

Bayesian networks

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Machine Learning

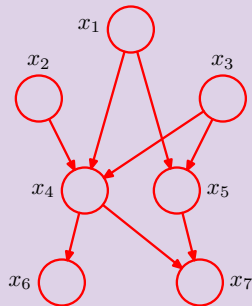
Why

- All probabilistic inference and learning amount at repeated applications of the sum and product rules
- *Probabilistic graphical models* are graphical representations of the *qualitative* aspects of probability distributions allowing to:
 - visualize the structure of a probabilistic model in a simple and intuitive way
 - discover properties of the model, such as conditional independencies, by inspecting the graph
 - express complex computations for inference and learning in terms of graphical manipulations
 - represent multiple probability distributions with the same graph, abstracting from their quantitative aspects (e.g. discrete vs continuous distributions)

Bayesian Networks (BN)

BN Semantics

- A BN structure (\mathcal{G}) is a *directed graphical model*
- Each node represents a random variable x_i
- Each edge represents a direct dependency between two variables



The structure encodes these independence assumptions:

$$\mathcal{I}_\ell(\mathcal{G}) = \{\forall i \ x_i \perp \text{NonDescendants}_{x_i} \mid \text{Parents}_{x_i}\}$$

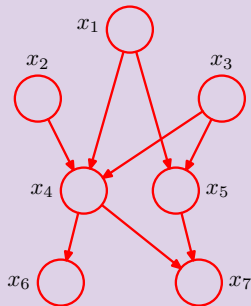
each variable is independent of its non-descendants given its parents

Bayesian Networks

Graphs and Distributions

- Let p be a joint distribution over variables \mathcal{X}
- Let $\mathcal{I}(p)$ be the set of independence assertions holding in p
- \mathcal{G} is an *independency map* (I-map) for p if p satisfies the local independences in \mathcal{G} :

$$\mathcal{I}_\ell(\mathcal{G}) \subseteq \mathcal{I}(p)$$



Note

The reverse is not necessarily true: there can be independences in p that are not modelled by \mathcal{G} .

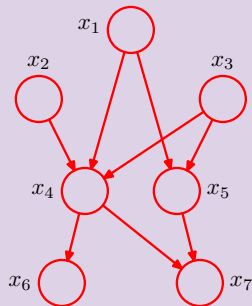
Bayesian Networks

Factorization

- We say that p factorizes according to \mathcal{G} if:

$$p(x_1, \dots, x_m) = \prod_{i=1}^m p(x_i | Pa_{x_i})$$

- If \mathcal{G} is an I-map for p , then p factorizes according to \mathcal{G}
- If p factorizes according to \mathcal{G} , then \mathcal{G} is an I-map for p



Example

$$p(x_1, \dots, x_7) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3) \\ p(x_5|x_1, x_3)p(x_6|x_4)p(x_7|x_4, x_5)$$

Proof: I-map \Rightarrow factorization

- 1 If \mathcal{G} is an I-map for p , then p satisfies (at least) these (local) independences:

$$\{\forall i \ x_i \perp NonDescendants_{x_i} | Parents_{x_i}\}$$

- 2 Let us order variables in a *topological order* relative to \mathcal{G} , i.e.:

$$x_i \rightarrow x_j \Rightarrow i < j$$

- 3 Let us decompose the joint probability using the chain rule as:

$$p(x_1, \dots, x_m) = \prod_{i=1}^m p(x_i | x_1, \dots, x_{i-1})$$

- 4 Local independences imply that for each x_i :

$$p(x_i | x_1, \dots, x_{i-1}) = p(x_i | Pa_{x_i})$$

Bayesian Networks

Proof: factorization \Rightarrow I-map

- 1 If p factorizes according to \mathcal{G} , the joint probability can be written as:

$$p(x_1, \dots, x_m) = \prod_{i=1}^m p(x_i | Pa_{x_i})$$

- 2 Let us consider the last variable x_m (repeat steps for the other variables). By the product and sum rules:

$$p(x_m | x_1, \dots, x_{m-1}) = \frac{p(x_1, \dots, x_m)}{p(x_1, \dots, x_{m-1})} = \frac{p(x_1, \dots, x_m)}{\sum_{x_m} p(x_1, \dots, x_m)}$$

- 3 Applying factorization and isolating the only term containing x_m we get:

$$= \frac{\prod_{i=1}^m p(x_i | Pa_{x_i})}{\sum_{x_m} \prod_{i=1}^m p(x_i | Pa_{x_i})} = \frac{p(x_m | Pa_{x_m}) \prod_{i=1}^{m-1} p(x_i | Pa_{x_i})}{\prod_{i=1}^{m-1} p(x_i | Pa_{x_i}) \sum_{x_m} p(x_m | Pa_{x_m})}$$

Definition

A Bayesian Network is a pair (\mathcal{G}, p) where p factorizes over \mathcal{G} and it is represented as a set of conditional probability distributions (cpd) associated with the nodes of \mathcal{G} .

Factorized Probability

$$p(x_1, \dots, x_m) = \prod_{i=1}^m p(x_i | Pa_{x_i})$$

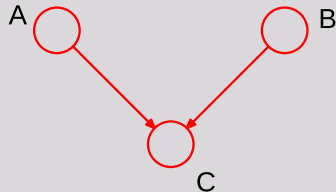
Bayesian Networks

Example: toy regulatory network

- Genes *A* and *B* have independent prior probabilities
- Gene *C* can be enhanced by both *A* and *B*

gene	value	P(value)
A	active	0.3
A	inactive	0.7

gene	value	P(value)
B	active	0.3
B	inactive	0.7



		A			
		active		inactive	
		B		B	
		active	inactive	active	inactive
C	active	0.9	0.6	0.7	0.1
C	inactive	0.1	0.4	0.3	0.9

Conditional independence

Introduction

- Two variables a, b are independent (written $a \perp b \mid \emptyset$) if:

$$p(a, b) = p(a)p(b)$$

- Two variables a, b are conditionally independent given c (written $a \perp b \mid c$) if:

$$p(a, b \mid c) = p(a \mid c)p(b \mid c)$$

- Independence assumptions can be verified by repeated applications of sum and product rules
- Graphical models allow to directly verify them through the *d-separation* criterion

Tail-to-tail

- Joint distribution:

$$p(a, b, c) = p(a|c)p(b|c)p(c)$$

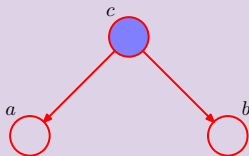
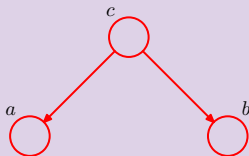
- a and b are **not independent**
(written $a \not\perp\!\!\!\perp b \mid \emptyset$):

$$p(a, b) = \sum_c p(a|c)p(b|c)p(c) \neq p(a)p(b)$$

- a and b are **conditionally independent given c** :

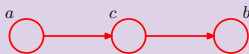
$$p(a, b|c) = \frac{p(a, b, c)}{p(c)} = p(a|c)p(b|c)$$

- c is *tail-to-tail* wrt to the path $a \rightarrow b$ as it is connected to the tails of the two arrows



Head-to-tail

- Joint distribution:

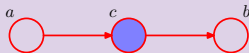


$$p(a, b, c) = p(b|c)p(c|a)p(a) = p(b|c)p(a|c)p(c)$$

- a and b are **not independent**:

$$p(a, b) = p(a) \sum_c p(b|c)p(c|a) \neq p(a)p(b)$$

- a and b are **conditionally independent given c** :



$$p(a, b|c) = \frac{p(b|c)p(a|c)p(c)}{p(c)} = p(b|c)p(a|c)$$

- c is *head-to-tail* wrt to the path $a \rightarrow b$ as it is connected to the head of an arrow and to the tail of the other one

Head-to-head

- Joint distribution:

$$p(a, b, c) = p(c|a, b)p(a)p(b)$$

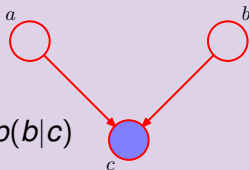
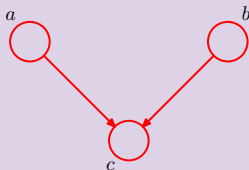
- a and b are **independent**:

$$p(a, b) = \sum_c p(c|a, b)p(a)p(b) = p(a)p(b)$$

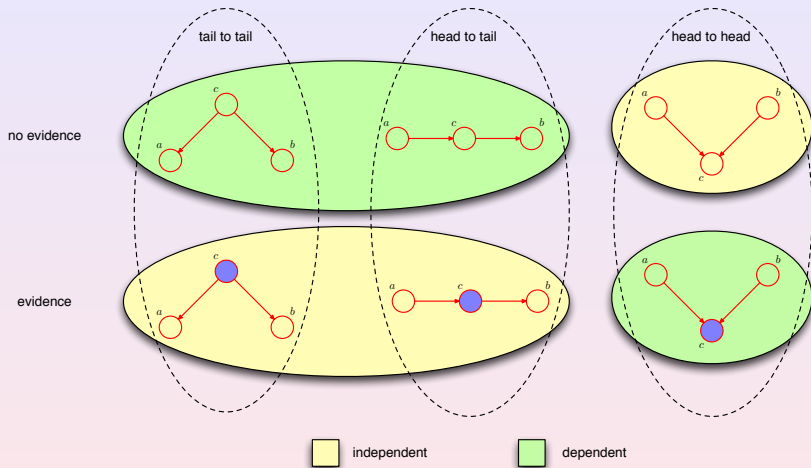
- a and b are **not conditionally independent given c** :

$$p(a, b|c) = \frac{p(c|a, b)p(a)p(b)}{p(c)} \neq p(a|c)p(b|c)$$

- c is *head-to-head* wrt to the path $a \rightarrow b$ as it is connected to the heads of the two arrows



d-separation: basic rules summary



Example of head-to-head connection

Setting

- A fuel system in a car:

battery B , either charged ($B = 1$) or flat ($B = 0$)

fuel tank F , either full ($F = 1$) or empty ($F = 0$)

electric fuel gauge G , either full ($G = 1$) or empty ($G = 0$)

Conditional probability tables (CPT)

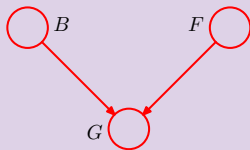
- Battery and tank have independent prior probabilities:

$$P(B = 1) = 0.9 \quad P(F = 1) = 0.9$$

- The fuel gauge is conditioned on both (unreliable!):

$$P(G = 1|B = 1, F = 1) = 0.8 \quad P(G = 1|B = 1, F = 0) = 0.2$$

$$P(G = 1|B = 0, F = 1) = 0.2 \quad P(G = 1|B = 0, F = 0) = 0.1$$



Example of head-to-head connection

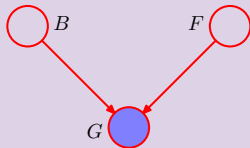
Probability of empty tank

- Prior:

$$P(F = 0) = 1 - P(F = 1) = 0.1$$

- Posterior after observing empty fuel gauge:

$$P(F = 0 | G = 0) = \frac{P(G = 0 | F = 0)P(F = 0)}{P(G = 0)} \simeq 0.257$$



Note

The probability that the tank is empty *increases* from observing that the fuel gauge reads empty (not as much as expected because of strong prior and unreliable gauge)

Example of head-to-head connection

Derivation

$$\begin{aligned}P(G = 0|F = 0) &= \sum_{B \in \{0,1\}} P(G = 0, B|F = 0) \\&= \sum_{B \in \{0,1\}} P(G = 0|B, F = 0)P(B|F = 0) \\&= \sum_{B \in \{0,1\}} P(G = 0|B, F = 0)P(B) = 0.81\end{aligned}$$

$$\begin{aligned}P(G = 0) &= \sum_{B \in \{0,1\}} \sum_{F \in \{0,1\}} P(G = 0, B, F) \\&= \sum_{B \in \{0,1\}} \sum_{F \in \{0,1\}} P(G = 0|B, F)P(B)P(F)\end{aligned}$$

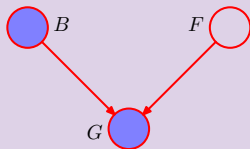
Example of head-to-head connection

Probability of empty tank

- Posterior after observing that the battery is also flat:

$$P(F = 0 | G = 0, B = 0) =$$

$$\frac{P(G = 0 | F = 0, B = 0)P(F = 0 | B = 0)}{P(G = 0 | B = 0)} \simeq 0.111$$



Note

- The probability that the tank is empty *decreases* after observing that the battery is also flat
- The battery condition *explains away* the observation that the fuel gauge reads empty
- The probability is still greater than the prior one, because the fuel gauge observation still gives some evidence in favour of an empty tank

General Head-to-head

- Let a *descendant* of a node x be any node which can be reached from x with a path following the direction of the arrows
- A head-to-head node c unblocks the dependency path between its parents if either itself or *any of its descendants* receives evidence

General d -separation criterion

d-separation definition

- Given a generic Bayesian network
- Given A, B, C arbitrary nonintersecting sets of nodes
- The sets A and B are d -separated by C ($dsep(A; B|C)$) if:
 - All paths from any node in A to any node in B are *blocked*
- A path is blocked if it includes at least one node s.t. either:
 - the arrows on the path meet tail-to-tail or head-to-tail at the node and it is in C , or
 - the arrows on the path meet head-to-head at the node and neither it nor any of its descendants is in C

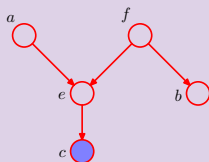
d-separation implies conditional independence

The sets A and B are independent given C ($A \perp B | C$) if they are d -separated by C .

Example of general d-separation

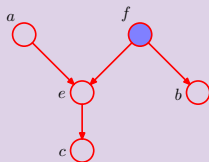
$$a \not\perp b | c$$

- Nodes a and b are **not d-separated** by c :
 - Node f is tail-to-tail and not observed
 - Node e is head-to-head and its child c is observed



$$a \perp b | f$$

- Nodes a and b are **d-separated** by f :
 - Node f is tail-to-tail and observed



Independence assumptions

- A BN structure \mathcal{G} encodes a set of *local* independence assumptions:

$$\mathcal{I}_\ell(\mathcal{G}) = \{\forall i x_i \perp \text{NonDescendants}_{x_i} \mid \text{Parents}_{x_i}\}$$

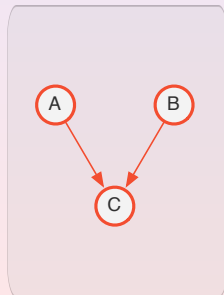
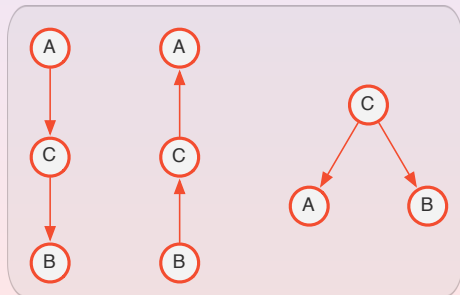
- A BN structure \mathcal{G} encodes a set of *global* (Markov) independence assumptions:

$$\mathcal{I}(\mathcal{G}) = \{(A \perp B \mid C) : \text{dsep}(A; B \mid C)\}$$

BN equivalence classes

I-equivalence

- Quite different BN structures can actually encode the exact same set of independence assumptions
- Two BN structures \mathcal{G} and \mathcal{G}' are *I-equivalent* if $\mathcal{I}(\mathcal{G}) = \mathcal{I}(\mathcal{G}')$
- The space of BN structures over \mathcal{X} is partitioned into a set of mutually exclusive and exhaustive *I-equivalence classes*



Minimal I-maps

- For a structure \mathcal{G} to be an I-map for p , it does not need to encode all its independences (e.g. a fully connected graph is an I-map of any p defined over its variables)
- A *minimal I-map* for p is an I-map \mathcal{G} which can't be “reduced” into a $\mathcal{G}' \subset \mathcal{G}$ (by removing edges) that is also an I-map for p .

Problem

A minimal I-map for p does not necessarily capture all the independences in p .

Perfect Maps (P-maps)

- A structure \mathcal{G} is a *perfect map* (P-map) for p if it captures all (and only) its independences:

$$\mathcal{I}(\mathcal{G}) = \mathcal{I}(p)$$

- There exists an algorithm for finding a P-map of a distribution which is exponential in the in-degree of the P-map.
- The algorithm returns an equivalence class rather than a single structure

Problem

Not all distributions have a P-map. Some cannot be modelled exactly by the BN formalism.

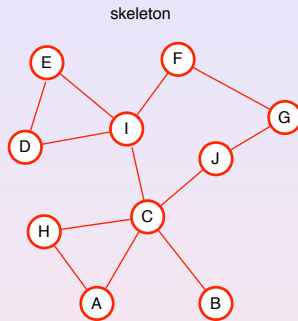
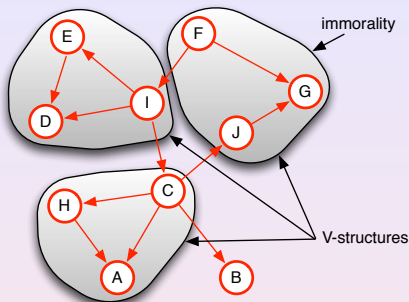
Practical Suggestions

- Get together with a domain expert
- Define variables for entities that can be *observed* or that you can be interested in *predicting* (latent variables can also be sometimes useful)
- Try following *causality* considerations in adding edges (more interpretable and sparser networks)
- In defining probabilities for configurations (almost) never assign zero probabilities
- If data are available, use them to help in *learning* parameters and structure (we'll see how)

Appendix

Additional reference material

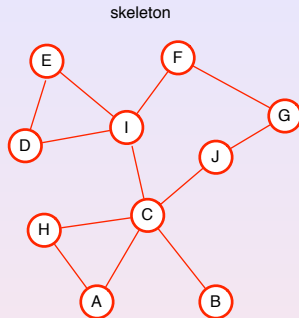
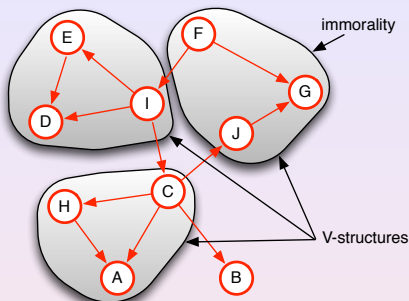
I-equivalence



Sufficient conditions

If two structures \mathcal{G} and \mathcal{G}' have the **same skeleton** and the **same set of v-structures** then they are I-equivalent

I-equivalence



Necessary and sufficient conditions

*Two structures \mathcal{G} and \mathcal{G}' are I-equivalent if and only if they have the **same skeleton** and the **same set of immoralities***

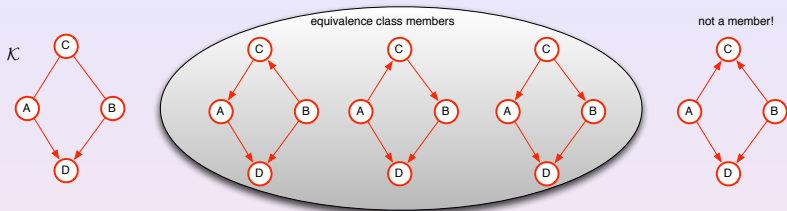
Partially directed acyclic graph (PDAG)

A PDAG is an acyclic graph with both directed and undirected edges

Representing an equivalence class

- An equivalence class for a structure \mathcal{G} can be represented by a PDAG \mathcal{K} such that:
 - If $x \rightarrow y \in \mathcal{K}$ then $x \rightarrow y$ should appear in all structures which are I-equivalent to \mathcal{G}
 - If $x - y \in \mathcal{K}$ then we can find a structure \mathcal{G}' that is I-equivalent to \mathcal{G} such that $x \rightarrow y \in \mathcal{G}'$

Equivalence class members



Generating members

- Representatives from \mathcal{K} can be obtained by adding directions to undirected edges
- One needs to check that the resulting structure has the **same set of immoralities** as \mathcal{K} (otherwise it's not in the equivalence class)

Markov blanket (or boundary)

Definition

- Given a directed graph with m nodes
- The *markov blanket* of node x_i is the minimal set of nodes making it x_i independent on the rest of the graph:

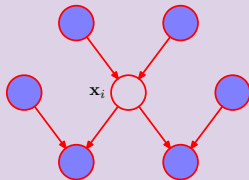
$$\begin{aligned} p(x_i | x_{j \neq i}) &= \frac{p(x_1, \dots, x_m)}{p(x_{j \neq i})} = \frac{p(x_1, \dots, x_m)}{\int p(x_1, \dots, x_m) dx_i} \\ &= \frac{\prod_{k=1}^m p(x_k | pa_k)}{\int \prod_{k=1}^m p(x_k | pa_k) dx_i} \end{aligned}$$

- All components which do not include x_i will cancel between numerator and denominator
- The only remaining components are:
 - $p(x_i | pa_i)$ the probability of x_i given its parents
 - $p(x_j | pa_j)$ where pa_j includes $x_i \Rightarrow$ the children of x_i with their *co-parents*

Markov blanket (or boundary)

d-separation

- Each parent x_j of x_i will be head-to-tail or tail-to-tail in the path btw x_i and any of x_j other neighbours \Rightarrow blocked
- Each child x_j of x_i will be head-to-tail in the path btw x_i and any of x_j children \Rightarrow blocked
- Each co-parent x_k of a child x_j of x_i be head-to-tail or tail-to-tail in the path btw x_j and any of x_k other neighbours \Rightarrow blocked



Example of i.i.d. samples

Maximum-likelihood

- We are given a set of instances $\mathcal{D} = \{x_1, \dots, x_N\}$ drawn from an univariate Gaussian with unknown mean μ
- All paths between x_i and x_j are blocked if we condition on μ
- The examples are independent of each other given μ :

$$p(\mathcal{D}|\mu) = \prod_{i=1}^N p(x_i|\mu)$$

- A set of nodes with the same variable type and connections can be compactly represented using the *plate* notation

