

Directed Graphical Models II

Independencies

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Recap

- ▶ Statistical independence assumptions facilitate the efficient representation of probabilistic models by limiting the number of variables that are allowed to directly interact with each other.
- ▶ Visualisation of factorised pdfs/pmfs as directed acyclic graphs (DAGs).
- ▶ DAGs to define sets of pdfs/pmfs in terms of a factorisation: directed graphical models
- ▶ The factors correspond to conditionals of the pdf/pmf, which defines a data generating process called ancestral sampling.

Program

1. Directed ordered Markov property
2. D-separation and the directed global Markov property
3. Further methods to determine independencies

Program

1. Directed ordered Markov property
 - Definition
 - Equivalence between factorisation and directed ordered Markov property
 - Examples
2. D-separation and the directed global Markov property
3. Further methods to determine independencies

Factorisation implies independencies

- ▶ Given a DAG G , we defined the directed graphical model to be the set of pdfs/pmfs that factorise as

$$p(x_1, \dots, x_d) = \prod_{i=1}^d k(x_i | \text{pa}_i)$$

for some conditional pdfs/pmfs $k(x_i | \text{pa}_i)$. We said that such $p(\mathbf{x})$ satisfy $F(G)$.

- ▶ We have seen that $k(x_i | \text{pa}_i) = p(x_i | \text{pa}_i) = p(x_i | \text{pre}_i)$ for any ordering of the variables that is topological to G .
- ▶ This means that $p(\mathbf{x})$ satisfies the independencies

$$x_i \perp\!\!\!\perp (\text{pre}_i \setminus \text{pa}_i) \mid \text{pa}_i \text{ for all } i$$

This holds for all orderings of the variables that are topological to G .

- ▶ We say that $p(\mathbf{x})$ satisfies the directed ordered Markov property relative to G , or $M_o(G)$ in short.

Equivalence between $F(G)$ and $M_o(G)$

- ▶ We can summarise the above as $F(G) \implies M_o(G)$.
- ▶ We use the chain rule to show the reverse, i.e. $M_o(G) \implies F(G)$:
 - ▶ Given G , order the variables topologically to the graph
 - ▶ Decompose $p(\mathbf{x})$ using the chain rule

$$p(\mathbf{x}) = \prod_i p(x_i | \text{pre}_i)$$

- ▶ Since $p(\mathbf{x})$ satisfies $M_o(G)$, we have $p(x_i | \text{pre}_i) = p(x_i | \text{pa}_i)$ and hence

$$p(\mathbf{x}) = \prod_i p(x_i | \text{pa}_i)$$

so that $p(\mathbf{x})$ satisfies $F(G)$.

- ▶ We thus have the equivalence $F(G) \iff M_o(G)$.

Two equivalent views on directed graphical models

1. Factorisation (generative) view point:

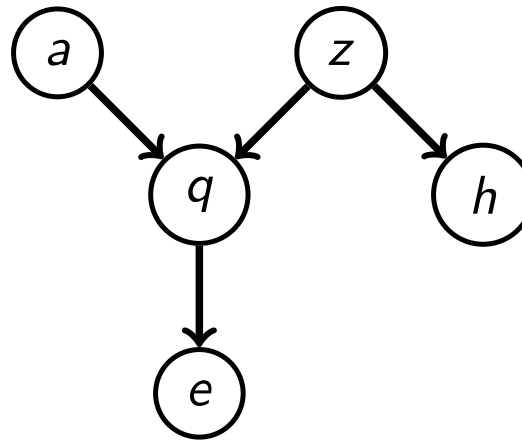
- ▶ We said the directed graphical model implied by a DAG G is the set of pdfs/pmfs that satisfy $F(G)$.
- ▶ It's the set of models that you obtain by looping over all possible factors $k(x_i|pa_i)$
- ▶ In other words, it's all the data that you can generate using ancestral sampling with different conditionals.

2. Independence (filtering) view point:

- ▶ Equivalently, we can say that the directed graphical model implied by a DAG G is the set of pdfs/pmfs that satisfy $M_o(G)$.
- ▶ It's the set of models that you obtain by filtering out from all possible models those that satisfy $M_o(G)$.
- ▶ In other words, it's all the data for which $M_o(G)$ holds.
(Similarly for further Markov properties that we will derive, the directed global Markov property $M_g(G)$ and the directed local Markov property $M_l(G)$.)

Example

DAG:



Topological ordering: (a, z, q, e, h)

Predecessor sets for the ordering:

$$\text{pre}_a = \emptyset, \text{pre}_z = \{a\}, \text{pre}_q = \{a, z\}, \text{pre}_e = \{a, z, q\}, \text{pre}_h = \{a, z, q, e\}$$

Parent sets

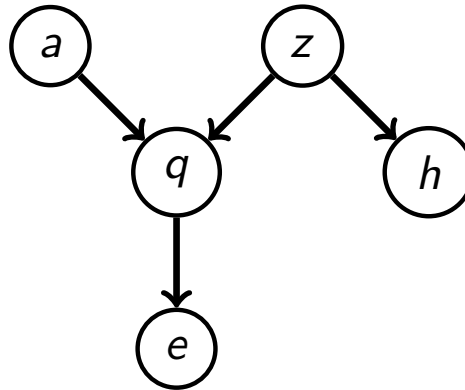
$$\text{pa}_a = \text{pa}_z = \emptyset, \text{pa}_q = \{a, z\}, \text{pa}_e = \{q\}, \text{pa}_h = \{z\}$$

All models defined by the DAG satisfy $x_i \perp\!\!\!\perp (\text{pre}_i \setminus \text{pa}_i) \mid \text{pa}_i$:

$$z \perp\!\!\!\perp a \quad e \perp\!\!\!\perp \{a, z\} \mid q \quad h \perp\!\!\!\perp \{a, q, e\} \mid z$$

Example (different topological ordering)

DAG:



Topological ordering: (a, z, h, q, e)

Predecessor sets for the ordering:

$$\text{pre}_a = \emptyset, \text{pre}_z = \{a\}, \text{pre}_h = \{a, z\}, \text{pre}_q = \{a, z, h\}, \text{pre}_e = \{a, z, h, q\}$$

Parent sets: as before

$$\text{pa}_a = \text{pa}_z = \emptyset, \text{pa}_h = \{z\}, \text{pa}_q = \{a, z\}, \text{pa}_e = \{q\}$$

All models defined by the DAG satisfy $x_i \perp\!\!\!\perp (\text{pre}_i \setminus \text{pa}_i) \mid \text{pa}_i$:

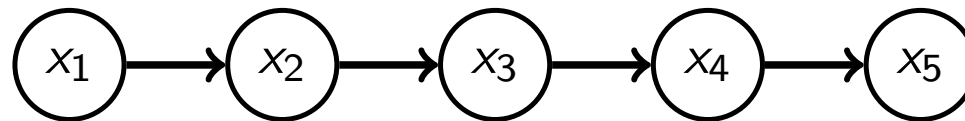
$$z \perp\!\!\!\perp a \quad h \perp\!\!\!\perp a \mid z \quad q \perp\!\!\!\perp h \mid a, z \quad e \perp\!\!\!\perp \{a, z, h\} \mid q$$

Note: the models also satisfy those obtained with the previous ordering:

$$z \perp\!\!\!\perp a \quad e \perp\!\!\!\perp \{a, z\} \mid q \quad h \perp\!\!\!\perp \{a, q, e\} \mid z$$

Example: Markov chain

DAG:



There is only one topological ordering: (x_1, x_2, \dots, x_5)

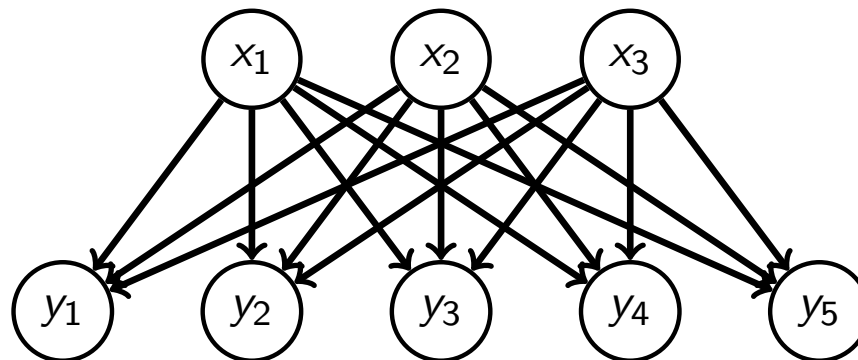
All models defined by the DAG satisfy: $x_{i+1} \perp\!\!\!\perp x_1, \dots, x_{i-1} \mid x_i$

(future independent of the past given the present)

Example: Probabilistic PCA, factor analysis, ICA

(PCA: principal component analysis; ICA: independent component analysis)

DAG:



Topological ordering $(x_1, x_2, x_3, y_1, y_2, y_3, y_4, y_5)$

All models defined by the DAG satisfy:

$$\begin{aligned} x_i &\perp\!\!\!\perp x_j & y_2 &\perp\!\!\!\perp y_1 \mid x_1, x_2, x_3 & y_3 &\perp\!\!\!\perp y_1, y_2 \mid x_1, x_2, x_3 \\ y_4 &\perp\!\!\!\perp y_1, y_2, y_3 \mid x_1, x_2, x_3 & y_5 &\perp\!\!\!\perp y_1, y_2, y_3, y_4 \mid x_1, x_2, x_3 \end{aligned}$$

y_5 is independent from all the other y_i given x_1, x_2, x_3 . Using further topological orderings shows that all y_i are independent from each other given x_1, x_2, x_3 .

(Marginally the y_i are not independent. The model explains possible dependencies between (observed) y_i through fewer (unobserved) x_i , see later.)

Remarks

- ▶ By using different topological orderings you can generate possibly different independence relations satisfied by the model.
- ▶ While they imply each other, deriving them from each other from the basic definition of independence may not be straightforward.
- ▶ Missing edges in a DAG cause the pa_i to be smaller than the pre_i , and thus lead to the independencies $x_i \perp\!\!\!\perp pre_i \setminus pa_i \mid pa_i$.
- ▶ Instead of “directed ordered Markov property”, we may just say “ordered Markov property” if it is clear that we are talking about DAGs.

Program

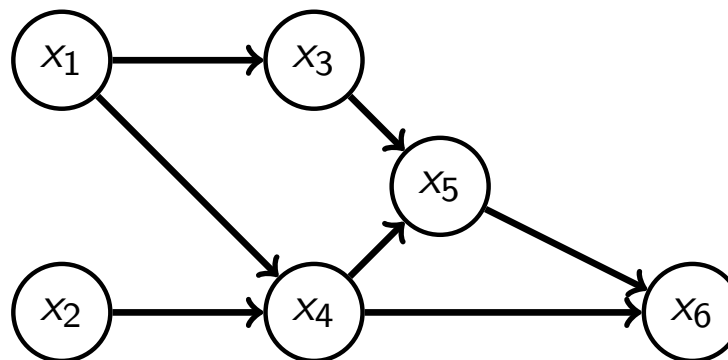
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Program

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 - Canonical connections
 - D-separation
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Further independence relations

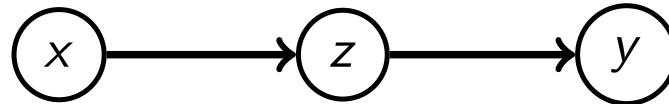
- ▶ Given the DAG below, what can we say about the independencies for the set of probability distributions that factorise over the graph?
- ▶ Is $x_1 \perp\!\!\!\perp x_2$? $x_1 \perp\!\!\!\perp x_2 \mid x_6$? $x_2 \perp\!\!\!\perp x_3 \mid \{x_1, x_4\}$?
- ▶ Ordered Markov properties give some independencies.
- ▶ Limitation: it only allows us to condition on parent sets.
- ▶ Directed separation (d-separation) gives further independencies.



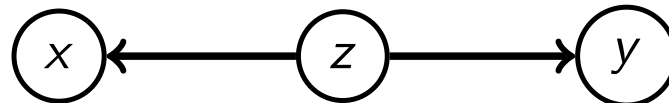
Three canonical connections in a DAG

In a DAG, two nodes x, y can be connected via a third node z in three ways:

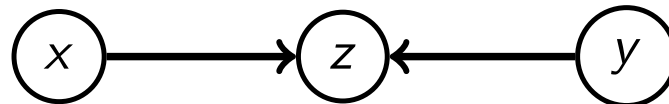
1. Serial connection (chain, head-tail or tail-head)



2. Diverging connection (fork, tail-tail)



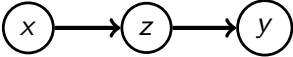
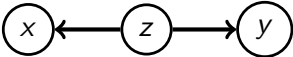
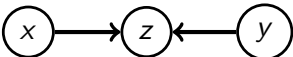
3. Converging connection (collider, head-head, v-structure)



Note: in any case, the sequence x, z, y forms a trail

Independencies for the three canonical connections

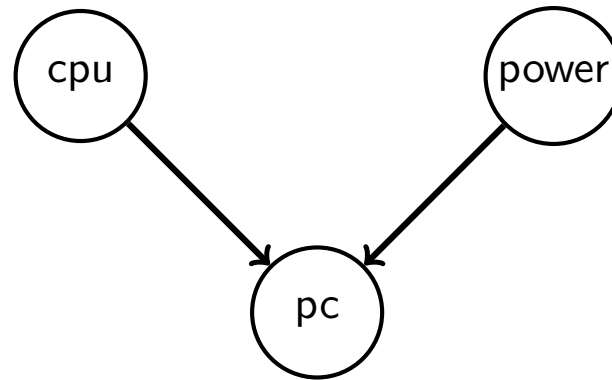
(Derived in the exercises)

Connection	$p(x, y)$	$p(x, y z)$	z node
	$x \not\perp y$	$x \perp y z$	default: open instantiated: closed
	$x \not\perp y$	$x \perp y z$	default: open instantiated: closed
	$x \perp y$	$x \not\perp y z$	default: closed with evidence: opens

Think of the z node as a valve or gate through which evidence (probability mass) can flow. Depending on the type of the connection, it's default state is either open or closed. Instantiation/evidence acts as a switch on the valve.

Colliders model “explaining away”

Example:



- ▶ One day your computer does not start and you bring it to a repair shop. You think the issue could be the power unit or the cpu.
- ▶ Investigating the power unit shows that it is damaged. Is the cpu fine?
- ▶ Without further information, finding out that the power unit is damaged typically reduces our belief that the cpu is damaged

power ~~⊥~~ cpu | pc

- ▶ Finding out about the damage to the power unit *explains away* the observed start-issues of the computer.

D-separation

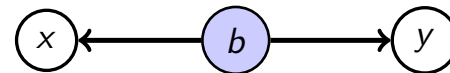
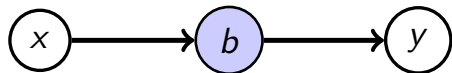
Let $X = \{x_1, \dots, x_n\}$, $Y = \{y_1, \dots, y_m\}$, and $Z = \{z_1, \dots, z_r\}$ be three disjoint sets of nodes in the graph. Assume all z_i are observed (instantiated).

- ▶ Two nodes x_i and y_j are said to be d-separated by Z if all trails between them are blocked by Z .
- ▶ The sets X and Y are said to be d-separated by Z if every trail from any variable in X to any variable in Y is blocked by Z .

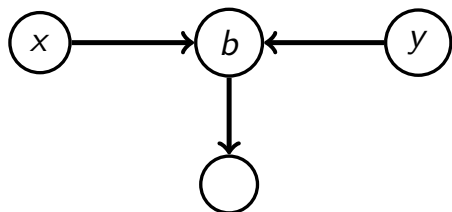
D-separation

A trail between nodes x and y is blocked by Z if there is a node b on the trail such that

1. either b is part of a head-tail or tail-tail connection along the trail and b is in Z ,



2. or b is part of a head-head (collider) connection along the trail and neither b nor any of its descendants are in Z .



It's like treating a segment of the trail as a canonical connection.

D-separation and conditional independence

Theorem: If X and Y are d-separated by Z then $X \perp\!\!\!\perp Y \mid Z$ for all probability distributions that factorise over the DAG.

For those interested: A proof can be found in Section 2.8 of *Bayesian Networks – An Introduction* by Koski and Noble (not examinable)

Important because:

1. the theorem allows us to read off (conditional) independencies from the graph
2. no restriction on the sets X, Y, Z
3. the theorem shows that statistical independencies detected by d-separation, which is purely a graph-based criterion, do always hold. They are “true positives” (“soundness of d-separation”).

Directed global Markov property $M_g(G)$

- ▶ Distributions $p(\mathbf{x})$ are said to satisfy the directed global Markov property with respect to the DAG G , or $M_g(G)$, if for any triple X, Y, Z of disjoint subsets of nodes such that X and Y are d-separated by Z in G , we have $X \perp\!\!\!\perp Y | Z$.
- ▶ *Global* Markov property because we do not restrict the sets X, Y, Z .
- ▶ The theorem says that $F(G) \implies M_g(G)$.
- ▶ We thus have so far $M_o(G) \iff F(G) \implies M_g(G)$.

What if two sets of nodes are not d-separated?

Theorem: If X and Y are not d-separated by Z then $X \not\perp\!\!\!\perp Y \mid Z$ in **some** probability distributions that factorise over the DAG.

For those interested: A proof sketch can be found in Section 3.3.1 of *Probabilistic Graphical Models* by Koller and Friedman (not examinable).

“not d-separated” is also called “d-connected”

$\not\perp\!\!\!\perp$ means statistically dependent

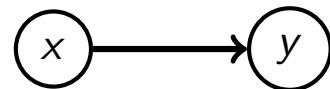
What if two sets of nodes are not d-separated?

- ▶ However, it can also be that d-connected variables are independent for some distributions that factorise over the graph.
- ▶ Example (Koller, Example 3.3): $p(x, y)$ with $x, y \in \{0, 1\}$ and

$$p(y = 0|x = 0) = a \quad p(y = 0|x = 1) = a$$

for $a > 0$ and some non-zero $p(x = 0)$.

- ▶ Graph has arrow from x to y . Variables are not d-separated.



- ▶ $p(y = 0) = ap(x = 0) + ap(x = 1) = a$,
which is $p(y = 0|x)$ for all x .
- ▶ $p(y = 1) = (1 - a)p(x = 0) + (1 - a)p(x = 1) = 1 - a$,
which is $p(y = 1|x)$ for all x .
- ▶ Hence: $p(y|x) = p(y)$ so that $x \perp\!\!\!\perp y$.

D-separation is not complete

- ▶ This means that d-separation does generally not reveal all independencies in all probability distributions that factorise over the graph.
- ▶ In other words, individual probability distributions that factorise over the graph may have further independencies not included in the set obtained by d-separation. This is because the graph criteria do not operate on the numerical values of the factors but only on “whom affects whom”, i.e. the parent-children relationships.
- ▶ We say that d-separation is not “complete” (“recall-rate” is not guaranteed to be 100%).

Recipe to determine whether two nodes are d-separated

1. Determine all trails between x and y (note: direction of the arrows does here not matter).
2. For each trail:
 - i Determine the default state of all nodes on the trail.
 - ▶ open if part of a head-tail or a tail-tail connection
 - ▶ closed if part of a head-head connection
 - ii Check whether the set of observed nodes Z switches the state of the nodes on the trail.
 - iii The trail is blocked if it contains a closed node.
3. The nodes x and y are d-separated if all trails between them are blocked.

Example: Are x_1 and x_2 d-separated?

Follows from ordered Markov property, but let us answer it with d-separation.

1. Determine all trails between x_1 and x_2

2. For trail x_1, x_4, x_2

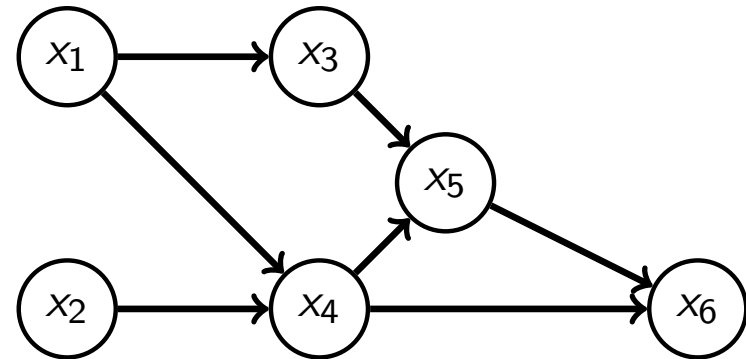
- i default state
- ii conditioning set is empty
- iii \Rightarrow Trail is blocked

For trail x_1, x_3, x_5, x_4, x_2

- i default state
- ii conditioning set is empty
- iii \Rightarrow Trail is blocked

Trail $x_1, x_3, x_5, x_6, x_4, x_2$ is blocked too (same arguments).

3. $\Rightarrow x_1$ and x_2 are d-separated.

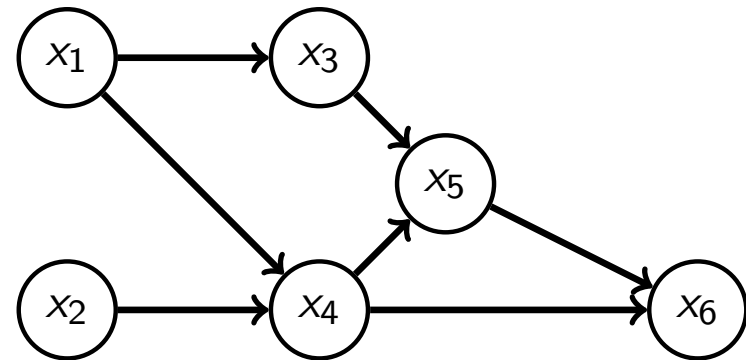


$x_1 \perp\!\!\!\perp x_2$ for all probability distributions that factorise over the graph.

Example: Are x_1 and x_2 d-separated by x_6 ?

1. Determine all trails between x_1 and x_2
2. For trail x_1, x_4, x_2
 - i default state
 - ii influence of x_6
 - iii \Rightarrow Trail not blocked

No need to check the other trails: x_1 and x_2 are not d-separated by x_6



$x_1 \not\perp\!\!\!\perp x_2 \mid x_6$ does not hold for all probability distributions that factorise over the graph.

Example: Are x_2 and x_3 d-separated by x_1 and x_4 ?

1. Determine all trails between x_2 and x_3

2. For trail x_3, x_1, x_4, x_2

i default state

ii influence of $\{x_1, x_4\}$

iii \Rightarrow Trail blocked

For trail x_3, x_5, x_4, x_2

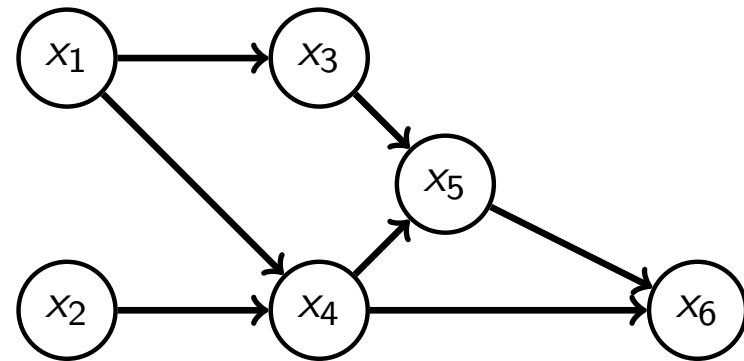
i default state

ii influence of $\{x_1, x_4\}$

iii \Rightarrow Trail blocked

Trail x_3, x_5, x_6, x_4, x_2 is blocked too (same arguments).

3. $\Rightarrow x_2$ and x_3 are d-separated by x_1 and x_4 .

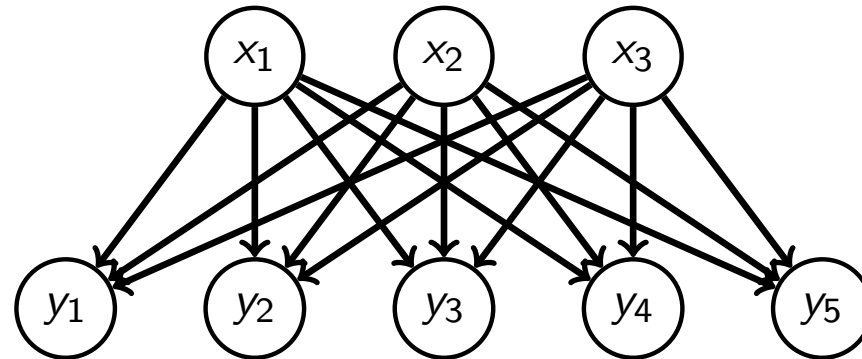


$x_2 \perp\!\!\!\perp x_3 \mid \{x_1, x_4\}$ for all probability distributions that factorise over the graph.

Example: Probabilistic PCA, factor analysis, ICA

(PCA: principal component analysis; ICA: independent component analysis)

DAG:



- ▶ From ordered Markov property: e.g.
 $y_5 \perp\!\!\!\perp y_1, y_2, y_3, y_4 \mid x_1, x_2, x_3$.
- ▶ Via d-separation: $y_i \not\perp\!\!\!\perp y_k$ since the x are in a tail-tail connection with the y 's.
- ▶ Via d-separation: $x_i \perp\!\!\!\perp x_j$ since all trails between them go through y 's that are in a collider configuration.
- ▶ Via d-separation: $x_i \not\perp\!\!\!\perp x_j \mid y_k$ for any $i, j, k, (i \neq j)$. This is the “explaining away” phenomenon.

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 - Directed local Markov property
 - Equivalences
 - Markov blanket

Directed local Markov property

- ▶ The independencies that you can obtain with the ordered Markov property depend on the topological ordering chosen.
- ▶ We next introduce the “directed local Markov property” that does not depend on the ordering but only on the graph.
- ▶ We say that $p(\mathbf{x})$ satisfies the directed local Markov property, $M_I(G)$ with respect to DAG G if

$$x_i \perp\!\!\!\perp (\text{nondesc}(x_i) \setminus \text{pa}_i) \mid \text{pa}_i$$

holds for all i , where pa_i denotes the parents and $\text{nondesc}(x_i)$ the non-descendants of x_i .

- ▶ In other words, $p(\mathbf{x})$ satisfying the directed local Markov property means that

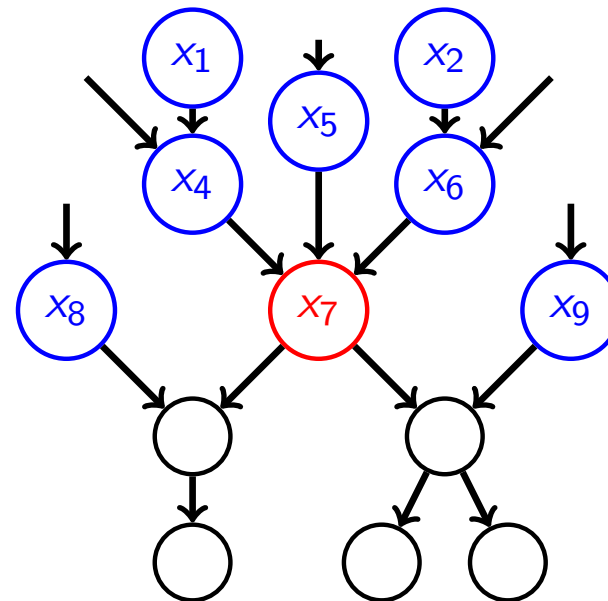
$$p(x_i | \text{nondesc}(x_i)) = p(x_i | \text{pa}_i) \quad \text{for all } i$$

Directed local Markov property

- ▶ We now show that $M_o(G) \iff M_l(G)$ for any DAG G .
- ▶ In words: If $p(\mathbf{x})$ satisfies the ordered Markov property it also satisfies the directed local Markov property and vice versa:

$$x_i \perp\!\!\!\perp (\text{pre}_i \setminus \text{pa}_i) \mid \text{pa}_i \iff x_i \perp\!\!\!\perp (\text{nondesc}(x_i) \setminus \text{pa}_i) \mid \text{pa}_i$$

$x_i \equiv x_7$
 $\text{pa}_7 = \{x_4, x_5, x_6\}$
 $\text{pre}_7 = \{x_1, x_2, \dots, x_6\}$
 $\text{nondesc}(x_7)$ in blue



Directed local Markov property

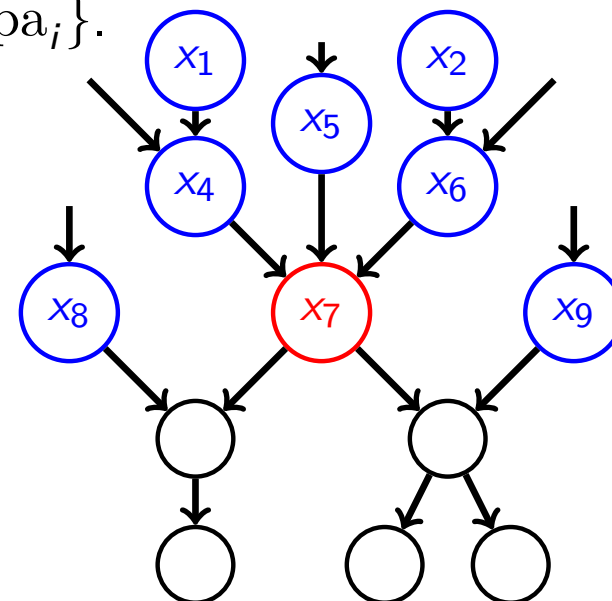
$x_i \perp\!\!\!\perp \text{pre}_i \setminus \text{pa}_i \mid \text{pa}_i \iff x_i \perp\!\!\!\perp \text{nondesc}(x_i) \setminus \text{pa}_i \mid \text{pa}_i$ follows because
(1) $\{x_1, \dots, x_{i-1}\} \subseteq \text{nondesc}(x_i)$ for all topological orderings, and
(2) $x \perp\!\!\!\perp \{y, w\} \mid z$ implies that $x \perp\!\!\!\perp y \mid z$ and $x \perp\!\!\!\perp w \mid z$.

For \Rightarrow , assume $p(\mathbf{x})$ follows the ordered Markov property. It then factorises over the graph and hence satisfies $M_g(G)$, and we can use d-separation to establish independence.

Consider all trails from x_i to $\{\text{nondesc}(x_i) \setminus \text{pa}_i\}$.

Two cases: move upwards or downwards:

- (1) upward trails are blocked by the parents
- (2) downward trails must contain a head-head (collider) connection because the $x_j \in \{\text{nondesc}(x_i) \setminus \text{pa}_i\}$ is a non-descendant. These paths are blocked because the collider node or its descendants are never part of pa_i .



The result follows because all paths from x_i to all elements in $\{\text{nondesc}(x_i) \setminus \text{pa}_i\}$ are blocked.

Equivalences so far

- ▶ For a DAG G , we have established the following relationships:

$$M_g(G) \iff F(G) \iff M_o(G) \iff M_l(G)$$

- ▶ We can close the loop by showing that $M_g(G) \implies M_l(G)$.
- ▶ If $p(\mathbf{x})$ satisfies $M_g(G)$ we can use d-separation to read our dependencies.
- ▶ The same reasoning as in the second part of the previous proof thus shows that $x_i \perp\!\!\!\perp (\text{nondesc}(x_i) \setminus \text{pa}_i) \mid \text{pa}_i$ holds.
- ▶ Hence $M_g(G) \implies M_l(G)$ and thus:

$$M_g(G) \iff F(G) \iff M_o(G) \iff M_l(G)$$

Summary of the equivalences

For a DAG G with nodes (random variables) x_i and parent sets pa_i , we have the following equivalences:

$$\begin{array}{lcl} p(\mathbf{x}) \text{ satisfies } F(G) & & p(\mathbf{x}) = \prod_{i=1}^d k(x_i | \text{pa}_i) \\ & \Downarrow & \\ p(\mathbf{x}) \text{ satisfies } M_o(G) & & x_i \perp\!\!\!\perp (\text{pre}_i \setminus \text{pa}_i) \mid \text{pa}_i \text{ for all } i \text{ and any topol. ordering} \\ & \Downarrow & \\ p(\mathbf{x}) \text{ satisfies } M_l(G) & & x_i \perp\!\!\!\perp (\text{nondesc}(x_i) \setminus \text{pa}_i) \mid \text{pa}_i \text{ for all } i \\ & \Downarrow & \\ p(\mathbf{x}) \text{ satisfies } M_g(G) & & \text{independencies asserted by d-separation} \end{array}$$

F : factorisation property, M_o : directed ordered MP, M_l : directed local MP, M_g : directed global MP (MP: Markov property)

Broadly speaking, the graph serves two related purposes:

1. it tells us how distributions factorise
2. it represents the independence assumptions made

What can we do with the equivalences?

The main things that we have covered:

- ▶ If we know the factorisation of a $p(\mathbf{x})$ in terms of conditional pdfs/pmfs, we can build a graph G such that $p(\mathbf{x})$ satisfies $F(G)$ and then use the graph to determine independencies that $p(\mathbf{x})$ satisfies.
- ▶ Similarly, if for some ordering of the random variables, we know the independencies $x_i \perp\!\!\!\perp (\text{pre}_i \setminus \pi_i) \mid \pi_i$ that $p(\mathbf{x})$ satisfies, where π_i is a minimal subset of the predecessors, we can obtain a graph G by identifying the π_i with the parents pa_i in a graph. By construction, $p(\mathbf{x})$ satisfies $M_o(G)$. From the graph we can obtain the factorisation of $p(\mathbf{x})$ and further independencies.
- ▶ We can start with the graph and check which independencies it implies, and, when happy, define a set of pdfs/pmfs that all satisfy the specified independencies.

What can we do with the equivalences?

What we haven't covered:

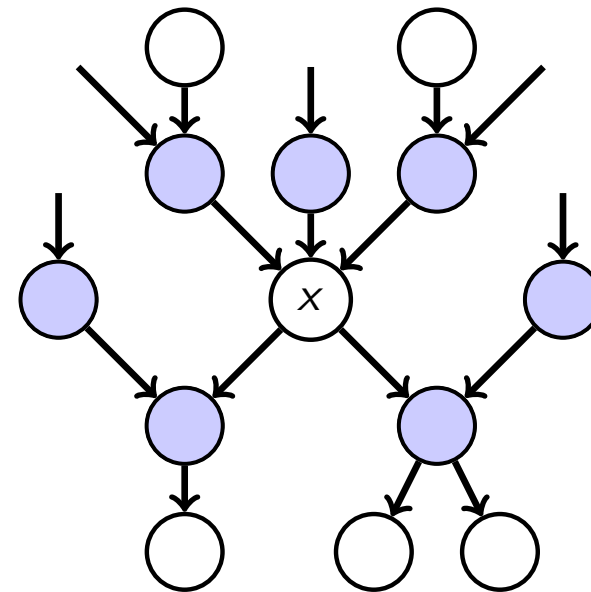
- ▶ How to determine a graph G from an arbitrary set of independencies
- ▶ How to learn the graph from samples from $p(\mathbf{x})$ (structure learning)
- ▶ These are difficult topics:
 - ▶ Multiple DAGs may express the same independencies and there may be no DAG that expresses all desired independencies (see later)
 - ▶ Learning the graph from samples involves independence tests which are not 100% accurate and errors propagate and may change the structure of the resulting DAG.
- ▶ Areas of active research, in particular in the field of causality.

Markov blanket

What is the minimal set of variables such that knowing their values makes x independent from the rest?

From d-separation:

- ▶ Isolate x from its ancestors
⇒ condition on parents
- ▶ Isolate x from its descendants
⇒ condition on children
- ▶ Deal with collider connection
⇒ condition on co-parents
(other parents of the children of x)



In directed graphical models, the parents, children, and co-parents of x are called its Markov blanket, denoted by $MB(x)$. We have $x \perp\!\!\!\perp \{\text{all vars} \setminus x \setminus MB(x)\} \mid MB(x)$.

Program recap

1. Directed ordered Markov property

- Definition
- Equivalence between factorisation and directed ordered Markov property
- Examples

2. D-separation and the directed global Markov property

- Canonical connections
- D-separation
- Recipe and examples

3. Further methods to determine independencies

- Directed local Markov property
- Equivalences
- Markov blanket

Further Reading

General material on DGMs and d-separation is covered in:

- ▶ Bishop (2006) secs. 8.1 and 8.2
- ▶ Barber (2012) secs. 3.1 and 3.3
- ▶ ... and many other sources

The details of the directed ordered Markov property, the directed local Markov property and the directed global Markov property are less widely available in the standard textbooks, and you are recommended to study the slides (by MG) on this topic

Credits

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