Directed Graphical Models

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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.
- Statistical independencies lead to a (partial) factorisation of pdfs/pmfs
- Equivalence between factorisation and ordered Markov property
- Visualisation of pdfs/pmfs as directed graph

- 1. Definition of directed graphical models
- 2. Three canonical connections in a DAG and their properties
- 3. Independencies in directed graphical models

Program

1. Definition of directed graphical models

- Definition via factorisation according to the graph
- Definition via ordered Markov property
- Derive independencies from the ordered Markov property with different topological orderings

2. Three canonical connections in a DAG and their properties

3. Independencies in directed graphical models

Directed graphical model

- We started with a pdf/pmf, wrote it in factorised form according to some ordering, and associated a DAG with it.
- We can also go the other way around and start with a DAG.
- Definition (via factorisation property) A directed graphical model based on a DAG with d nodes and associated random variables x_i is the set of pdfs/pmfs that factorise as

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

where pa_i denotes the parents of x_i in the graph.

Remark: a pdf/pmf p(x₁,...,x_d) that can be written in the above form is said to "factorise over the graph".

Example

DAG:



Random variables: *a*, *z*, *q*, *e*, *h*

 $\text{Parent sets: } \text{pa}_{\textit{a}} = \text{pa}_{\textit{z}} = \varnothing, \text{pa}_{\textit{q}} = \{\textit{a}, \textit{z}\}, \text{pa}_{\textit{e}} = \{\textit{q}\}, \text{pa}_{\textit{h}} = \{\textit{z}\}.$

Directed graphical model: set of pdfs/pmfs p(a, z, q, e, h) that factorise as:

$$p(a, z, q, e, h) = p(a)p(z)p(q|a, z)p(e|q)p(h|z)$$

Alternative definition of directed graphical models

- For any DAG with d nodes we can always find an ordering of the associated random variables that is topological to the DAG. Re-label the nodes accordingly as x₁,...,x_d.
- Recall: in topological orderings, the parents always come before the children.
- Hence: $pa_i \subseteq pre_i$ whatever topological ordering we picked.
- The derived equivalence of factorisation and ordered Markov property, with the pa_i as the π_i , thus yields the result:

$$p(\mathbf{x}) = \prod_{i=1}^{d} p(x_i | pa_i) \iff x_i \perp (pre_i \setminus pa_i) | pa_i \text{ for all } i$$

A since pa_i ⊆ pre_i whatever the topological ordering, the result holds for all topological orderings.

Alternative definition of directed graphical models

Two consequences:

- For a given DAG, the independencies derived from the ordered Markov property with any topological ordering imply the independencies derived with any other topological ordering.
- The insensitivity to the particular topological ordering used provides an alternative definition of directed graphical models.
- Definition (via ordered Markov property) A directed graphical model based on a DAG with d nodes and associated random variables x_i is the set of pdfs/pmfs that satisfy the ordered Markov property

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

for an ordering x_1, \ldots, x_d of the x_i that is topological to the DAG.

Example

DAG:



Random variables: a, z, q, e, hOrdering: (a, z, q, e, h) (meaning: $x_1 = a, x_2 = z, x_3 = q, x_4 = e, x_5 = h$) Predecessor sets for the ordering: $pre_a = \emptyset, pre_z = \{a\}, pre_q = \{a, z\}, pre_e = \{a, z, q\}, pre_h = \{a, z, q, e\}$ Parent sets: as before $pa_a = pa_z = \emptyset, pa_q = \{a, z\}, pa_e = \{q\}, pa_h = \{z\}$ All models in the set defined by the DAG satisfy $x_i \perp (pre_i \setminus pa_i) \mid pa_i$:

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

Example (different topological ordering)

DAG:



Ordering: (a, z, h, q, e)

Predecessor sets for the ordering:

 $\operatorname{pre}_{a} = \varnothing, \operatorname{pre}_{z} = \{a\}, \operatorname{pre}_{h} = \{a, z\}, \operatorname{pre}_{q} = \{a, z, h\}, \operatorname{pre}_{e} = \{a, z, h, q\}$

Parent sets: as before

 $\mathrm{pa}_{\textit{a}} = \mathrm{pa}_{\textit{z}} = \varnothing, \mathrm{pa}_{\textit{h}} = \{z\}, \mathrm{pa}_{\textit{q}} = \{a, z\}, \mathrm{pa}_{\textit{e}} = \{q\}$

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

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

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

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

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.
- The directed graphical model corresponds to a set of probability distributions. Two views according to the two definitions: The set includes all those distributions that you get
 - by looping over all possible conditionals $p(x_i | pa_i)$,
 - by retaining, from all possible joint distributions over the x_i, those that satisfy the independencies given by the ordered Markov property
- Individual pdfs/pmf in the set are typically also called a directed graphical model ("overloading" of the name of the set and its elements).
- Other names for directed graphical models: belief network, Bayesian network, Bayes network.

Example: Markov model

DAG:

$$(x_1) \longrightarrow (x_2) \longrightarrow (x_3) \longrightarrow (x_4) \longrightarrow (x_5)$$

All models, i.e. pdfs/pmfs $p(\mathbf{x})$, in the set factorise as $p(\mathbf{x}) = p(x_1)p(x_2|x_1)p(x_3|x_2)p(x_4|x_3)p(x_5|x_4)$

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

By ordered Markov property: all models in the set satisfy: $x_{i+1} \perp x_1, \ldots, x_{i-1} \mid x_i$ (future independent of the past given the present)

Example: Probabilistic PCA, factor analysis, ICA

(PCA: principal component analysis; ICA: independent component analysis) DAG: (x_1) (x_2) (x_3)



Explains properties of (observed) y_i through fewer (unobserved) x_i . Different further assumptions lead to different methods (more later).

All models in the set factorise as $p(x_1, x_2, x_3, y_1, ..., y_5) =$ $p(x_1)p(x_2)p(x_3)p(y_1|x_1, x_2, x_3)p(y_2|x_1, x_2, x_3) ... p(y_5|x_1, x_2, x_3)$ With topological ordering $(x_1, x_2, x_3, y_1, y_2, y_3, y_4, y_5)$: All satisfy: $x_i \perp x_j \quad y_2 \perp y_1 \mid x_1, x_2, x_3 \quad y_3 \perp y_1, y_2 \mid x_1, x_2, x_3$ $y_4 \perp y_1, y_2, y_3 \mid x_1, x_2, x_3 \quad y_5 \perp y_1, y_2, y_3, y_4 \mid x_1, x_2, x_3$

Program

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2. Three canonical connections in a DAG and their properties

3. Independencies in directed graphical models

Further independence properties?

- Parent-child links in the graph encode (conditional) independence properties.
- Ordered Markov property yields sets of independence assertions.
- Questions:
 - For any triple of random variables (x, y, z), can we determine whether x ⊥⊥ y | z holds?
 - Does the graph induce or impose additional independencies on any probability distribution that factorises over the graph?
- Important because
 - it yields increased understanding of the properties of the model
 - we can exploit the independencies e.g. for inference and learning
- Approach: Investigate how probabilistic evidence that becomes available at a node can "flow" through the DAG and influence our belief about another node.

1. Definition of directed graphical models

- 2. Three canonical connections in a DAG and their properties
 - Serial connection
 - Diverging connection
 - Converging connection
 - I-equivalence

3. Independencies in directed graphical models

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

Serial connection $\xrightarrow{\times} \xrightarrow{\simeq} \xrightarrow{\vee}$

- Markov model is made up of serial connections
- Graph: x influences z, which in turn influences y but no direct influence from x to y.
- Factorisation: p(x, z, y) = p(x)p(z|x)p(y|z)
- Ordered Markov property: y II x | z If the state or value of z is known (i.e. if the random variable z is "instantiated"), evidence about x will not change our belief about y, and vice versa.

We say that the z node is "closed" and that the trail between x and y is "blocked" by the instantiated z. In other words, knowing the value of z blocks the flow of evidence between x and y.

- What can we say about the marginal distribution of (x, y)?
- By sum rule, joint probability distribution of (x, y) is

$$p(x, y) = \int p(x)p(z|x)p(y|z)dz$$
$$= p(x)\int p(z|x)p(y|z)dz$$
$$\neq p(x)p(y)$$

- In a serial connection, if the state of z is unknown, then evidence or information about x will influence our belief about y, and the other way around. Evidence can flow through z between x and y.
- We say that the z node is "open" and the trail between x and y is "active".

Diverging connection $x \rightarrow z \rightarrow y$

- Graph for probabilistic PCA, factor analysis, ICA has such connections (z correspond to the latents, x and y to the observed)
- Graph: z influences both x and y. No directed connection between x and y.
- Factorisation: p(x, y, z) = p(z)p(x|z)p(y|z)
- Ordered Markov property (with ordering z, x, y): y \product x | z If the state or value z is known, evidence about x will not change our belief about y, and vice versa.
- As in serial connection, knowing z closes the z node, which blocks the trail between x and y.

Diverging connection $x \rightarrow y$

- What can we say about the marginal distribution of (x, y)?
- By sum rule, joint probability distribution of (x, y) is

$$p(x, y) = \int p(z)p(x|z)p(y|z)dz$$
$$\neq p(x)p(y)$$

- In a diverging connection, as in the serial connection, if the state of z is unknown, then evidence or information about x will influence our belief about y, and the other way around. Evidence can flow through z between x and y.
- ► The *z* node is open and the trail between *x* and *y* is active.

Converging connection $\xrightarrow{}$

- Graph for probabilistic PCA, factor analysis, ICA has such connections (z corresponds to an observed, x and y to two latents)
- Graph: x and y influence z. No direction connection between x and y.
- Factorisation: p(x, y, z) = p(x)p(y)p(z|x, y)
- Ordered Markov property: x III y When we do not have evidence about z, evidence about x will not change our belief about y, and vice versa.
- If no evidence about z is available, the z node is closed, which blocks the trail between x and y.

Converging connection $x \rightarrow x \rightarrow y$

- This means that the marginal distribution of (x, y) factorises:
 p(x, y) = p(x)p(y)
- Conditional distribution of (x, y) given z?

$$p(x, y|z) = \frac{p(x, y, z)}{p(z)} = \frac{p(x)p(y)p(z|x, y)}{\int p(x)p(y)p(z|x, y) dx dy}$$

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

This means that $x \not\perp y \mid z$.

- If evidence or information about z is available, evidence about x will influence the belief about y, and vice versa.
- Information about z opens the z-node, and evidence can flow between x and y.
- Note: information about z means that z or one of its descendents is observed (see tutorials).
 (A node w is a descendant of z if there is a directed path from z to w.)

Explaining away



- 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.

Connection	z node	p(x, y)	p(x, y z)
$x \rightarrow z \rightarrow y$	default: open instantiated: closed	х⊥⊈у	x
$x \leftarrow z \rightarrow y$	default: open instantiated: closed	х ∦_ у	$x \perp \!\!\!\perp y \mid z$
$x \rightarrow z \leftarrow y$	default: closed with evidence: opens	х	x

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.

I-equivalence

- Same independence assertions for
 - $(x \longrightarrow z \longrightarrow y) \qquad (x \longleftarrow z \longleftarrow y) \qquad (x \longleftarrow z \longrightarrow y)$
- The graphs have different causal interpretations Consider e.g. $x \equiv$ rain; $z \equiv$ street wet; $y \equiv$ car accident
- This means that based on statistical dependencies (observational data) alone, we cannot select among the graphs and thus determine what causes what.
- The three directed graphs are said to be independence-equivalent (I-equivalent).

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3. Independencies in directed graphical models

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- D-separation
- Directed local Markov property
- Equivalences of the different Markov properties and the factorisation
- Markov blanket

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.



Let $X = \{x_1, \ldots, x_n\}$, $Y = \{y_1, \ldots, y_m\}$, and $Z = \{z_1, \ldots, z_r\}$ 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.

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*.



D-separation and conditional independence

Theorem: If X and Y are d-separated by Z then $X \perp Y \mid Z$ 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 out (conditional) independencies from the graph
- 2. no restriction on the sets X, Y, Z
- the theorem shows that independencies detected by d-separation do always hold. They are "true positives" ("soundness of d-separation").

Theorem: If X and Y are not d-separated by Z then $X \not\perp Y \mid Z$ 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"

D-separation and conditional independence

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

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

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 $x \perp y$.

D-separation and conditional independence

- 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.
- 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 closed.

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 ⇒ Trail is blocked
 - Ear trail ve ve ve ve
 - 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 ity distributions th blocked too (same arguments). ise over the graph.

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



 $x_1 \perp x_2$ 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



 $x_1 \perp x_2 \mid x_6$ does generally not hold for 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 .



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

Directed local Markov property

- The independencies that you can obtain with the ordered Markov property depend on the topological ordering chosen.
- We introduce the "directed local Markov property" that does not depend on the ordering but only on the graph.
- We say that p(x) satisfies the directed local Markov property with respect to a given DAG with parent sets pa_i if

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

holds for all *i*, where nondesc(x_i) denotes the non-descendants of x_i .

In other words, p(x) satisfying the directed local Markov property means that

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

Directed local Markov property

- We now use d-separation to show an equivalence between p(x) satisfying the ordered and the local Markov property.
- Result: If p(x) satisfies the ordered Markov property it also satisfies the directed local Markov property and vice versa:

 $x_i \perp (\operatorname{pre}_i \setminus \operatorname{pa}_i) | \operatorname{pa}_i \iff x_i \perp (\operatorname{nondesc}(x_i) \setminus \operatorname{pa}_i) | \operatorname{pa}_i$

where nondesc(x_i) denotes the non-descendants of x_i .

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



Directed local Markov property

 $x_i \perp \operatorname{pre}_i \setminus \operatorname{pa}_i | \operatorname{pa}_i \leftarrow x_i \perp \operatorname{nondesc}(x_i) \setminus \operatorname{pa}_i | \operatorname{pa}_i$ follows because $\{x_1, \ldots, x_{i-1}\} \subseteq \operatorname{nondesc}(x_i)$ for all topological orderings

For \Rightarrow consider all trails from x_i to {nondesc(x_i) \ pa_i }.

Two cases: move upwards or downwards:

(1) upward trails are blocked by the parents (2) downward trails must contain a headhead (collider) connection because the $x_j \in$ {nondesc(x_i) \ 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 now follows because all paths from x_i to all elements in $\{\text{nondesc}(x_i) \setminus \text{pa}_i\}$ are blocked.



Summary of the equivalences

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

 $p(\mathbf{x})$ factorises over the DAG $p(\mathbf{x}) = \prod_{i=1}^{d} p(x_i | pa_i)$ $p(\mathbf{x})$ satisfies the ordered MP $x_i \perp pre_i \setminus pa_i | pa_i \text{ for all } i$ $p(\mathbf{x})$ satisfies the directed local MP $x_i \perp nondesc(x_i) \setminus pa_i | pa_i \text{ for all } i$ $p(\mathbf{x})$ satisfies the directed global MPindependencies asserted by d-separation (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

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

 \Rightarrow condition on parents

 Isolate x from its descendants

 \Rightarrow condition on children

- Deal with collider connection
 - $\Rightarrow \text{ condition on}$ 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 $x \perp \{ \text{all vars } \setminus x \setminus MB(x) \} \mid MB(x).$

Program recap

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- Definition via ordered Markov property
- Derive independencies from the ordered Markov property with different topological orderings
- 2. Three canonical connections in a DAG and their properties
 - Serial connection
 - Diverging connection
 - Converging connection
 - I-equivalence
- 3. Independencies in directed graphical models
 - D-separation
 - Directed local Markov property
 - Equivalences of the different Markov properties and the factorisation
 - Markov blanket