{pmatrix}$$

where $\mathbf{\Omega}_{1,1}$ is $(p-1) \times (p-1)$, $\omega_{1,2}$ is $(p-1) \times 1$, $\omega_{2,2}$ 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

$$\begin{aligned} \begin{pmatrix} \mathbf{W}_{1,1} & \mathbf{w}_{1,2} \\ \mathbf{w}'_{1,2} & w_{2,2} \end{pmatrix} &= \begin{pmatrix} \left(\mathbf{\Omega}_{1,1} - \frac{\omega_{1,2} \omega'_{1,2}}{\omega_{2,2}} \right)^{-1} & -\mathbf{W}_{1,1} \frac{\omega_{1,2}}{\omega_{2,2}} \\ \frac{1}{\omega_{2,2}} - \frac{\omega'_{1,2} \mathbf{W}_{1,1} \omega_{1,2}}{\omega_{2,2}^2} & \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{\Omega}_{1,1}^{-1} + \frac{\mathbf{\Omega}_{1,1}^{-1} \omega_{1,2} \omega'_{1,2} \mathbf{\Omega}_{1,1}^{-1}}{\omega_{2,2} - \omega'_{1,2} \mathbf{\Omega}_{1,1}^{-1} \omega_{1,2}} & -\frac{\mathbf{\Omega}_{1,1}^{-1} \omega_{1,2}}{\omega_{2,2} - \omega'_{1,2} \mathbf{\Omega}_{1,1}^{-1} \omega_{1,2}} \\ \frac{1}{\omega_{2,2} - \omega'_{1,2} \mathbf{\Omega}_{1,1}^{-1} \omega_{1,2}} & \end{pmatrix} \end{aligned}$$

References

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