Fundamentals of Probabilistic Data Mining Chapter II - Probabilistic Graphical Models

Xavier Alameda-Pineda

Ensimag/Inria

Table of Today's Contents

Conditional Dependency

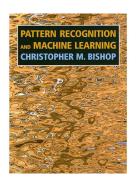
2 D-separation: beyond 3 variables

Markovian dependencies

References

There is a lot of bibliography on probabilistic graphical models.

I strongly suggest the following book:



Pattern Recognition and Machine Learning, from Christopher M. Bishop (Springer)

The concepts discussed in FPDM correspond to different parts of Ch. 2, 8, 9, 10, 12, 13.

Conditional Dependency

Conditional Independence: reminder

Definition

Let X, Y, and Z be random variables, we say that X and Y are **conditionally independent** given Z, and write $X \perp\!\!\!\perp Y \mid Z$, iff one of the following equivalent expressions holds:

- p(x, y|z) = p(x|z)p(y|z)

Proof of the equivalence: Any questions?

Conditional Independence: reminder (2)



Two-kids
$$p(x, y, z) = p(z|x)p(y|x)p(x)$$
:

$$p(y,z|x) = p(y|x)p(z|x)$$
 and $p(y,z) \neq p(y)p(z)$.

Conditional Independence: reminder (2)



Two-kids p(x, y, z) = p(z|x)p(y|x)p(x):

$$p(y,z|x) = p(y|x)p(z|x)$$
 and $p(y,z) \neq p(y)p(z)$.



Two-parents p(x, y, z) = p(z|x, y)p(y)p(x):

$$p(x,y|z) \neq p(x|z)p(y|z)$$
 and $p(x,y) = p(x)p(y)$.

Conditional Independence: reminder (2)



Two-kids p(x, y, z) = p(z|x)p(y|x)p(x):

$$p(y,z|x) = p(y|x)p(z|x)$$
 and $p(y,z) \neq p(y)p(z)$.



Two-parents p(x, y, z) = p(z|x, y)p(y)p(x):

$$p(x,y|z) \neq p(x|z)p(y|z)$$
 and $p(x,y) = p(x)p(y)$.

Never forget that...

"Independence" and "Conditional Independence" are **two different** things.

Conditional Independence: 3 Gaussian variables

Let X, Y and Z three random variables following:

Conditional Independence: 3 Gaussian variables

Let X, Y and Z three random variables following:

Then, the joint probability p(x, y, z) is a **multivariate Gaussian**:

$$p(x,y,z) = \frac{1}{\sqrt{|2\pi\Sigma|}} \exp\Big(-\frac{1}{2}(v-\mu)^{\top}\Sigma^{-1}(v-\mu)\Big),$$

where $v = (x, y, z)^{\top}$ is the joint vector and Σ and μ are the so-called **covariance matrix** and **mean vector**.

(\rightarrow check Bishop's book, section 2.3 until 2.3.4).

Homework: (i) prove that you obtain such a Gaussian, (ii) compute μ .

Conditional Independence: 3 Gaussian variables (II)

 Σ in the previous equation takes the following form:

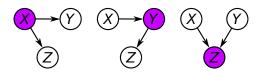
$$\Sigma^{-1} = \begin{pmatrix} \frac{1}{\nu_x} + \frac{p^2}{\nu_y} + \frac{c^2}{\nu_z} & \frac{p}{\nu_y} & \frac{c}{\nu_z} \\ \frac{p}{\nu_y} & \frac{1}{\nu_y} + \frac{k^2}{\nu_z} & \frac{k}{\nu_z} \\ \frac{c}{\nu_z} & \frac{k}{\nu_z} & \frac{1}{\nu_z} \end{pmatrix}$$

Conditional Independence: 3 Gaussian variables (II)

 Σ in the previous equation takes the following form:

$$\Sigma^{-1} = \begin{pmatrix} \frac{1}{\nu_x} + \frac{\rho^2}{\nu_y} + \frac{c^2}{\nu_z} & \frac{\rho}{\nu_y} & \frac{c}{\nu_z} \\ \frac{\rho}{\nu_y} & \frac{1}{\nu_y} + \frac{k^2}{\nu_z} & \frac{k}{\nu_z} \\ \frac{c}{\nu_z} & \frac{k}{\nu_z} & \frac{1}{\nu_z} \end{pmatrix}$$

For which values of p, k, c you obtain the models: two-parents, two-kids and cascaded ? You've got 5 minutes.

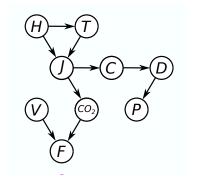


Homework: prove the expression for Σ .

D-separation

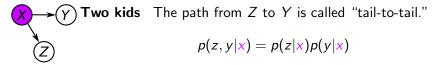
D-separation: motivation

Recall...

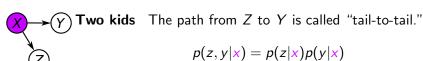


Is $P \perp \!\!\! \perp V \mid T$? How would you do it? Is this strategy scalable?

Let us recall the 3-var models:



Let us recall the 3-var models:



$$(X)$$
 Two parents The path from X to Y is called "head-to-head."



Let us recall the 3-var models:



) **Two kids** The path from Z to Y is called "tail-to-tail."

$$p(z,y|x) = p(z|x)p(y|x)$$



Two parents The path from X to Y is called "head-to-head."

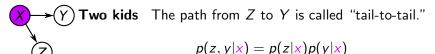
$$p(x, y|z) \neq p(x|z)p(y|z)$$

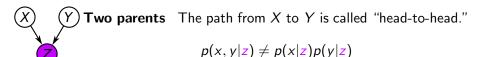


Cascaded The path from X to Z is called "head-to-tail."

$$p(x,z|y) = p(x|y)p(z|y)$$

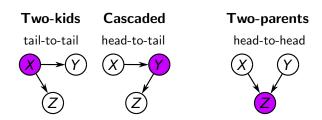
Let us recall the 3-var models:

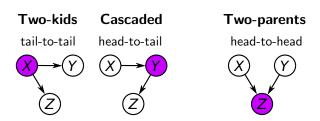




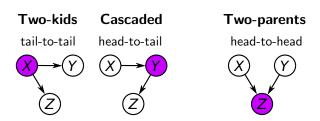
Cascaded The path from
$$X$$
 to Z is called "head-to-tail."
$$p(x,z|y) = p(x|y)p(z|y)$$

Please check Section 8.2 of Bishop's book.



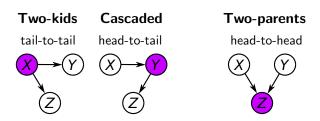


The purple node "blocks" the path in two-kids/tail-to-tail & cascaded/head-to-tail \to conditional independence.



The purple node "blocks" the path in two-kids/tail-to-tail & cascaded/head-to-tail \rightarrow conditional independence.

The purple node "unblocks" the path in two-parents/head-to-head \rightarrow conditional dependence.

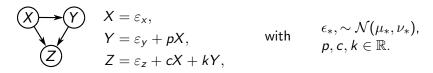


The purple node "blocks" the path in two-kids/tail-to-tail & cascaded/head-to-tail \rightarrow conditional independence.

The purple node "unblocks" the path in two-parents/head-to-head \rightarrow conditional dependence.

In the two-parents, Z or any descendant of Z will unblock the path.

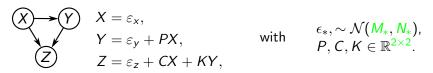
[1D] Let X, Y and Z three random variables following:



[1D] Let X, Y and Z three random variables following:

$$X = \varepsilon_{x},$$
 $Y = \varepsilon_{y} + pX,$ with $\epsilon_{*}, \sim \mathcal{N}(\mu_{*}, \nu_{*}),$ $Z = \varepsilon_{z} + cX + kY,$

[2D] Let X, Y and Z three random vectors following:



[1D] Let X, Y and Z three random variables following:

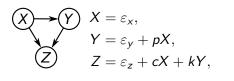
$$X = \varepsilon_{x},$$
 $Y = \varepsilon_{y} + pX,$ with $\epsilon_{*}, \sim \mathcal{N}(\mu_{*}, \nu_{*}),$ $Z = \varepsilon_{z} + cX + kY,$

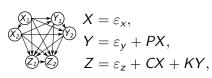
[2D] Let X, Y and Z three random vectors following:

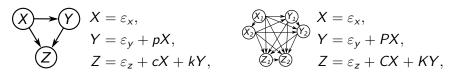
In this case, $M_* \in \mathbb{R}^2$ and $N_* \in \mathbb{R}^{2 \times 2}$.

Each ϵ_* is a **multivariate Gaussian**.

 $V = (X^\top, Y^\top, Z^\top)^\top$ is also a multivariate Gaussian.





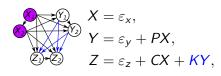


The covariance matrix Σ in the 2D-case writes (check Bishop's book):

$$\Sigma^{-1} = \left(\begin{array}{ccc} N_x^{-1} + P^\top N_y^{-1} P + C^\top N_z^{-1} C & N_y^{-1} P & N_z^{-1} C \\ P^\top N_y^{-1} & N_y^{-1} + K^\top N_z^{-1} K & N_z^{-1} K \\ C^\top N_z^{-1} & K^\top N_z^{-1} & N_z^{-1} \end{array} \right)$$

$$X = \varepsilon_x,$$

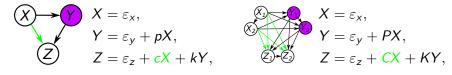
 $Y = \varepsilon_y + pX,$
 $Z = \varepsilon_z + cX + kY,$



The covariance matrix Σ in the 2D-case writes (check Bishop's book):

$$\Sigma^{-1} = \left(\begin{array}{ccc} N_x^{-1} + P^\top N_y^{-1} P + C^\top N_z^{-1} C & N_y^{-1} P & N_z^{-1} C \\ P^\top N_y^{-1} & N_y^{-1} + K^\top N_z^{-1} K & N_z^{-1} K \\ C^\top N_z^{-1} & K^\top N_z^{-1} & N_z^{-1} \end{array} \right)$$

Two-kids (tail-to-tail): p(y, z|x) = p(y|x)p(z|x)

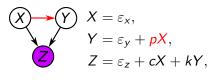


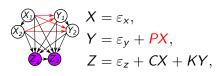
The covariance matrix Σ in the 2D-case writes (check Bishop's book):

$$\Sigma^{-1} = \left(\begin{array}{ccc} N_x^{-1} + P^\top N_y^{-1} P + C^\top N_z^{-1} C & N_y^{-1} P & N_z^{-1} C \\ P^\top N_y^{-1} & N_y^{-1} + K^\top N_z^{-1} K & N_z^{-1} K \\ C^\top N_z^{-1} & K^\top N_z^{-1} & N_z^{-1} \end{array} \right)$$

Two-kids (tail-to-tail):
$$p(y, z|x) = p(y|x)p(z|x)$$

Cascaded (head-to-tail): $p(x, z|y) = p(x|y)p(z|y)$





The covariance matrix Σ in the 2D-case writes (check Bishop's book):

$$\Sigma^{-1} = \left(\begin{array}{ccc} N_x^{-1} + P^\top N_y^{-1} P + C^\top N_z^{-1} C & N_y^{-1} P & N_z^{-1} C \\ P^\top N_y^{-1} & N_y^{-1} + K^\top N_z^{-1} K & N_z^{-1} K \\ C^\top N_z^{-1} & K^\top N_z^{-1} & N_z^{-1} \end{array} \right)$$

Two-kids (tail-to-tail): p(y, z|x) = p(y|x)p(z|x)

Cascaded (head-to-tail): p(x, z|y) = p(x|y)p(z|y)

Two-parents (head-to-head): $p(x, y|z) \neq p(x|z)p(y|z)$

$$X \rightarrow Y$$
 $X = \varepsilon_x$,
 $Y = \varepsilon_y + pX$,
 $Z = \varepsilon_z + cX + kY$,

$$X = \varepsilon_{x},$$
 $Y = \varepsilon_{y} + PX,$
 $Z = \varepsilon_{z} + CX + KY,$

The covariance matrix Σ in the 2D-case writes (check Bishop's book):

$$\Sigma^{-1} = \left(\begin{array}{ccc} N_x^{-1} + P^\top N_y^{-1} P + C^\top N_z^{-1} C & N_y^{-1} P & N_z^{-1} C \\ P^\top N_y^{-1} & N_y^{-1} + K^\top N_z^{-1} K & N_z^{-1} K \\ C^\top N_z^{-1} & K^\top N_z^{-1} & N_z^{-1} \end{array} \right)$$

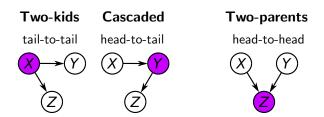
Two-kids (tail-to-tail): p(y, z|x) = p(y|x)p(z|x)

Cascaded (head-to-tail): p(x, z|y) = p(x|y)p(z|y)

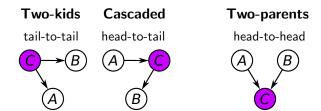
Two-parents (head-to-head): $p(x, y|z) \neq p(x|z)p(y|z)$

This gives us hope for more complicated models!

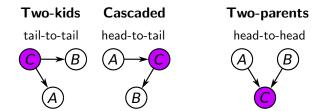
Remember?



Remember? Let me change the variable names...

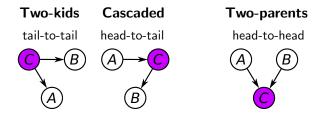


Remember? Let me change the variable names...



Tail-to-tail & head-to-tail $\rightarrow A \perp\!\!\!\perp B \mid C$.

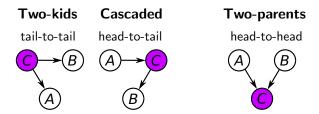
Remember ? Let me change the variable names...



Tail-to-tail & head-to-tail $\rightarrow A \perp\!\!\!\perp B \mid C$.

Head-to-head $\rightarrow A \not\perp \!\!\! \perp B \mid C$ or any descendant of C.

Remember ? Let me change the variable names...



Tail-to-tail & head-to-tail $\rightarrow A \perp\!\!\!\perp B \mid C$.

Head-to-head $\rightarrow A \not\perp \!\!\! \perp B \mid C$ or any descendant of C.

 \Rightarrow Nodes within tail-to-tail or head-to-tail can be in C and nodes within head-to-head or any of their descendents must not be in C.

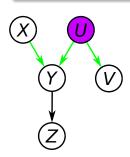
Definition: blocked path

- the path meets tail-to-tail or head-to-tail at the node and the node is in C;
- the path meets head-to-head at the node and neither the node nor any of its descendants are in C.

Definition: blocked path

Let A, B and C be three non-intersecting sets of nodes of a directed acyclic graph. A path from A to B is said to be blocked by C if it includes a node that either:

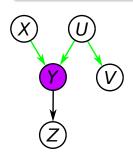
- the path meets tail-to-tail or head-to-tail at the node and the node is in C;
- the path meets head-to-head at the node and neither the node nor any of its descendants are in C.



Is the path from X to V blocked by U?

Definition: blocked path

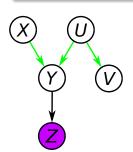
- the path meets tail-to-tail or head-to-tail at the node and the node is in C;
- the path meets head-to-head at the node and neither the node nor any of its descendants are in C.



- Is the path from X to V blocked by U? Yes
- Is the path from X to V blocked by Y?

Definition: blocked path

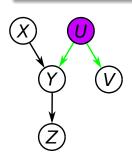
- the path meets tail-to-tail or head-to-tail at the node and the node is in C;
- the path meets head-to-head at the node and neither the node nor any of its descendants are in C.



- Is the path from X to V blocked by U? Yes
- Is the path from X to V blocked by Y? No
- Is the path from X to V blocked by Y?

Definition: blocked path

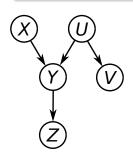
- the path meets tail-to-tail or head-to-tail at the node and the node is in C;
- the path meets head-to-head at the node and neither the node nor any of its descendants are in C.



- Is the path from X to V blocked by U? Yes
- Is the path from X to V blocked by Y? No
- Is the path from X to V blocked by Y? No, because of Z.
- Is the path from Y to V blocked by U?

Definition: blocked path

- the path meets tail-to-tail or head-to-tail at the node and the node is in C;
- the path meets head-to-head at the node and neither the node nor any of its descendants are in C.

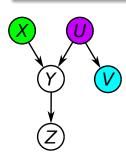


- Is the path from X to V blocked by U? Yes
- Is the path from X to V blocked by Y? No
- Is the path from X to V blocked by Y? No, because of Z.
- Is the path from Y to V blocked by U? Yes

Definition: D-separation

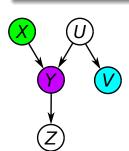
Definition: D-separation

Let A, B and C be three non-intersecting sets of nodes of a directed acyclic graph. A and B are D-separated by C, if all paths from any node from A to B are blocked by C.



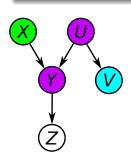
• Is $\{X\}$ D-separated from $\{V\}$ by $\{U\}$?

Definition: D-separation



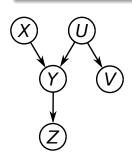
- Is $\{X\}$ D-separated from $\{V\}$ by $\{U\}$? Yes
- Is $\{X\}$ D-separated from $\{V\}$ by $\{Y\}$?

Definition: D-separation



- Is $\{X\}$ D-separated from $\{V\}$ by $\{U\}$? Yes
- Is $\{X\}$ D-separated from $\{V\}$ by $\{Y\}$? No
- Is $\{X\}$ D-separated from $\{V\}$ by $\{Y, U\}$?

Definition: D-separation

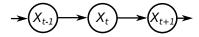


- Is $\{X\}$ D-separated from $\{V\}$ by $\{U\}$? Yes
- Is $\{X\}$ D-separated from $\{V\}$ by $\{Y\}$? No
- ullet Is $\{X\}$ D-separated from $\{V\}$ by $\{Y,U\}$? Yes

Markovian dependencies

Markov models: introduction

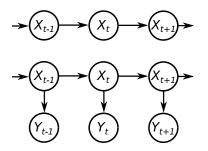
Principle: each variable depends only on its closer neighbours. Examples:



Markov chain.

Markov models: introduction

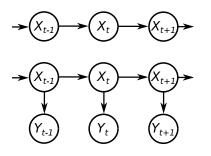
Principle: each variable depends only on its closer neighbours. Examples:



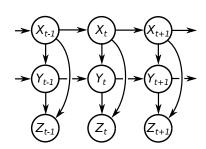
Markov chain (top). Hidden Markov chain (bottom).

Markov models: introduction

Principle: each variable depends only on its closer neighbours. Examples:

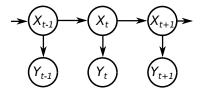


Markov chain (top). Hidden Markov chain (bottom).

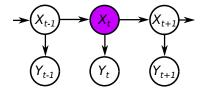


Double hidden Markov chain.

With the following model:



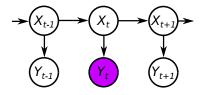
With the following model:



Is $\{X_{t-1}\}$ D-separated from $\{Y_{t+1}\}$ by ...

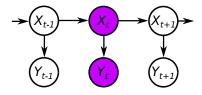
• $\{X_t\}$? [1 minute]

With the following model:



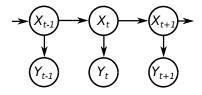
- $\{X_t\}$? Yes
- $\{Y_t\}$? [1 minute]

With the following model:



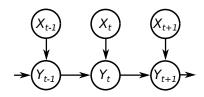
- $\{X_t\}$? Yes
- $\{Y_t\}$? No
- $\{X_t, Y_t\}$? [1 minute]

With the following model:

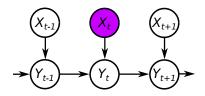


- $\{X_t\}$? Yes
- $\{Y_t\}$? No
- $\{X_t, Y_t\}$? Yes

With the following model:



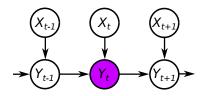
With the following model:



Is $\{X_{t-1}\}$ D-separated from $\{Y_{t+1}\}$ by ...

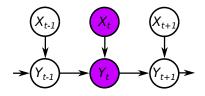
• $\{X_t\}$? [1 minute]

With the following model:



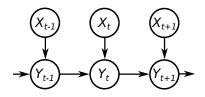
- $\{X_t\}$? No
- $\{Y_t\}$? [1 minute]

With the following model:



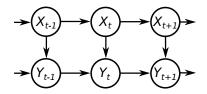
- $\{X_t\}$? No
- $\{Y_t\}$? Yes
- $\{X_t, Y_t\}$? [1 minute]

With the following model:

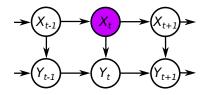


- $\{X_t\}$? No
- $\{Y_t\}$? Yes
- $\{X_t, Y_t\}$? Yes

With the following model:



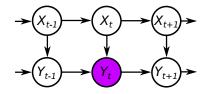
With the following model:



Is $\{X_{t-1}\}$ D-separated from $\{Y_{t+1}\}$ by ...

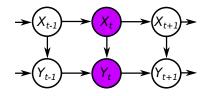
• $\{X_t\}$? [1 minute]

With the following model:



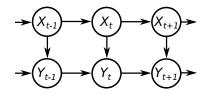
- $\{X_t\}$? No
- $\{Y_t\}$? [1 minute]

With the following model:



- $\{X_t\}$? No
- $\{Y_t\}$? No
- $\{X_t, Y_t\}$? [1 minute]

With the following model:



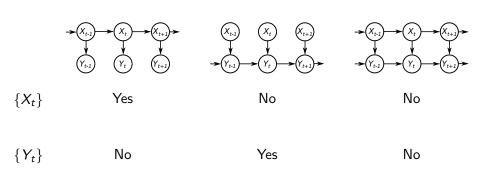
- $\{X_t\}$? No
- $\{Y_t\}$? No
- $\{X_t, Y_t\}$? Yes

D-separation in Markov models: summary

 $\{X_t, Y_t\}$

Yes

Is $\{X_{t-1}\}$ D-separated from $\{Y_{t+1}\}$ by (left column) in (top row)?



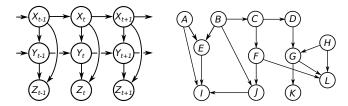
Yes

23 / 28

Yes

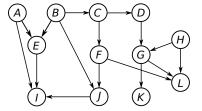
More complex models

Let's play a little bit with these two models:

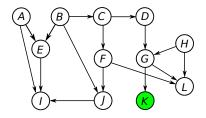


Find one example of D-separation and one example of non D-separation (in whatever case). [You've got 5 minutes]

Model example:



Model example:

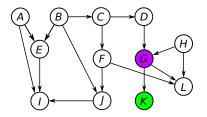


For a given node K, what is the minimal set of variables \mathcal{B}_K so that:

$$p(K|\text{all except }K) = p(K|\mathcal{B}_K)$$
?

You've got 3 minutes!

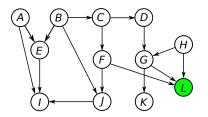
Model example:



For a given node K, what is the minimal set of variables \mathcal{B}_K so that:

$$p(K|\text{all except }K) = p(K|\mathcal{B}_K)$$
? $\mathcal{B}_K = \{G\}$

Model example:

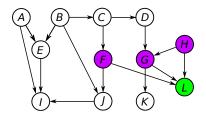


For a given node K, what is the minimal set of variables \mathcal{B}_K so that:

$$p(K|\text{all except } K) = p(K|\mathcal{B}_K)$$
? $\mathcal{B}_K = \{G\}$

For L? You've got 3 minutes!

Model example:

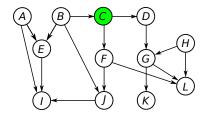


For a given node K, what is the minimal set of variables \mathcal{B}_K so that:

$$p(K|\text{all except } K) = p(K|\mathcal{B}_K)$$
? $\mathcal{B}_K = \{G\}$

For L? $\mathcal{B}_L = \{F, G, H\}$ because F, G, H are **parents** of L.

Model example:

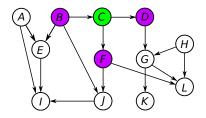


For a given node K, what is the minimal set of variables \mathcal{B}_K so that:

$$p(K|\text{all except } K) = p(K|\mathcal{B}_K)$$
? $\mathcal{B}_K = \{G\}$

For L? $\mathcal{B}_L = \{F, G, H\}$ because F, G, H are **parents** of L. For C? You've got 3 minutes!

Model example:



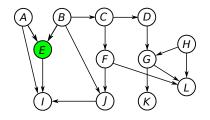
For a given node K, what is the minimal set of variables \mathcal{B}_K so that:

$$p(K|\text{all except }K) = p(K|\mathcal{B}_K)?$$
 $\mathcal{B}_K = \{G\}$

For L? $\mathcal{B}_L = \{F, G, H\}$ because F, G, H are **parents** of L.

For C? $\mathcal{B}_C = \{B, D, F\}$ because B(F, D) is parent (**children**) of C.

Model example:



For a given node K, what is the minimal set of variables \mathcal{B}_K so that:

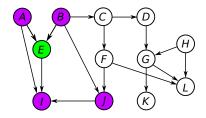
$$p(K|\text{all except }K) = p(K|\mathcal{B}_K)?$$
 $\mathcal{B}_K = \{G\}$

For L? $\mathcal{B}_L = \{F, G, H\}$ because F, G, H are **parents** of L.

For C? $\mathcal{B}_C = \{B, D, F\}$ because B(F, D) is parent (**children**) of C.

For E? You've got 3 minutes!

Model example:



For a given node K, what is the minimal set of variables \mathcal{B}_K so that:

$$p(K|\text{all except } K) = p(K|\mathcal{B}_K)$$
? $\mathcal{B}_K = \{G\}$

For L?
$$\mathcal{B}_L = \{F, G, H\}$$
 because F, G, H are parents of L .

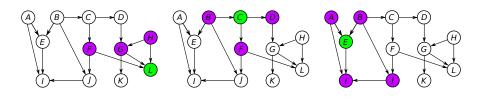
For
$$C$$
? $\mathcal{B}_C = \{B, D, F\}$ because $B(F, D)$ is parent (**children**) of C .

For E? $\mathcal{B}_E = \{A, B, I, J\}$ because A, B (I) are parents (children) of E and J is **co-parent** of E.

Markov blanket: definition

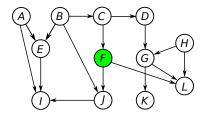
Definition of Markov blanket

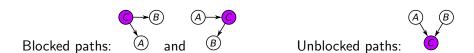
The Markov blanket is the minimal set that D-separates a set of nodes from the rest of the graph.

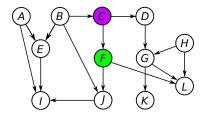


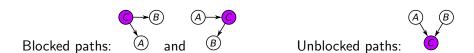
Construction of the Markov blanket

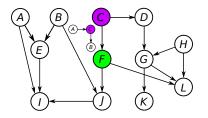
Given a directed acyclic graph, and a node X on that graph, the Markov blanket of X, \mathcal{B}_{x} is the set of all parents, children and co-parents of X.

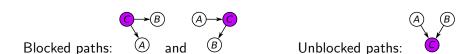


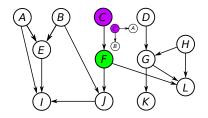


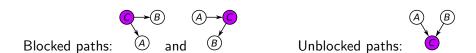


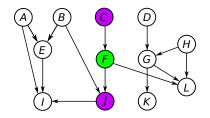


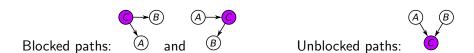


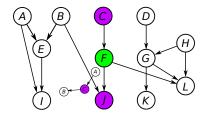


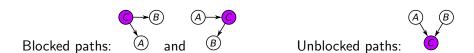


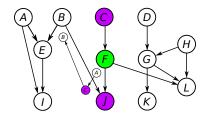


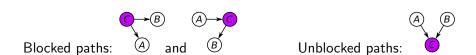


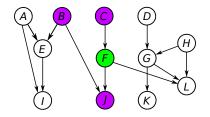


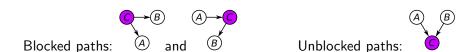


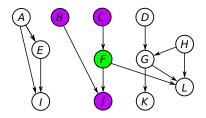


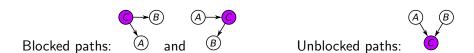


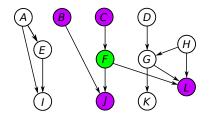


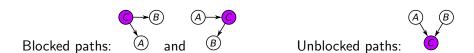


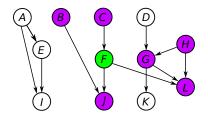


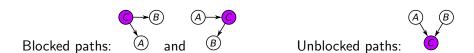


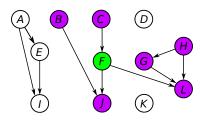


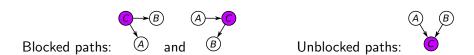






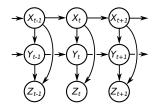






Markov blanket: practice

Homerwork: Find the Markov blanket of X_t , of Y_t and of Z_t in:



Next two sessions Fei will explain the GMM in detail and the expectation-maximization (EM) algorithm. This provides the basis for the rest of the semester and for practical session #1.

See you in three weeks!!!