# Mod 6: Gaussian Graphical Models

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Graphical Models

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Graphical model:

$$\mathcal{G} = (V, E)$$

$$V = \{1, 2, ..., m\}$$
 set of nodes

 $E \subseteq V \times V$  set of edges

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Adjacent nodes and neighborhoods:

*i* and *j* are neighbors 
$$\Leftrightarrow$$
  $(i, j) \in E$ 

Undirected graph:

## $(i,j) \in E \Leftrightarrow (j,i) \in E$

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Path from i to j:

ordered set 
$$\{i_1, i_2, ..., i_l\} \subseteq V$$

$$i_1 = i$$
 ,  $i_l = j$   
 $(i_k, i_{k+1}) \in E$ ,  $k = 1, ..., l-1$ 

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Let A, B, C, be disjoint subsets of V.

C separates A and B if all path from A to B goes through some element of C.



Gaussian graphical model:

$$\mathbf{X} = \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_m \end{pmatrix} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

# $(i,j) \in E \Leftrightarrow Corr(X_i, X_j \mid \text{all other variables}) \neq 0$

Conditional Independence (denoted by  $\perp$ )

$$X_{1} \perp X_{2} \mid X_{3} \Leftrightarrow f(x_{1}, x_{2} \mid x_{3}) = f(x_{1} \mid x_{3}) f(x_{2} \mid x_{3})$$

**Notation:** Let  $A = \{i_1, ..., i_l\} \subseteq V$ 

$$\mathbf{X}_{A} \;\; = \;\; \left( egin{array}{c} X_{i_1} \ X_{i_2} \ dots \ X_{i_l} \ dots \ X_{i_l} \end{array} 
ight)$$

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Image: Image:

Suppose that A, B and C are disjoint. Then

$$\mathbf{X}_{A} \perp \mathbf{X}_{B} \mid \mathbf{X}_{C} \Leftrightarrow f(\mathbf{x}_{A}, \mathbf{x}_{B} \mid \mathbf{x}_{C}) = f(\mathbf{x}_{A} \mid \mathbf{x}_{C}) f(\mathbf{x}_{B} \mid \mathbf{x}_{C})$$

Some general properties of  $\bot$ 

• 
$$\mathbf{X}_{A} \perp \mathbf{X}_{B} \mid \mathbf{X}_{C} \Rightarrow \mathbf{X}_{B} \perp \mathbf{X}_{A} \mid \mathbf{X}_{C}$$
  
•  $\mathbf{X}_{A} \perp \mathbf{X}_{B} \mid \mathbf{X}_{C}$  and  $\mathbf{U} = h(\mathbf{X}_{A}) \Rightarrow \mathbf{U} \perp \mathbf{X}_{B} \mid \mathbf{X}_{C}$   
•  $\mathbf{X}_{A} \perp \mathbf{X}_{B} \mid \mathbf{X}_{C}$  and  $\mathbf{U} = h(\mathbf{X}_{A}) \Rightarrow \mathbf{X}_{A} \perp \mathbf{X}_{B} \mid (\mathbf{X}_{C}, \mathbf{U})$   
•  $\mathbf{X}_{A} \perp \mathbf{X}_{B} \mid \mathbf{X}_{C}$  and  $\mathbf{X}_{A} \perp \mathbf{W} \mid (\mathbf{X}_{B}, \mathbf{X}_{C}) \Rightarrow \mathbf{X}_{A} \perp (\mathbf{W}, \mathbf{X}_{B}) \mid \mathbf{X}_{C}$ 

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Node neighborhood:

$$\mathcal{A}_i = \{j \neq i : (i,j) \in E\}$$

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**Markov-Like Properties** 

Local Markov property: for all *i*,

$$X_i \perp \mathbf{X}_{V \setminus \overline{\mathcal{A}}_i} \mid \mathbf{X}_{\mathcal{A}_i}, \quad ext{ with } \overline{\mathcal{A}}_i = \mathcal{A}_i \cup \{i\}$$

Global Markov property: let A, B, C, be disjoint subsets of V

if C separates A and B then  $\mathbf{X}_A \perp \mathbf{X}_B \mid \mathbf{X}_C$ 

Some important notes:

- If the distribution of **X** has a positive and continuous density (w.r.l.m.), then these Markov properties are equivalent.
- Moreover, in this case, both Markov properties hold when *E* is defined by the condition



Parametrization of the GGM

1) In terms of the conditional correlations:

$$E = \left\{ (j, l) \in V^2 : Corr\left(X_j, X_l | X_{V \setminus \{j, l\}}\right) \neq 0 \right\}$$

2) In terms of the entries of the precision matrix  $(\omega_{pq}) = \Omega = \Sigma^{-1}$ 

$$E = \left\{ (j, l) \in V^2 : \omega_{jl} \neq 0 \right\}$$

**Note:** it can be shown that  $Corr\left(X_j, X_l | X_{V \setminus \{j,l\}}\right) = 0 \iff \omega_{jl} = 0$  (see "Reading")

3) In terms of the Pearson correlation of the regression residuals

a) Let 
$$e_j = X_j - E\left(X_j | X_{V \setminus \{j,l\}}
ight)$$
 and  $e_l = X_l - E\left(X_l | X_{V \setminus \{j,l\}}
ight)$ 

b) Let  $\beta_{jl} = \textit{Corr}\left(\textit{e}_{j},\textit{e}_{l}
ight)$ 

$$E = \left\{ (j, l) \in V^2 : \beta_{jl} \neq 0 \right\}$$

**Note:** it can be shown that  $Corr\left(X_j, X_l | X_{V \setminus \{j,l\}}\right) = \beta_{jl}$  (see "Reading")

GLASSO proposed by Friedman, Hastie and Tibshirani (2008):

$$\widehat{\Omega} = \arg\min_{\Omega \succ 0} \left\{ tr\left(S\Omega\right) - \log \det\left(\Omega\right) + \lambda \sum_{i \neq j} |\omega_{ij}| \right\}$$

where

- S is the sample covariance matrix, and
- $\Omega = \Sigma^{-1}$  is the precision matrix See the package "glasso" in CRAN

#### Stepwise GGM

Set the entry threshold  $\overline{\beta}$  (a number between 0 and 1)

- Given a system of neighborhoods  $\left\{\mathcal{A}_{j}^{(k)}\right\}$  compute the regression residuals  $\mathbf{e}_{j}$  by regressing  $X_{j}$  on  $\mathbf{X}_{\mathcal{A}_{j}^{(k)}}$
- For each  $l \notin \mathcal{A}_{j}^{(k)}$  (and therefore  $j \notin \mathcal{A}_{j}^{(k)}$ ) compute the Pearson correlation

$$\widehat{eta}_{jl} = rac{\mathbf{e}_j' \mathbf{e}_l}{\sqrt{\mathbf{e}_j' \mathbf{e}_j} \sqrt{\mathbf{e}_l' \mathbf{e}_l}}$$

Let

$$\begin{split} \left|\widehat{\beta}_{j_0l_0}\right| &= \max_{l\notin\mathcal{A}_j^{(k)}, j\in V} \left|\widehat{\beta}_{jl}\right| \\ \bullet \ \mathsf{lf} \left|\widehat{\beta}_{j_0l_0}\right| \geq \overline{\beta}, \ \mathsf{set} \ \mathcal{A}_{j_0}^{(k+1)} = \mathcal{A}_{j_0}^{(k)} \cup \{l_0\}, \ \mathcal{A}_{l_0}^{(k+1)} = \mathcal{A}_{l_0}^{(k)} \cup \{j_0\}, \\ \mathcal{A}_j^{(k+1)} = \mathcal{A}_j^{(k)} \ \text{ for } j \neq j_0, \ l_0 \ \text{ and continue.} \end{split}$$

• If 
$$\left|\widehat{eta}_{j_0 l_0}
ight| < \overline{eta}$$
, stop

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