Faithfulness assumption in concentration and covariance graphical models

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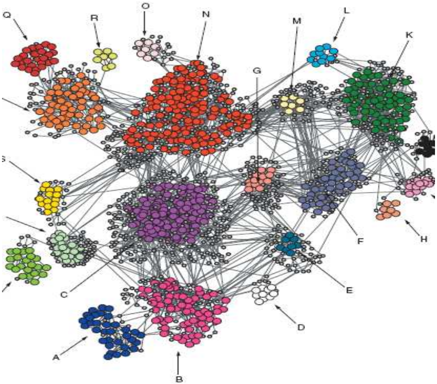
Motivation

yeast FOCI coexpression network. (Magwene et Kim *2004*[1])



1. P. Magwene and J. Kim. Estimating genomic coexpression networks using first-order conditional independence. *Genom Biol.*, 5(12), 2004.

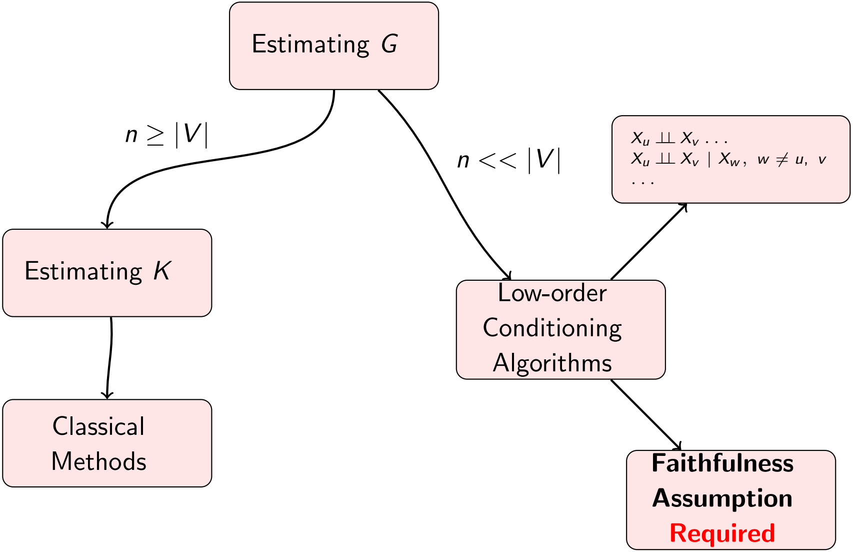
Motivation

- Estimating Gene Network Interaction (GNI) from Genomic Data ?
- GNI = Gaussian Concentration Graph.
  - $G = (V, E)$ undirected graph, V set of genes
  - $\mathbf{X}_V = (X_u, \in u \in V)' \sim \mathcal{N}(\mu = 0, K = \Sigma^{-1})$ where $X_u = X(g_u)$ expression level of g_u.

No interaction between

$$
\begin{aligned}
g_u \text{ and } g_v \quad &\Longleftrightarrow \quad u \not\sim_G v \\
&\Longleftrightarrow \quad X_u \perp\!\!\!\perp X_v \mid \mathbf{X}_{V \setminus \{u,v\}} \\
&\Longleftrightarrow \quad k_{uv} = 0
\end{aligned}
$$

Motivation



Estimating G
$n \geq |V|$
$n << |V|$
Estimating K
Classical Methods
Low-order Conditioning Algorithms
$X_u \perp\!\!\!\perp X_v \ldots$
$X_u \perp\!\!\!\perp X_v \mid X_w, \; w \neq u, \; v$
$\ldots$
Faithfulness Assumption Required

Outline

1. Graphical models
   - Preliminaries
   - Concentration graphical models
   - Covariance graphical models
2. Faithfulness assumption
   - Definition
   - Implications of faithful assumption
3. Faithfulness assumption for Gaussian tree models

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Undirected graphs

Definition

An undirected graph $G = (V, E)$ is a pair of sets V and $E \subseteq (V \times V) \setminus \{(u, u),\ u \in V\}$ such that

$$\forall\, (u, v) \in E \iff (v, u) \in E$$

- We write $u \sim_G v$ when $(u, v) \in E$ and we say that u and v are *adjacent* in G.
- A path connecting two distinct vertices u and v in G is a sequence $(u_0, u_1, \dots, u_n)$ where $u_0 = u$ and $u_n = v$ where $\forall\, i = 0, \dots, n-1,\ u_i \sim_G u_{i+1}$.
- We denote by $\mathcal{P}(u, v, G)$ the set of paths between u and v

Undirected graphs...*Separators*

- In a connected graph, a *separator* $S \subseteq V$ such that $\exists\ u \not\sim_G v$ such that $u, v \notin S$ and

$$\forall p \in \mathcal{P}(u, v, G), \quad p \cap S \neq \emptyset$$

- An $\emptyset$ separates u and v iff there is no path between u and v, i.e., they belong to different connected components.
- (A, B, S) a triplet of disjoint subset of V, S separates A and B in G iff S separates any $(u, v) \in A \times B$.
- A *separation statement*, (A, B, S) is a triplet of pairwise disjoint subsets. S separates A and B in G iff S is a separator of any pair of vertices $(u, v) \in A \times B$.

Graphical Models

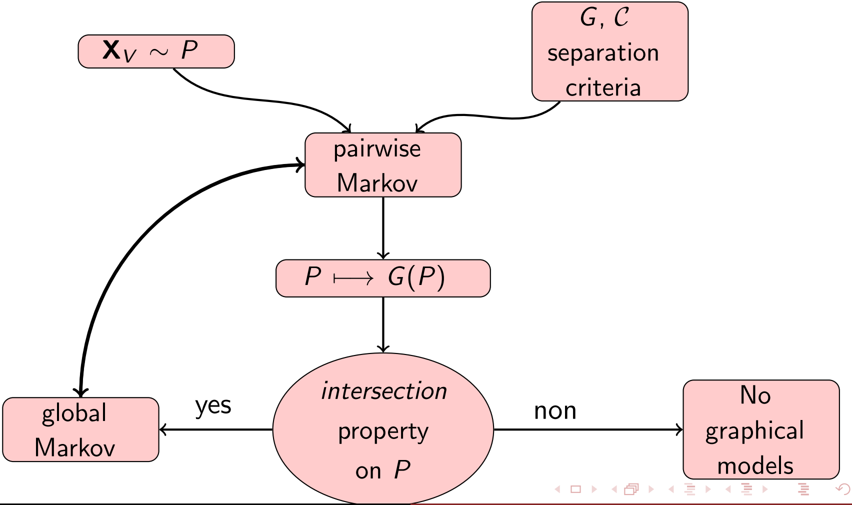
- V is a finite set
- $\mathbf{X} = (X_v, v \in V)'$ is a random vector with probability distribution P.
- $G = (V, E)$ is a graph where $E \subseteq V \times V$.

Definition

We say that P is Markov to G if

$$\left(\begin{array}{l} \text{A } \textit{separation} \\ \text{statement read on } G \end{array} \right) \Rightarrow \left(\begin{array}{l} \text{Conditional independence} \\ \text{statement read on } P \end{array} \right)$$

Basic Concept



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Concentration graphical models

$\mathbf{X} = (X_v, v \in V)' \sim P$ and $G = (V, E)$ an undirected graph.

Definition

G is the concentration graph associated with P iff

$$u \not\sim_G v \iff X_u \perp\!\!\!\perp X_v \mid \mathbf{X}_{V \setminus \{u,v\}}$$

where $\mathbf{X}_{V\setminus\{u,v\}} := (X_w,\ w \neq u \text{ and } w \neq v)'$.

Question :

Can we read additional conditional independence statements in the graph G ?

Concentration intersection property

Theorem (Lauritzen *1996*)

Assume that

i. *G is the concentration graph associated with P.*

ii. *P satisfies the concentration intersection property, i.e., $\forall$ A, B and $C \subseteq V$ and pairwise disjoints*

$$\mathbf{X}_A \perp\!\!\!\perp \mathbf{X}_B \mid \mathbf{X}_{C\cup D} \ \text{ and } \ \mathbf{X}_A \perp\!\!\!\perp \mathbf{X}_C \mid \mathbf{X}_{B\cup D} \ \Rightarrow \ \mathbf{X}_A \perp\!\!\!\perp \mathbf{X}_{B\cup C} \mid \mathbf{X}_D. \tag{1}$$

Then P is concentration global Markov to G, i.e., $\forall(A, B, S)$,

$$\text{if } S \text{ separates } A \text{ and } B \text{ in } G \Rightarrow \mathbf{X}_A \perp\!\!\!\perp \mathbf{X}_B \mid \mathbf{X}_S. \tag{2}$$

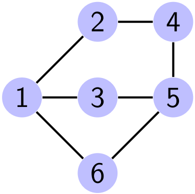
Example :

As $\{2, 5\}$ separates $\{1\}$ and $\{4\}$ then

$$X_1 \perp\!\!\!\perp X_4 \mid (X_2,\ X_5).$$

As $\{2, 3, 6\}$ separates $\{4, 5\}$ and $\{1\}$ then

$$X_1 \perp\!\!\!\perp (X_4, X_5) \mid (X_2, X_3, X_6).$$



Covariance graphical models

$\mathbf{X} = (X_v, v \in V)' \sim P$ and $G_0 = (V, E_0)$ an undirected graph.

Definition

G_0 is the covariance graph associated with P iff

$$u \not\sim_{G_0} v \iff X_u \perp\!\!\!\perp X_v$$

where $\mathbf{X}_{V\setminus\{u,v\}} := (X_w,\ w \neq u \text{ and } w \neq v)'$.

Question :

Can we read additional conditional independence statements in the graph G_0 ?

Covariance intersection property

Theorem (Kauermann *1996*)

Assume that

i. G_0 *is the covariance graph associated with* P.

ii. P *satisfies the covariance intersection property, i.e.,* $\forall\ A, B, C \subseteq V$ *and pairwise disjoints*

$$\mathbf{X}_A \perp\!\!\!\perp \mathbf{X}_B \ \text{ and } \ \mathbf{X}_A \perp\!\!\!\perp \mathbf{X}_C \ \Rightarrow \ \mathbf{X}_A \perp\!\!\!\perp \mathbf{X}_{B \cup C}. \tag{3}$$

Then P *is covariance global Markov to* G_0*, i.e.,* $\forall (A, B, S)$,

$$\text{if } V \setminus (S \cup A \cup B) \text{ separates } A \text{ and } B \text{ in } G_0 \Rightarrow \mathbf{X}_A \perp\!\!\!\perp \mathbf{X}_B \mid \mathbf{X}_S.$$

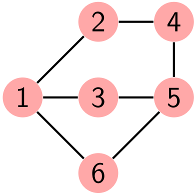
Example :

As $\{2,5\} = V \setminus (\{3,6\} \cup \{1\} \cup \{4\})$ separates $\{1\}$ and $\{4\}$ then

$$X_1 \perp\!\!\!\perp X_4 \mid (X_3,\ X_6).$$

As $\{2,3,6\} = V \setminus (\emptyset \cup \{1\} \cup \{4,5\})$ separates $\{4,5\}$ and $\{1\}$ then

$$X_1 \perp\!\!\!\perp (X_4, X_5).$$



Faithfulness assumption

Definition

We say that P is faithful to G if

$$\left(\begin{array}{l} \text{A } \textit{separation} \\ \text{statement read on } G \end{array}\right) \Longleftrightarrow \left(\begin{array}{l} \text{Conditional independence} \\ \text{statement read on } P \end{array}\right)$$

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Assume that G is the concentration graph and G_0 is the covariance graph associated with P.

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Assume that G is the concentration graph and G_0 is the covariance graph associated with P.

- P is concentration faithful to G if $\forall\,(A, B, S)$

$$S \text{ separates } A \text{ and } B \text{ in } G \iff \mathbf{X}_A \perp\!\!\!\perp \mathbf{X}_B \mid \mathbf{X}_S .$$

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- P is concentration faithful to G if $\forall\,(A, B, S)$

$$S \text{ separates } A \text{ and } B \text{ in } G \iff \mathbf{X}_A \perp\!\!\!\perp \mathbf{X}_B \mid \mathbf{X}_S.$$

- P is covariance faithful to G_0 if $\forall\,(A, B, S)$

$$S \text{ separates } A \text{ and } B \text{ in } G_0 \iff \mathbf{X}_A \perp\!\!\!\perp \mathbf{X}_B \mid \mathbf{X}_{V\setminus(A\cup B\cup S)}.$$

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Implication of concentration faithful assumption

Theorem (Malouche and Rajaratnam *2010a*)

- $\mathbf{X}_V = (X_v, v \in V)' \sim P$
- *Assume that P satisfies the concentration and the covariance intersection properties ((1) and (3)).*
- *Assume that P has a positive density.*
- $G = (V, E)$ *and* $G_0 = (V, E_0)$ *denote respectively the concentration and the covariance graph associated with* P.

If P is concentration faithful to G, then

i. *all the connected components of G_0 are complete.*

ii. *G and G_0 have the same connected components.*

The proof : the concentration graph case...

- if G is connected,

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$$\begin{aligned} u \not\sim_{G_0} v \quad &\Longleftrightarrow \quad X_u \perp\!\!\!\perp X_v \\ &\Longleftrightarrow \quad \emptyset \text{ separates } u \text{ and } v \text{ in } G \\ &\qquad\ \ \textit{faithful assumption} : \ \text{impossible} \end{aligned}$$

The proof : the concentration graph case...

- if G is connected,

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- if G is not connected, we have to prove : if G_A is a connected component of G then $G_A = G(P_A)$ where $\mathbf{X}_A = (X_u,\ u \in A)' \sim P_A$.

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- if G is not connected, we have to prove : if G_A is a connected component of G then $G_A = G(P_A)$ where $\mathbf{X}_A = (X_u,\, u \in A)' \sim P_A$.

  Equivalently

$$X_u \perp\!\!\!\perp X_v \mid \mathbf{X}_{V\setminus\{u,v\}} \Longleftrightarrow X_u \perp\!\!\!\perp X_v \mid \mathbf{X}_{A\setminus\{u,v\}}$$

Implication of covariance faithful assumption

Theorem (Malouche and Rajaratnam *2010a*)

- $\mathbf{X}_V = (X_v,\, v \in V)' \sim P$
- *Assume that P satisfies the concentration and the covariance intersection properties ((1) and (3)).*
- *$G = (V, E)$ and $G_0 = (V, E_0)$ denote respectively the concentration and the covariance graph associated with P.*

If P is covariance faithful to G_0, then

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- if G_0 is not connected. W.l.o.g assume that G_0 have two connected components $(G_0)_A$ and $(G_0)_B$, where $A \cup B = V$ and $A \cap B = \emptyset$.

Claim 1 $u \sim_G v \iff u, v \in A$ or $u, v \in B$

The proof : the covariance graph case...

- if G_0 is connected,

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Claim 1 $u \sim_G v \iff u, v \in A$ or $u, v \in B$

Claim 2 A and B generate also two connected components in G.

Gaussian graphical Models

- $\mathbf{X} = (X_v,\ v \in V)' \sim P = \mathcal{N}_{|V|}(\mu, K = \Sigma^{-1})$, with density

$$f(\mathbf{x}) = \frac{1}{(2\pi)^{|V|/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\mu)'\Sigma^{-1}(\mathbf{x}-\mu)'\right),$$

  $K = (k_{uv})$ precision matrix and $\Sigma = (\sigma_{uv})$ Gaussian distribution.

- P satisfies concentration and covariance intersection properties ((1) and (3)).

- Concentration graph : $G = (V, E)$

$$u \not\sim_G v \iff k_{uv} = 0.$$

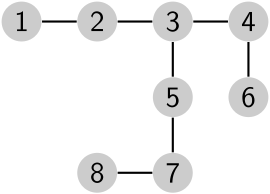
- Covariance graph associated with P : $G_0 = (V, E_0)$ defined by

$$u \not\sim_{G_0} v \iff \sigma_{uv} = 0.$$

Undirected graphs... *Trees*

Definition

A graph G is called a *tree* if any pair of vertices (u, v) in G are connected by exactly one path, i.e., $|\mathcal{P}(u, v, G)| = 1 \ \forall \ u, v \in V$.



Lemma

If G is a tree, any subgraph of G induced by a subset of V is a union of connected components, each of which are trees.

Concentration faithful Trees

Theorem (Becker, Geiger and Meek *2005*)

Assume that

i. *P is a Gaussian distribution*
ii. *G is the concentration graph associated with P.*

If G is a tree then P is concentration faithful to G.

Covariance faithful Trees

Theorem (Malouche and Rajaratnam *2010b*)

Assume that

i. *P is a Gaussian distribution*

ii. *G_0 is the covariance graph associated with P.*

If G_0 is a tree then P is covariance faithful to G_0.

Computing inverse matrices using graphs

Lemma (Brualdi and Cvetkovic *2008*, Jones and West *2005*)

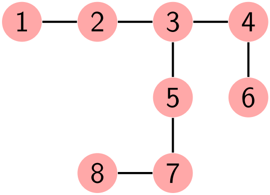
Let $K = (k_{uv})$ and $\Sigma = (\sigma_{uv})$ be $d \times d$ matrices and let $G_0 = (V, E_0)$ be an undirected graph :

$$u \not\sim_{G_0} v \iff \sigma_{uv} = 0.$$

If $K = \Sigma^{-1}$, then $\forall (u, v) \in V \times V$

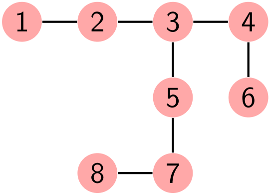
$$k_{uv} = \sum_{\substack{p \in \mathcal{P}(u,v,G_0) \\ p = (u_0, \ldots, u_n)}} (-1)^{|p|+1} \sigma_{u_0 u_1} \sigma_{u_1 u_2} \ldots \sigma_{u_{n-1} u_n} \frac{|\Sigma \setminus p|}{|\Sigma|}$$

Example



- G_0 covariance graph of $\mathbf{X} = (X_1, \ldots, X_8)'$
- $S = \{4, 6\}$ does not separate $A = \{1, 2\}$, $B = \{5\}$.
- $V \setminus (A \cup B \cup S) = \{3, 8, 7\}$
- Question : $\mathbf{X}_{\{1,2\}} \perp\!\!\!\perp X_{\{5\}} \mid \mathbf{X}_{\{3,8,7\}}$?

Example



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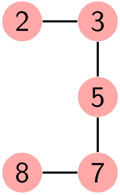

$(G_0)_{\{2,5,3,7,8\}}$ covariance graph of $\mathbf{X}_{\{2,5,3,7,8\}}$

$$k_{25|387} = (-1)^{2+1} \sigma_{23}\, \sigma_{35} \frac{|\Sigma(\{8,7\})|}{|\Sigma(\{2,5,3,8,7\})|} \neq 0$$

$$X_2 \not\!\perp\!\!\!\perp X_5 \mid \mathbf{X}_{\{3,8,7\}} \Rightarrow \mathbf{X}_{\{1,2\}} \not\!\perp\!\!\!\perp X_{\{5\}} \mid \mathbf{X}_{\{3,8,7\}}$$

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