Introduction to Statistical Machine Learning

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(Many figures from C. M. Bishop, "Pattern Recognition and Machine Learning")

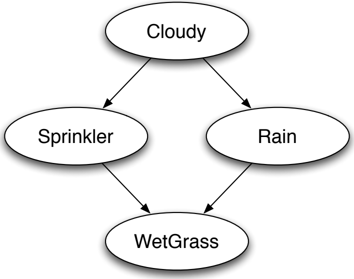
Outlines

Part XIII

Probabilistic Graphical Models 1

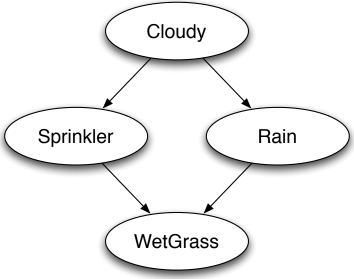
Motivation via Independence

- Why is the grass wet?



Motivation via Independence

- Why is the grass wet?



- Introduce four Boolean variables :
  $C(loudy), S(prinkler), R(ain), W(etGrass) \in \{F(alse), T(rue)\}$.

Motivation via Independence

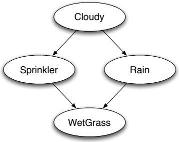
- Model the conditional probabilities

p(C = F)	p(C = T)
0.2	0.8

C	p(S = F)	p(S = T)
F	0.5	0.5
T	0.9	0.1

C	p(R = F)	p(R = T)
F	0.8	0.2
T	0.2	0.8

S R	p(W = F)	p(W = T)
F F	1.0	0.0
T F	0.1	0.9
F T	0.1	0.9
T T	0.01	0.99

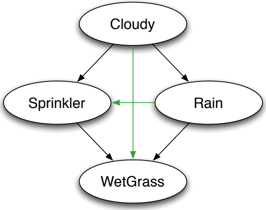


Motivation via Independence

- If everything depends on everything

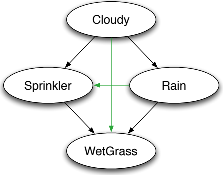
C S R W	p(C, S, R, W)
F F F F	...
F F F T	...
...	...
T T T F	...
T T T T	...

$$
\begin{aligned}
p(W, S, R, C) &= p(W \mid S, R, C)\, p(S, R, C) \\
&= p(W \mid S, R, C)\, p(S \mid R, C)\, p(R, C) \\
&= p(W \mid S, R, C)\, p(S \mid R, C)\, p(R \mid C)\, p(C)
\end{aligned}
$$

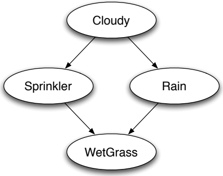


Motivation via Independence

$$p(W) = \sum_{S,R,C} p(W \mid S, R, C)\, p(S \mid R, C)\, p(R \mid C)\, p(C)$$



$$p(W) = \sum_{S,R} p(W \mid S, R) \sum_{C} p(S \mid C)\, p(R \mid C)\, p(C)$$



Motivation via Distributive Law

- Two key observations when dealing with probabilities
  1. Distributive Law can save operations

$$\underbrace{a(b+c)}_{\text{2 operations}} = \underbrace{ab+ac}_{\text{3 operations}}$$

  2. If some probabilities do not depend on all random variables, we might be able to factor them out. For example, assume

$$p(x_1, x_3 \mid x_2) = p(x_1 \mid x_2)\, p(x_3 \mid x_2),$$

then (using $\sum_{x_3} p(x_3 \mid x_2) = 1$)

$$\begin{aligned} p(x_1) &= \sum_{x_2, x_3} p(x_1, x_2, x_3) = \sum_{x_2, x_3} p(x_1, x_3 \mid x_2)\, p(x_2) \\ &= \underbrace{\sum_{x_2, x_3} p(x_1 \mid x_2)\, p(x_3 \mid x_2)\, p(x_2)}_{O(|\mathcal{X}_1||\mathcal{X}_2||\mathcal{X}_3|)} = \underbrace{\sum_{x_2} p(x_1 \mid x_2)\, p(x_2)}_{O(|\mathcal{X}_1||\mathcal{X}_2|)} \end{aligned}$$

Motivation via Complexity Reduction

- How to deal with more complex expression?

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

Motivation via Complexity Reduction

- How to deal with more complex expression?

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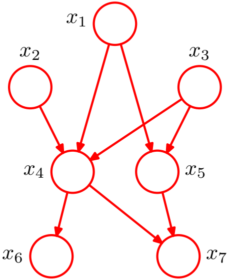
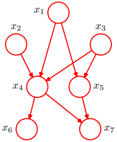
- Graphical models



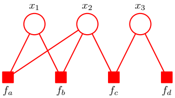
Probabilistic Graphical Models

Graphical models

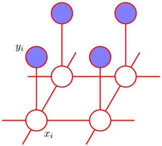
- Visualise the structure of a probabilistic model
- Complex computations with formulas $\rightarrow$ manipulations with graphs
- Obtain insights into model properties by inspection
- Develop and motivate new models



Bayesian Network



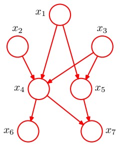
Factor Graph



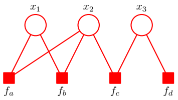
Markov Random Field

Probabilistic Graphical Models

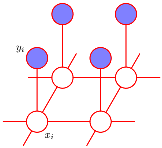
- Graph
  1. Nodes (vertices) : a random variable
  2. Edges (links, arcs; directed or undirected) : probabilistic relationship
- Directed Graph : Bayesian Network (also called Directed Graphical Model) expressing causal relationship between variables
- Undirected Graph : Markov Random Field expressing soft constraints between variables
- Factor Graph : convinient for solving inference problems (derived from Bayesian Networks or Markov Random Fields).



Bayesian Network



Factor Graph



Markov Random Field

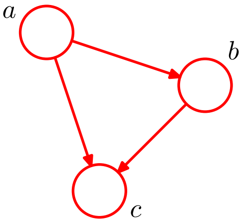
Bayesian Network

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

Bayesian Network

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

1. Draw a node for each conditional distribution associated with a random variable.
2. Draw an edge from each conditional distribution associated with a random variable to all other conditional distribution which are conditioned on this variable.



- We have chosen a particular ordering of the variables !

Bayesian Network

- General case for K variables

$$p(x_1, \dots, x_K) = p(x_K \,|\, x_1, \dots, x_{K-1}) \dots p(x_2 \,|\, x_1)\, p(x_1)$$

- The graph of this distribution is fully connected. (Prove it.)
- What happens if we deal with a distribution represented by a graph which is not fully connected?
- Can not be the most general distribution anymore.
- The absence of edges carries important information.

Bayesian Network - Joint Distribution $\rightarrow$ Graph

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

Bayesian Network - Joint Distribution $\rightarrow$ Graph

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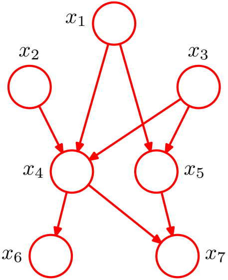
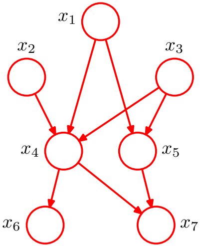
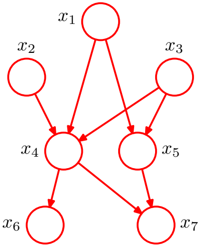


Bayesian Network - Graph → Joint Distribution



Can we get the expression from the graph?

Bayesian Network - Graph $\rightarrow$ Joint Distribution



Can we get the expression from the graph?

1. Write a product of probability distributions, one for each associated random variable. $\leftrightarrow$ Draw a node for each conditional distribution associated with a random variable.
2. Add all random variables associated with parent nodes to the list of conditioning variables. $\leftrightarrow$ Draw an edge from each conditional distribution associated with a random variable to all other conditional distribution which are conditioned on this variable.

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

Bayesian Network - Joint Distribution $\leftrightarrow$ Graph

- The joint distribution defined by a graph is given by the product, over all of the nodes of the graph, of a conditional distribution for each node conditioned on the variables corresponding to the parents of the node in the graph.

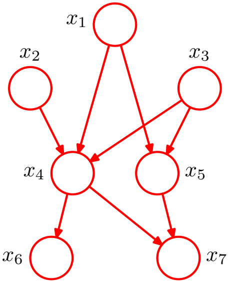
$$p(\mathbf{x}) = \prod_{k=1}^{K} p(x_k \mid \mathrm{pa}(x_k))$$

  where $\mathrm{pa}(x_k)$ denotes the set of parents of x_k and $\mathbf{x} = (x_1, \dots, x_K)$.

- Restriction : Graph must be a directed acyclic graph (DAG).

Bayesian Network - Joint Distribution $\leftrightarrow$ Graph

- Restriction : Graph must be a directed acyclic graph (DAG).
- There are no closed paths in the graph when moving along the directed edges.
- Or equivalently: There exists an ordering of the nodes such that there are no edges that go from any node to any lower numbered node.



- Extension: Can also have sets of variables, or vectors at a node.

Bayesian Network - Joint Distribution $\leftrightarrow$ Graph

- Given

$$p(\mathbf{x}) = \prod_{k=1}^{K} p(x_k \mid \mathrm{pa}(x_k)).$$

- Is $p(\mathbf{x})$ normalised, $\sum_{\mathbf{x}} p(\mathbf{x}) = 1$?

Bayesian Network - Joint Distribution $\leftrightarrow$ Graph

- Given
$$p(\mathbf{x}) = \prod_{k=1}^{K} p(x_k \mid \mathrm{pa}(x_k)).$$
- Is $p(\mathbf{x})$ normalised, $\sum_{\mathbf{x}} p(\mathbf{x}) = 1$?
- As graph is DAG, there always exists a node with no outgoing edges, say x_i.

$$\sum_{\mathbf{x}} p(\mathbf{x}) = \sum_{x_1,\dots,x_{i-1},x_{i+1},\dots,x_K} \prod_{\substack{k=1 \\ k \neq i}}^{K} p(x_k \mid \mathrm{pa}(x_k)) \quad \underbrace{\sum_{x_i} p(x_i \mid \mathrm{pa}(x_i))}_{=1}$$

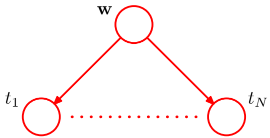
because $\sum_{x_i} p(x_i \mid \mathrm{pa}(x_i)) = \sum_{x_i} \frac{p(x_i, \mathrm{pa}(x_i))}{p(\mathrm{pa}(x_i))} = \frac{p(\mathrm{pa}(x_i))}{p(\mathrm{pa}(x_i))} = 1$

- Repeat, until no node left.

Bayesian Network - Plate Notation

- Bayesian polynomial regression : observed inputs $\mathbf{x}$, observed targets $\mathbf{t}$, noise variance σ^2, hyperparameter α controlling the priors for $\mathbf{w}$.
- Focusing on $\mathbf{t}$ and $\mathbf{w}$ only

$$p(\mathbf{t}, \mathbf{w}) = p(\mathbf{w}) \prod_{k=1}^{N} p(t_n \mid \mathbf{w})$$



Bayesian Network - Plate Notation

- Bayesian polynomial regression : observed inputs **x**, observed targets **t**, noise variance σ^2, hyperparameter α controlling the priors for $\mathbf{w}$.
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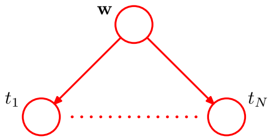
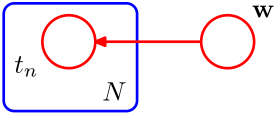
$$p(\mathbf{t}, \mathbf{w}) = p(\mathbf{w}) \prod_{k=1}^{N} p(t_n \mid \mathbf{w})$$





A plate.

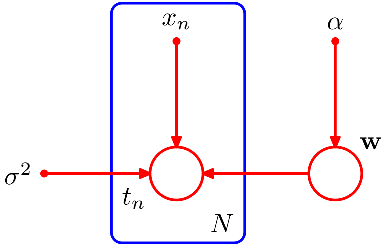
Bayesian Network - Plate Notation

- Include also the parameters into the graphical model

$$p(\mathbf{t}, \mathbf{w} \mid \mathbf{x}, \alpha, \sigma^2) = p(\mathbf{w} \mid \alpha) \prod_{k=1}^{N} p(t_n \mid \mathbf{w}, x_n, \sigma^2)$$

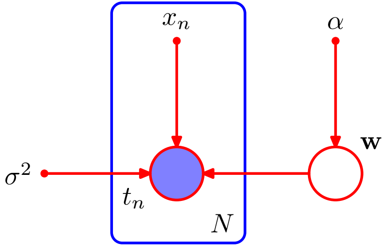
Random variables = open circles

Deterministic variables = smaller solid circles



Bayesian Network - Plate Notation

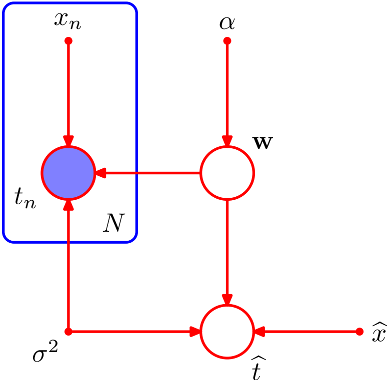
- Random variables
  - Observed random variables, e.g. $\mathbf{t}$
  - Unobserved random variables, e.g. $\mathbf{w}$, (latent random variables, hidden random variables)
- Shade the observed random variables in the graphical model.



Bayesian Network - Plate Notation

- Prediction : new data point $\widehat{x}$. Want to predict $\widehat{t}$.

$$p(\widehat{t}, \mathbf{t}, \mathbf{w} \,|\, \widehat{x}, \mathbf{x}, \alpha, \sigma^2) = \left[\prod_{k=1}^{N} p(t_n \,|\, x_n, \mathbf{w}, \sigma^2)\right] p(\mathbf{w} \,|\, \alpha)\, p(\widehat{t} \,|\, \widehat{x}, \mathbf{w}, \sigma^2)$$



Polynomial regression model including prediction.

Bayesian Network - Conditional Independence

Definition (Conditional Independence)

If for three random variables a, b, and c the following holds

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

then a is conditionally independent of b given c.
Notation : $a \perp\!\!\!\perp b \,|\, c$.

- The above equation must hold for all possible values of c.
- Consequence :

$$\begin{aligned} p(a, b \,|\, c) &= p(a \,|\, b, c)\, p(b \,|\, c) \\ &= p(a \,|\, c)\, p(b \,|\, c) \end{aligned}$$

- Conditional independence simplifies
  - the structure of the model
  - the computations needed to perform interference/learning.

Bayesian Network - Conditional Independence

Rules for Conditional Independence

Symmetry : $X \perp\!\!\!\perp Y \mid Z \Longrightarrow Y \perp\!\!\!\perp X \mid Z$

Decomposition : $Y, W \perp\!\!\!\perp X \mid Z \Longrightarrow Y \perp\!\!\!\perp X \mid Z$ and $W \perp\!\!\!\perp X \mid Z$

Weak Union : $X \perp\!\!\!\perp Y, W \mid Z \Longrightarrow X \perp\!\!\!\perp Y \mid Z, W$

Contraction : $X \perp\!\!\!\perp W \mid Z, Y$

and $X \perp\!\!\!\perp Y \mid Z \Longrightarrow X \perp\!\!\!\perp W, Y \mid Z$

Intersection : $X \perp\!\!\!\perp Y \mid Z, W$

and $X \perp\!\!\!\perp W \mid Z, Y \Longrightarrow X \perp\!\!\!\perp Y, W \mid Z$

Note: Intersection is only valid for $p(X), p(Y), p(Z), p(W) > 0$.

Bayesian Network - Conditional Independence

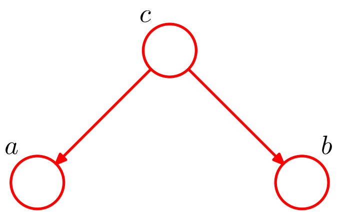
- Can we work with the graphical model directly?
- Check the simplest examples containing only three nodes.
- First example has joint distribution

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

- Marginalise both sides over c

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

- Does not hold : $a \perp\!\!\!\perp b \,|\, \emptyset$ (where $\emptyset$ is the empty set).

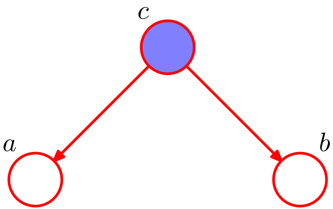


Bayesian Network - Conditional Independence

- Now condition on c.

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

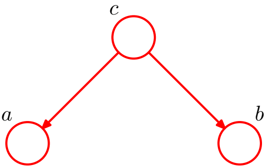
- Therefore $a \perp\!\!\!\perp b \mid c$.



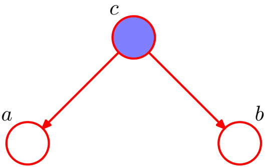
Bayesian Network - Conditional Independence

Graphical interpretation

- In both graphical models there is a path from a to b.
- The node c is called tail-to-tail (TT) with respect to this path because the node c is connected to the tails of the arrows in the path.
- The presence of the TT-node c in the path left renders a dependend on b (and b dependend on a).
- Conditioning on c blocks the path from a to b and causes a and b to become conditionally independent on c.



Not $a \perp\!\!\!\perp b \mid \emptyset$



$a \perp\!\!\!\perp b \mid c$

Bayesian Network - Conditional Independence

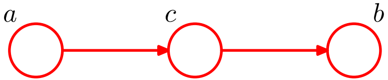
- Second example.

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

- Marginalise over c to test for independence.

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

- Does not hold : $a \perp\!\!\!\perp b \mid \emptyset$.

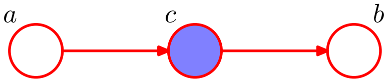


Bayesian Network - Conditional Independence

- Now condition on c.

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

  where we used Bayes' theorem $p(c \mid a) = p(a \mid c)\, p(c) / p(a)$.
- Therefore $a \perp\!\!\!\perp b \mid c$.



Bayesian Network - Conditional Independence

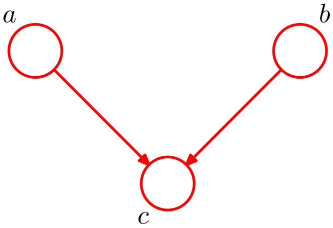
- Third example. (A little bit more subtle.)

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

- Marginalise over c to test for independence.

$$\begin{aligned} p(a, b) &= \sum_c p(a)\, p(b)\, p(c \mid a, b) = p(a)\, p(b) \sum_c p(c \mid a, b) \\ &= p(a)\, p(b) \end{aligned}$$

- a and b are independent if NO variable is observed: $a \perp\!\!\!\perp b \mid \emptyset$.



Bayesian Network - Conditional Independence

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

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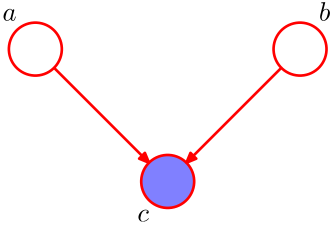
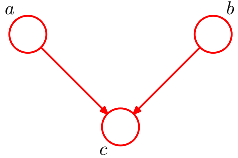


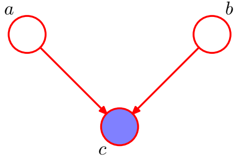
Bayesian Network - Conditional Independence

Graphical interpretation

- In both graphical models there is a path from a to b.
- The node c is called head-to-head (HH) with respect to this path because the node c is connected to the heads of the arrows in the path.
- The presence of the HH-node c in the path left makes a independent of b (and b independent of a). The unobserved c blocks the path from a to b.



$a \perp\!\!\!\perp b \mid \emptyset$

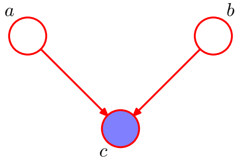


Not $a \perp\!\!\!\perp b \mid c$

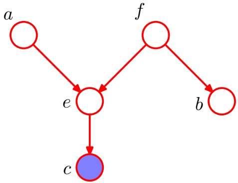
Bayesian Network - Conditional Independence

Graphical interpretation

- Conditioning on c unblocks the path from a to b, and renders a conditionally dependent on b given c.
- Some more terminology: Node y is a descendant of node x if there is a path from x to y in which each step follows the directions of the arrows.
- A HH-path will become unblocked if either the node, or any of its descendants, is observed.



Not $a \perp\!\!\!\perp b \mid c$



Not $a \perp\!\!\!\perp f \mid c$

Conditional Independence - Factorisation

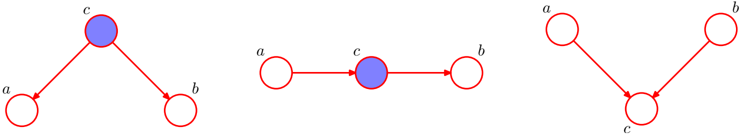
- Conditional Independence and Factorisation have been shown to be equivalent for all possible configuration of three nodes.
- Are they equivalent for any Bayesian Networks?
- Characterise which conditional independence statements hold for an arbitrary factorisation and check whether a distribution satisfying those statements will have such a factorisation.

Bayesian Network - D-Separation

Definition (Blocked Path)

A blocked path is a path which contains

- an observed TT- or HT-node, or
- an unobserved HH-node whose descendants are all unobserved.



Bayesian Network - D-Separation

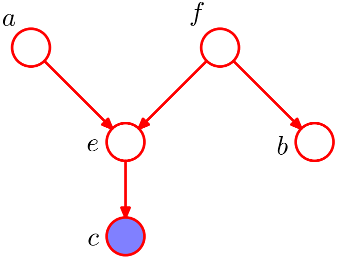
- Consider a general directed graph in which A, B, and C are arbitrary non-intersecting sets of nodes. (There may be other nodes in the graph which are not contained in the union of A, B, and C.)
- Consider all possible paths from any node in A to any node in B.
- Any such path is blocked, if it includes a node such that either
  - the node is HT or TT, and the node is in set C, or
  - the node is HH, and neither the node, nor any of the descendants, is in set C.
- If all paths are blocked, then A is $d-$ separated from B by C, and the joint distribution over all the variables in the graph will satisfy $A \perp\!\!\!\perp B \mid C$.

(Note: D-separation stands for 'directional' separation.)

Bayesian Network - D-separation

Example

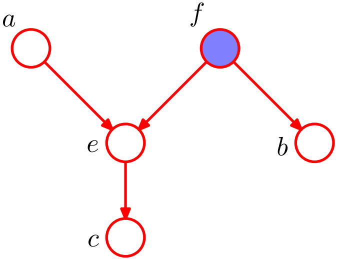
- The path from a to b is not blocked by f because f is a TT-node and unobserved.
- The path from a to b is not blocked by e because e is a HH-node, and although unobserved itself, one of its descendants (node c) is observed.



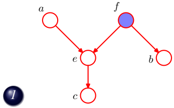
Bayesian Network - D-separation

Another example

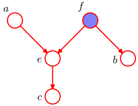
- The path from a to b is blocked by f because f is a TT-node and observed. Therefore, $a \perp\!\!\!\perp b \mid f$.
- Furthermore, the path from a to b is also blocked by e because e is a HH-node, and neither it nor its descendants are observed. Therefore $a \perp\!\!\!\perp b \mid f$.



Finding $p(a, b \mid f)$ - 'Analytical' method



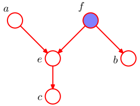
Finding $p(a, b \mid f)$ - 'Analytical' method

1. 

2. Conditional probability with the given observable(s):

$$p(a, b, c, e \mid f)$$

Finding $p(a, b \mid f)$ - 'Analytical' method

1. 

2. Conditional probability with the given observable(s):

$$p(a, b, c, e \mid f)$$

3. Rewrite it as a joint distribution over all variables

$$p(a, b, c, e \mid f) = \frac{p(a, b, c, e, f)}{p(f)}$$

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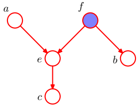
1. 

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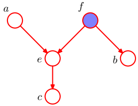
4. Factorise the joint probability according to the graph

$$p(a, b, c, e \mid f) = \frac{p(a, b, c, e, f)}{p(f)} = \frac{p(a)\, p(f)\, p(e \mid a, f)\, p(b \mid f)\, p(c \mid e)}{p(f)}$$

Finding $p(a, b \mid f)$ - 'Analytical' method

1. 

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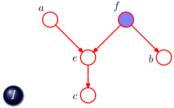
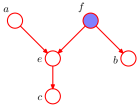
5. Marginalise over all variables we don't care about

$$p(a, b \mid f) = \sum_{c,e} \frac{p(a)\, p(f)\, p(e \mid a, f)\, p(b \mid f)\, p(c \mid e)}{p(f)} = p(a)\, p(b \mid f)$$

Finding $p(a, b \mid f)$ - 'Graphical' method

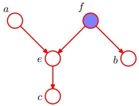


Finding $p(a, b \mid f)$ - 'Graphical' method

1. 

2. Check whether $a \perp\!\!\!\perp b \mid f$ holds or not.
Result : $a \perp\!\!\!\perp b \mid f$ holds.
    - Reason : The path from a to b is blocked by f because f is a TT-node and observed. Therefore, $a \perp\!\!\!\perp b \mid f$.

Finding $p(a, b \mid f)$ - 'Graphical' method

1. 

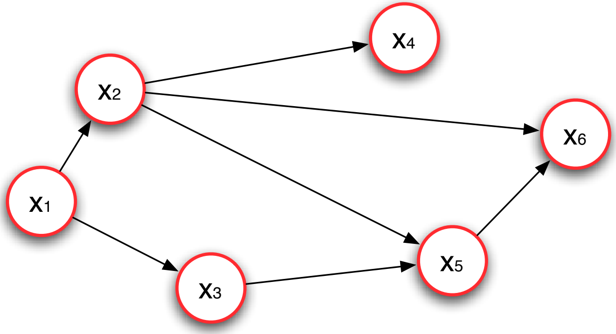
2. Check whether $a \perp\!\!\!\perp b \mid f$ holds or not.
   Result : $a \perp\!\!\!\perp b \mid f$ holds.
   - Reason : The path from a to b is blocked by f because f is a TT-node and observed. Therefore, $a \perp\!\!\!\perp b \mid f$.
3. Write down the factorisation

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

Bayesian Network - D-separation

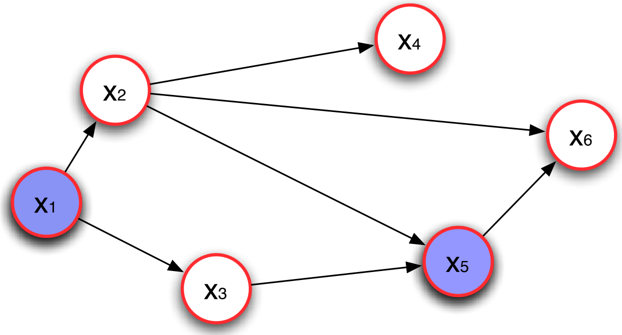
A third example

- Is x_3 d-separated from x_6 given x_1 and x_5 ?
- Mark x_1 and x_5 as observed.



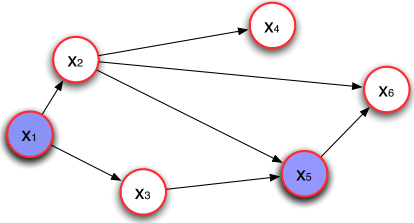
Bayesian Network - D-separation

- Is x_3 d-separated from x_6 given x_1 and x_5 ?



Bayesian Network - D-separation

- Is x_3 d-separated from x_6 given x_1 and x_5 ?
- 4 paths between x_3 and x_6.
- $\{x_3, x_1, x_2\}$ is blocked because x_1 is TT-node and observed.
- $\{x_3, x_5, x_6\}$ is blocked because x_5 is a HT-node and observed.
- $\{x_3, x_5, x_2\}$ is not blocked because x_5 is a HH-node and observed.
- $\{x_5, x_2, x_6\}$ is not blocked because x_2 is a TT-node and unobserved.
- Therefore, x_3 is not d-separated from x_6 given x_1 and x_5 as not all paths between x_3 and x_6 are blocked.



Conditional Independence $\Leftrightarrow$ Factorisation

Theorem (Factorisation $\Rightarrow$ Conditional Independence)

If a probability distribution factorises according to a directed acyclic graph, and if A, B and C are disjoint subsets of nodes such that A is d-separated from B by C in the graph, then the distribution satisfies $A \perp\!\!\!\perp B \mid C$.

Theorem (Conditional Independence $\Rightarrow$ Factorisation)

If a probability distribution satisfies the conditional independence statements implied by d-separation over a particular directed graph, then it also factorises according to the graph.

Conditional Independence $\Leftrightarrow$ Factorisation

Why is Conditional Independence $\Leftrightarrow$ Factorisation relevant?

- Conditional Independence statements are usually what a domain expert knows about the problem at hand.
- Needed is a model $p(\mathbf{x})$ for computation.
- The Conditional Independence $\Rightarrow$ Factorisation provides $p(x)$ from Conditional Independence statements.
- One can build a global model for computation from local conditional independence statements.

Conditional Independence ⇔ Factorisation

- Given a set of Conditional Independence statements.
- Adding another statement will in general produce other statements.
- All statements can be read as d-separation in a DAG.
- However, there are sets of Conditional Independence statements which cannot be satisfied by any Bayesian Network.

Conditional Independence ⇔ Factorisation

The broader picture

- A directed graphical model can be viewed as a filter accepting probability distributions $p(\mathbf{x})$ and only letting these through which satisfy the factorisation property. The set of all possible distribution $p(\mathbf{x})$ which pass through the filter is denoted as $\mathcal{DF}$.
- Alternatively, only these probability distributions $p(\mathbf{x})$ pass through the filter (graph), which respect the conditional independencies implied by the d-separation properties of the graph.
- The d-separation theorem says that the resulting set $\mathcal{DF}$ is the same in both cases.