

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.

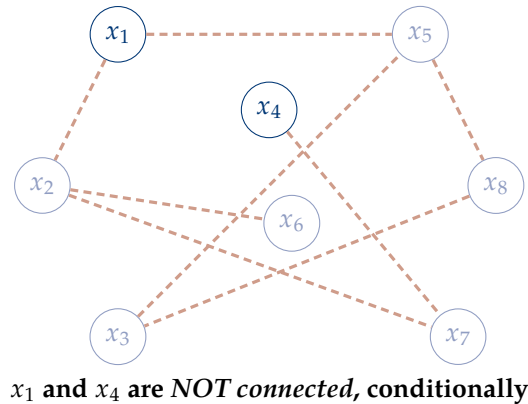
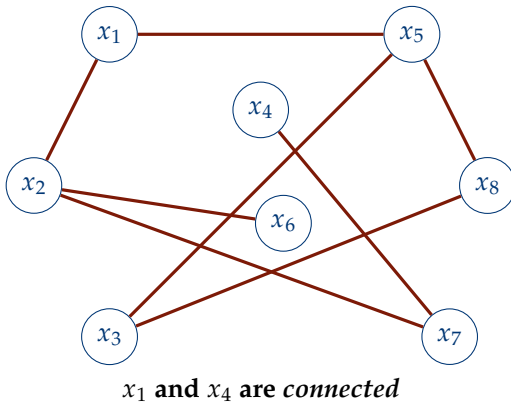
Sparse precision matrix for the Gaussian vector mentioned above $\mathbf{x} \sim \mathcal{N}(\mathbf{0}, \Sigma)$, we have $\forall u, v$

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

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.



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 $\mathcal{L}(\Omega)$. Let the sample covariance matrix $\mathbf{S} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i'$

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

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