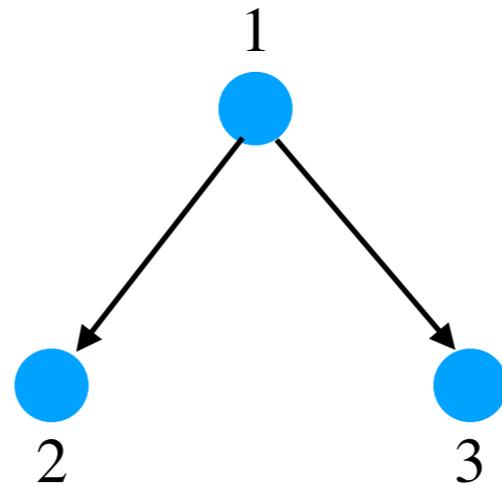


# Graphical Models

Sullivant – Algebraic Statistics – Ch. 13

# Roadmap



	Directed	Undirected
Multivariate Gaussian	?	?
Discrete	?	?

**Graph + random variable  
indexed by the nodes**

**Implicit conditions**

$$X_2 \perp\!\!\!\perp X_3 | X_1$$

**Explicit parametrization**

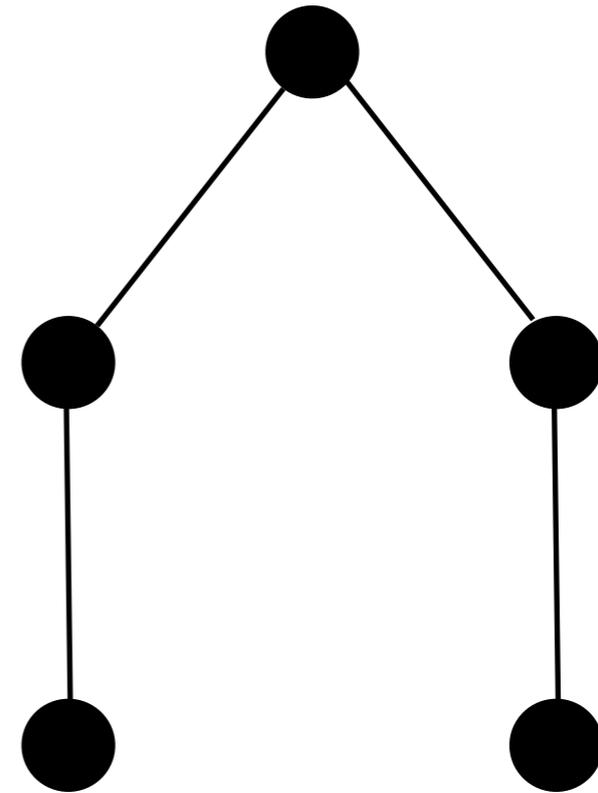
$$p(x) = p(x_1)p(x_2|x_1)p(x_3|x_1)$$

# Undirected Graphs

Notation:  $G = (V, E)$ ,  $V =$  vertices,  
 $E =$  edges.

$N(v) =$  neighbors of  $v$ .

$X$ : random vector indexed by  $V$ .



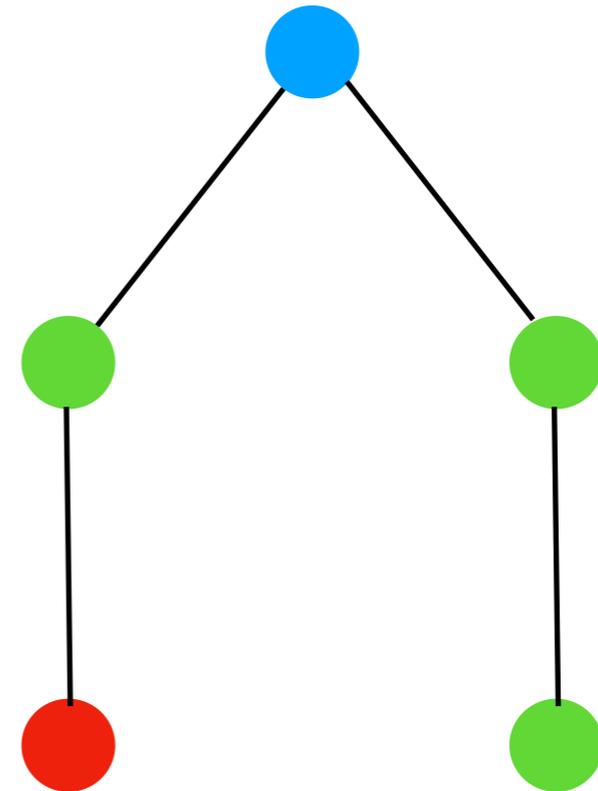
# Markov Properties

Pairwise Markov property:

$$X_u \perp\!\!\!\perp X_v \mid X_{V \setminus \{u,v\}}$$

for all

$$\{u, v\} \notin E$$



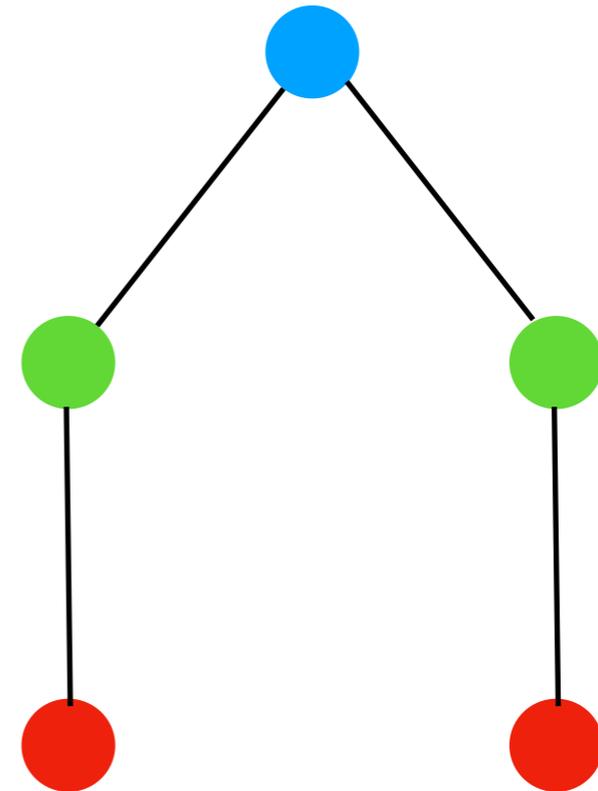
# Markov Properties

Local Markov property

$$X_v \perp\!\!\!\perp X_{V \setminus (N(v) \cup v)} \mid X_{N(v)}$$

for all

$$v \in V$$

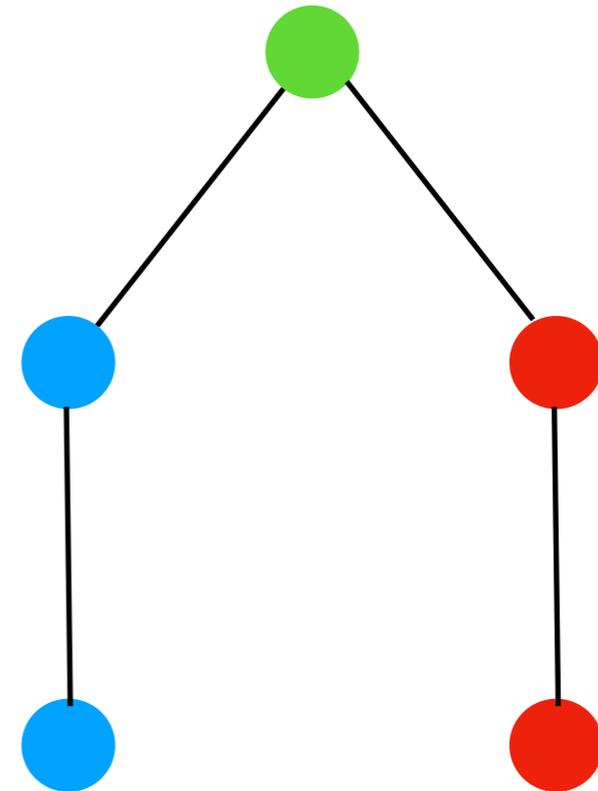


# Markov Properties

Global Markov property

$$X_A \perp\!\!\!\perp X_B \mid X_C$$

for all disjoint  $A, B, C$  such that  $C$   
separates  $A$  and  $B$



# Theorem 13.1.4

Intersection axiom  $\Rightarrow$  the Markov properties are equivalent.

In part.: if

$$P_X(x) > 0$$

for all  $x$ , then the Markov properties are equivalent for all  $G$ .

# Example: Multivariate Gaussian

$X$ : multivariate Gaussian with nonsingular covariance matrix  $\Sigma$

Satisfies the intersection axiom

# Example: Multivariate Gaussian

$$\begin{aligned} X_u \perp\!\!\!\perp X_v \mid X_{V \setminus \{u,v\}} &\Leftrightarrow \det \Sigma_{V \setminus u, V \setminus v} = 0 \\ &\Leftrightarrow \Sigma_{u,v}^{-1} = 0 \end{aligned}$$

# Example: Multivariate Gaussian

$A, B, C$  disjoint subsets of  $V$  such that  $C$  does *not* separate  $A$  and  $B$

$\Rightarrow$  there exists  $\Sigma$  such that  $X$  satisfies all global Markov statements but

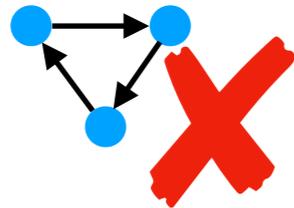
$$X_A \not\perp X_B \mid X_C$$

Path not sep. by  $C$

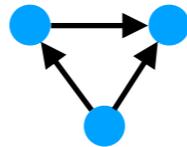
$$\Sigma^{-1} = \left( \begin{array}{c|c} \begin{array}{cccc} 1 & \varepsilon & & \\ \varepsilon & 1 & \ddots & \\ & \ddots & \ddots & \varepsilon \\ & & \varepsilon & 1 \end{array} & \\ \hline & \begin{array}{ccc} 1 & & \\ & \ddots & \\ & & 1 \end{array} \end{array} \right)$$

Rest of the graph

# Directed Acyclic Graphs



Directed cycle



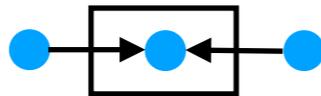
Undirected cycle



Undirected path

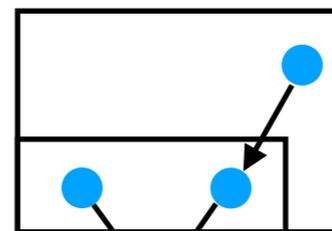


Directed path

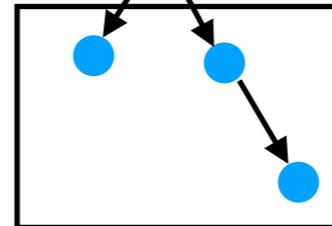


Collider

Parents of  $v$ :  $pa(v)$



Descendants of  $v$



Ancestors of  $v$ :  $an(v)$

Nondescendants of  $v$ :  $nd(v)$



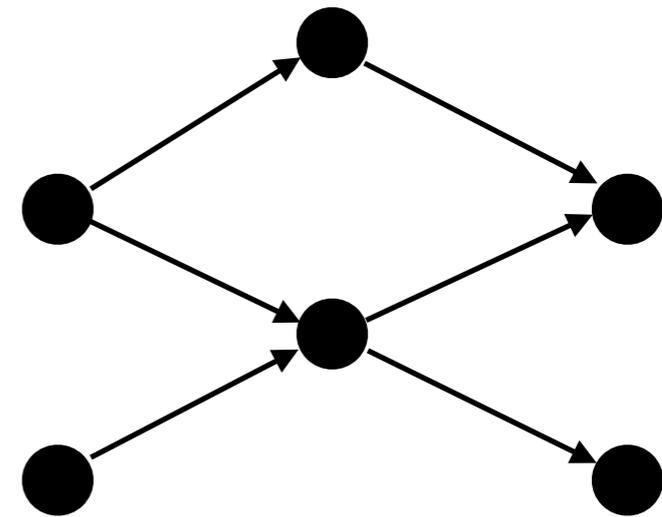
# d-separation

$C \subset V$ , d-separates  $v, w \in V$ :

for all undirected paths  $\pi$  between  $v$   
and  $w$ , in induced subgraph of  $\pi$   
there exists

a collider in  $C \cup \text{an}(C)$ ,

**or** a non-collider in  $C$ ,



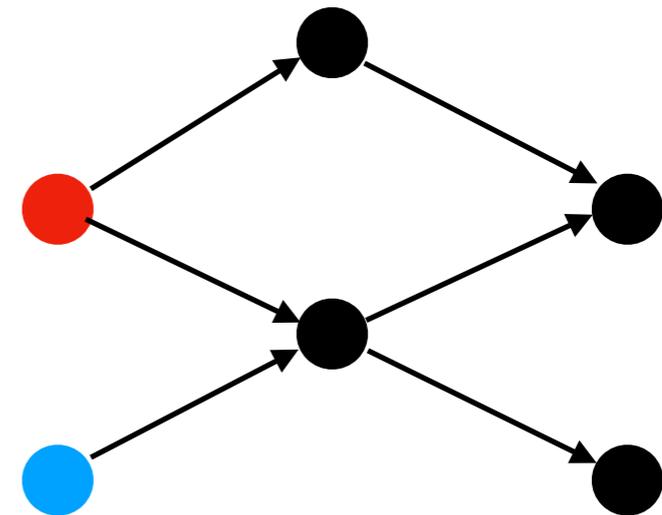
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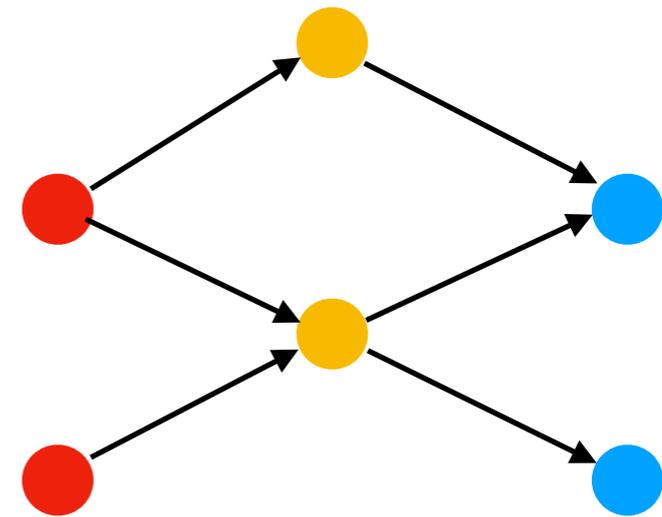
**or** a non-collider in  $C$ ,



# d-separation

$C \subset V$  d-separates  $A, B \subset V$ :

$C$  d-separates all pairs  $a \in A, b \in B$



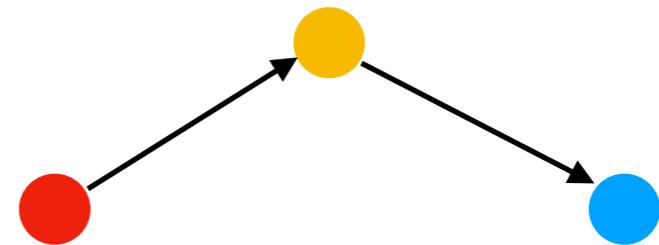
# d-separation

$C \subset V$ , d-separates  $v, w \in V$ :

for all undirected paths  $\pi$  between  $v$   
and  $w$ , in induced subgraph of  $\pi$   
there exists

a collider in  $C \cup \text{an}(C)$ ,

**or** a non-collider in  $C$ ,



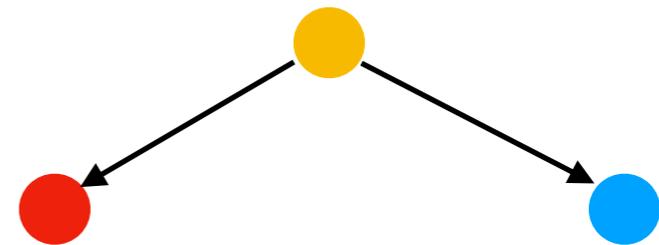
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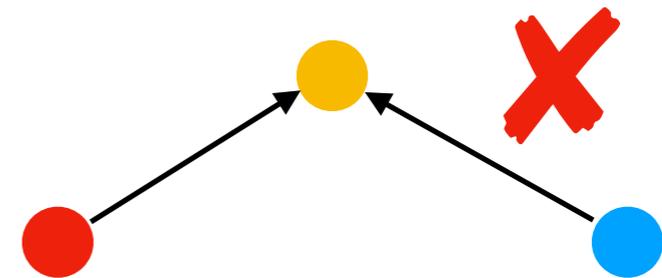
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there exists

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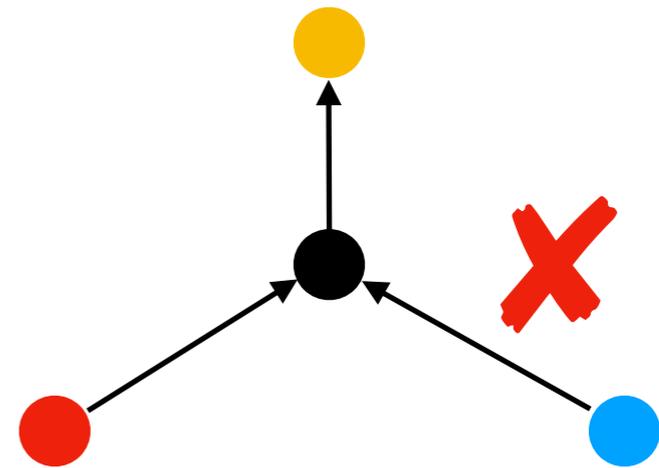
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**or** a non-collider in  $C$ ,



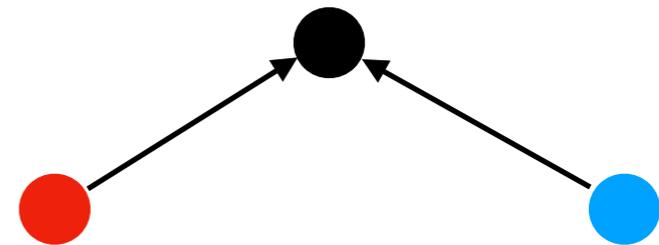
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for all undirected paths  $\pi$  between  $v$   
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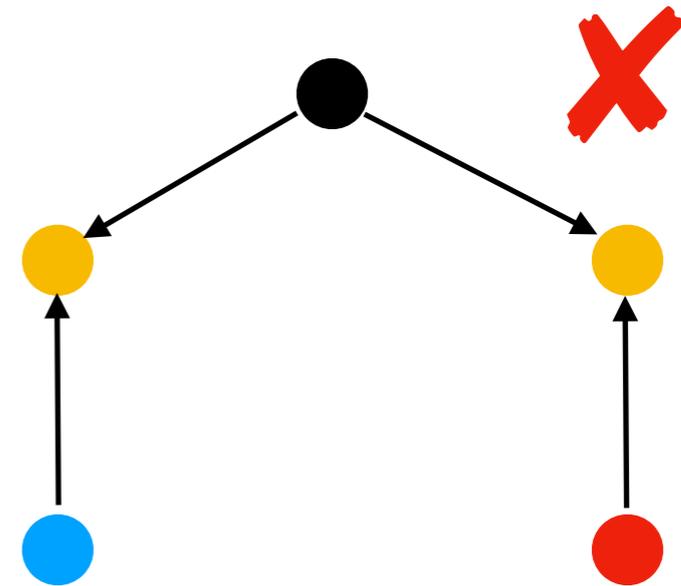
# d-separation

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for all undirected paths  $\pi$  between  $v$   
and  $w$ , in induced subgraph of  $\pi$   
there exists

a collider in  $C \cup \text{an}(C)$ ,

**or** a non-collider in  $C$ ,



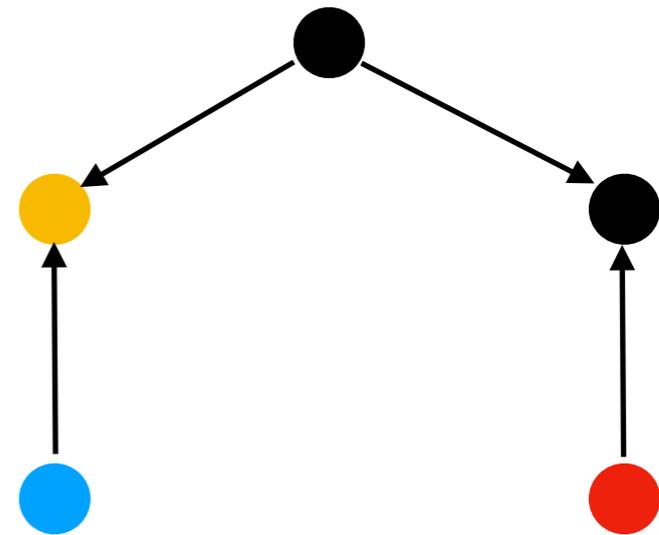
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for all undirected paths  $\pi$  between  $v$   
and  $w$ , in induced subgraph of  $\pi$   
there exists

a collider in  $C \cup \text{an}(C)$ ,

**or** a non-collider in  $C$ ,

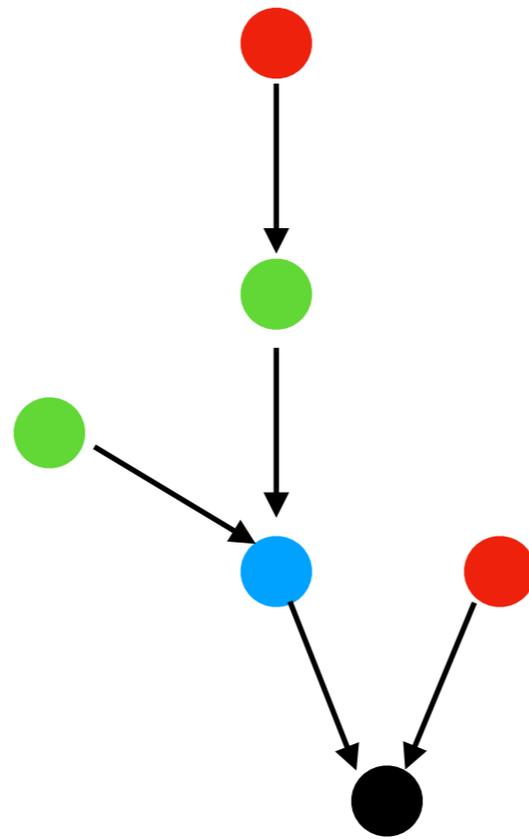


# Markov Properties

**Definition 13.1.9.** Let  $G = (V, E)$  be a directed acyclic graph.

- (i) The *directed pairwise Markov property* associated to  $G$  consists of all conditional independence statements  $X_u \perp\!\!\!\perp X_v \mid X_{\text{nd}(u) \setminus \{v\}}$  where  $(u, v)$  is not an edge of  $G$ .
- (ii) The *directed local Markov property* associated to  $G$  consists of all conditional independence statements  $X_v \perp\!\!\!\perp X_{\text{nd}(v) \setminus \text{pa}(v)} \mid X_{\text{pa}(v)}$  for all  $v \in V$ .
- (iii) The *directed global Markov property* associated to  $G$  consists of all conditional independence statements  $X_A \perp\!\!\!\perp X_B \mid X_C$  for all disjoint sets  $A$ ,  $B$ , and  $C$  such that  $C$  d-separates  $A$  and  $B$  in  $G$ .

# Local Markov property



# Parametrized undirected graphical model

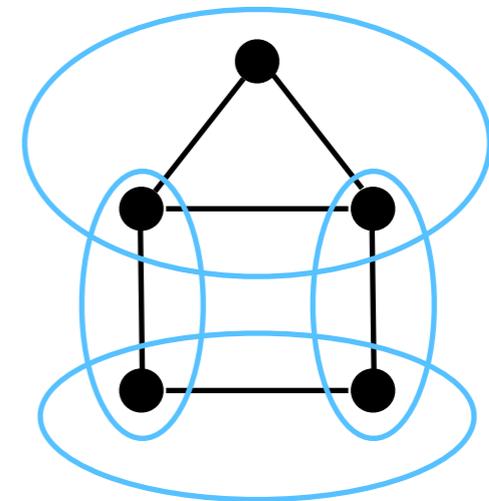
**Density function:**

$$f(x) = \frac{1}{Z} \prod_{C \in \mathcal{C}(G)} \phi_C(x_C) \quad \text{"Factorizes according to } G\text{"}$$

$\mathcal{C}(G)$ : set of all maximal cliques

$\phi_C: X_C \rightarrow \mathbb{R}_{>0}$  potential functions

$Z$ : normalizing constant



$$f(x_1, x_2, x_3, x_4, x_5) = \frac{1}{Z} \phi_{123}(x_1, x_2, x_3) \phi_{25}(x_2, x_5) \phi_{34}(x_3, x_4) \phi_{45}(x_4, x_5).$$

**Theorem 13.2.3** (Hammersley–Clifford). A continuous positive probability density  $f$  on  $\mathcal{X}$  satisfies the pairwise Markov property on the graph  $G$  if and only if it factorizes according to  $G$ .

**Proof.**  $\Leftarrow$ : let  $f = \frac{1}{Z} \prod_C \phi_C$  and let  $i, j \in V$  not connected by an edge.

$$\text{Then } f(x_i, x_j, x_R) = \frac{1}{Z} (\prod_{i \in C} \phi_C) (\prod_{j \in C} \phi_C) (\prod_{i, j \notin C} \phi_C)$$

Hence for all  $x_i, y_i, x_j, y_j, x_R$ :  $f(x_i, x_j, x_R) f(y_i, y_j, x_R) = f(x_i, y_j, x_R) f(y_i, x_j, x_R)$

$$\text{Average over the } y_i, y_j: \text{ get } \frac{f(x_i, x_j, x_R)}{f(x_i, x_R)} = \frac{f(x_j, x_R)}{f(x_R)}$$

$\Rightarrow$ : Let  $f$  satisfy the pairwise Markov property w.r.t.  $G$ , Let  $y \in \mathcal{X}$  arbitrary.

$$C \subset V \rightsquigarrow \phi_C(x_C) := \prod_{S \subseteq C} f(x_S, y_{V \setminus S})^{(-1)^{|C| - |S|}}$$

Möbius inversion on the power set of  $V$  gives

$$f(x) = \prod_{C \subseteq V} \phi_C(x_C)^{\mu(V, C)}$$

It suffices to show:  $\phi_C \equiv 1$  if  $C$  is not a clique

For this, choose  $i, j \in C$  not connected by an edge, write down  $\phi_C$ , and use the Markov property of  $i$  and  $j$ .

# Corollary

Let  $P$  be a distribution that factors according to  $G$ . Then  $P$  satisfies the global Markov property on  $G$ .

*Proof:* the global Markov property is a closed condition and the statement is correct when  $P$  has positive density.

# Parametric directed graphical model

All densities  $f$  with  $f(x) = \prod_{j \in V} f(x_j | x_{\text{pa}(j)})$

"Recursive Factorization Property"

Idea: we always have  $f(x) = f(x_1)f(x_2|x_1)f(x_3|x_1, x_2) \cdots f(x_n|x_1, \dots, x_{n-1})$

Here, the ordering of the vertices respects parenthood.

But the graph says that the information from the parents suffices.

**Theorem 13.2.10** (Recursive Factorization). *A probability density satisfies the recursive factorization property (13.2.2) associated to the directed acyclic graph  $G$  if and only if it satisfies the directed local Markov property associated to  $G$ .*

**Proof.** ( $\Rightarrow$ ) Let  $f$  factorize. Then it satisfies the *global* Markov property

Indeed, let  $C$  d-separate  $A, B$ , W.l.o.g.  $V = \text{an}(A \cup B \cup C)$

Then  $C$  separates  $A$  and  $B$  in the *moralization*  $G^{\text{mor}}$  of  $G$



Moralization makes  $\{j\} \cup \text{pa}(j)$  into a clique, hence  $f$  factorizes according to  $G^{\text{mor}}$

By the Corollary,  $X_A \perp\!\!\!\perp X_B | X_C$

( $\Leftarrow$ ) carry out the Idea  $f(x) = f(x_1)f(x_2|x_1) \cdots f(x_n|x_1, \dots, x_n)$

# Theorem

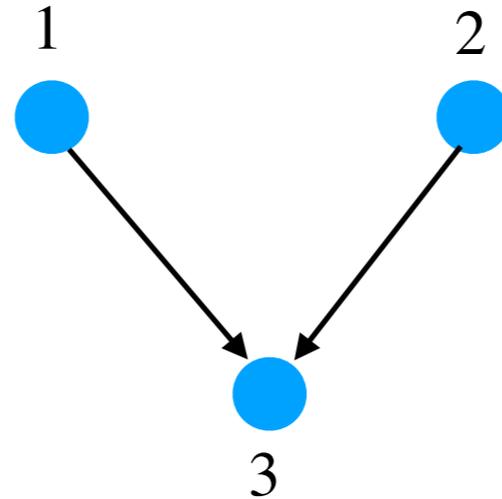
For any random variable  $X$ , directed graph  $G$ :

Local directed Markov w.r.t.  $G \Rightarrow$  Global directed Markov w.r.t.  $G$



Recursive factorization property w.r.t.  $G$

# Example: discrete case



$$X_i \in \{0, 1\}$$

$$f(x_1, x_2, x_3) = f(x_1)f(x_2)f(x_3|x_1, x_2)$$

$$\begin{array}{ll} p_{0,0,0} = \theta_0^{(1)} \theta_0^{(2)} \theta_{0|0,0}^{(3)} & p_{1,0,0} = \theta_1^{(1)} \theta_0^{(2)} \theta_{0|1,0}^{(3)} \\ p_{0,0,1} = \theta_0^{(1)} \theta_0^{(2)} \theta_{1|0,0}^{(3)} & p_{1,0,1} = \theta_1^{(1)} \theta_0^{(2)} \theta_{1|1,0}^{(3)} \\ p_{0,1,0} = \theta_0^{(1)} \theta_1^{(2)} \theta_{0|0,1}^{(3)} & p_{1,1,0} = \theta_1^{(1)} \theta_1^{(2)} \theta_{0|1,1}^{(3)} \\ p_{0,1,1} = \theta_0^{(1)} \theta_1^{(2)} \theta_{1|0,1}^{(3)} & p_{1,1,1} = \theta_1^{(1)} \theta_1^{(2)} \theta_{1|1,1}^{(3)} \end{array}$$

$$\Delta_1 \times \Delta_1 \times \Delta_1^4 \rightarrow \Delta_7$$

# Multivariate Gaussian case

$X$  multivariate Gaussian  $\Rightarrow X_i$  univariate Gaussian

$X_j | X_{\text{pa}(j)}$  multivariate Gaussian

$$f(x) = \prod_j f(x_j | x_{\text{pa}(j)}) \Rightarrow X_i = \sum_{j \in \text{pa}(i)} \lambda_{i,j} X_j + \varepsilon_i$$

Where  $\varepsilon_i \sim \mathcal{N}(\nu_i, \omega_i)$

We have  $X = (\text{Id} - \Lambda)^{-T} \varepsilon$

Where  $\Lambda_{i,j} = \lambda_{i,j}$  if  $(i, j) \in E$ , 0 else.

$$\Rightarrow \Sigma = (\text{Id} - \Lambda)^{-T} \Omega (\text{Id} - \Lambda)^{-1}$$

With  $\Omega = \text{diag}(\omega_1, \dots, \omega_n)$

**Proposition 13.2.12.** *The parametrized Gaussian graphical model associated to the directed acyclic graph  $G$  consists of all pairs  $(\mu, \Sigma) \in \mathbb{R}^m \times PD_m$  such that  $\Sigma = (Id - \Lambda)^{-T} \Omega (Id - \Lambda)^{-1}$  for some  $\Omega$  diagonal with positive entries and upper triangular  $\Lambda \in \mathbb{R}^E$ .*

$$\mathcal{M}_{\text{paramGaussian}} = \text{image of } (\Lambda, \Omega) \mapsto \Sigma$$

Ideal of the closure:  $I_G$

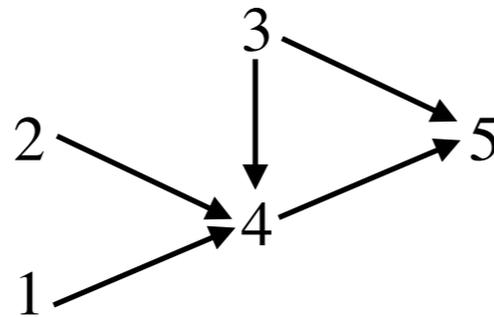
Ideal  $I_{\text{glob}}$  of conditional independent statements for  $X \sim \mathcal{N}(\mu, \Sigma)$ :

$$\text{Ideal } I_{\text{glob}} = \sum_{A \perp_d B|C} I_{A \perp B|C}$$

$$I_{A \perp B|C} = \langle (|C| + 1)\text{-minors of } \Sigma_{A \cup C, B \cup C} \rangle$$

Question: when does  $I_{\text{glob}} = I_G$ ?

# Example



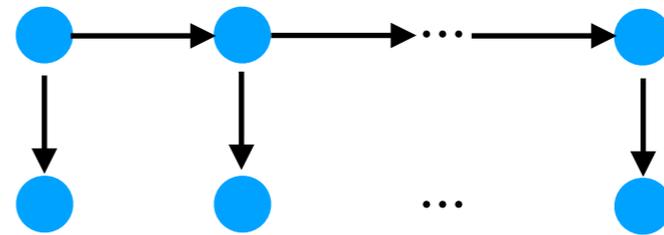
$$\det(\Sigma_{12,45}) \in I_G \setminus I_{\text{glob}}$$

$$I_G = I_{\text{glob}} + \langle \det(\Sigma_{12,45}) \rangle$$

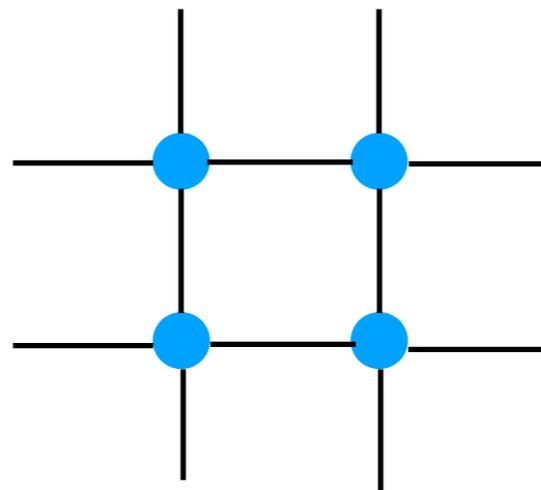
# Examples of graphical models



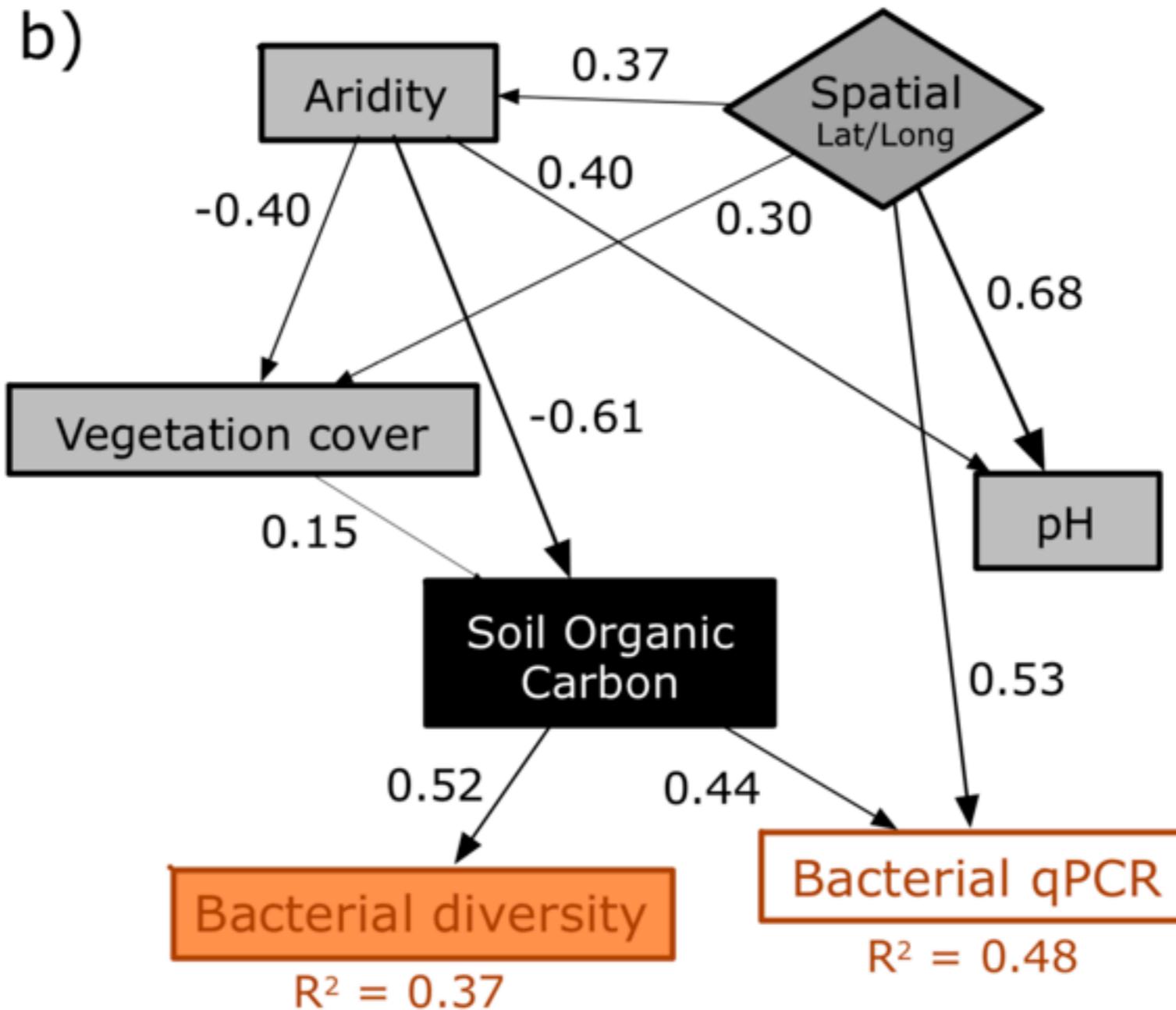
Markov chain



Hidden Markov model



Ising model



(Guerra, Eisenhauer, Pereira: *Synthesising Soil Ecosystem Multifunctionality*)

**Talk to Eliana or me about this!**