COMP 562: Introduction to Machine Learning

Lecture 10 : Learning Bayesian Networks

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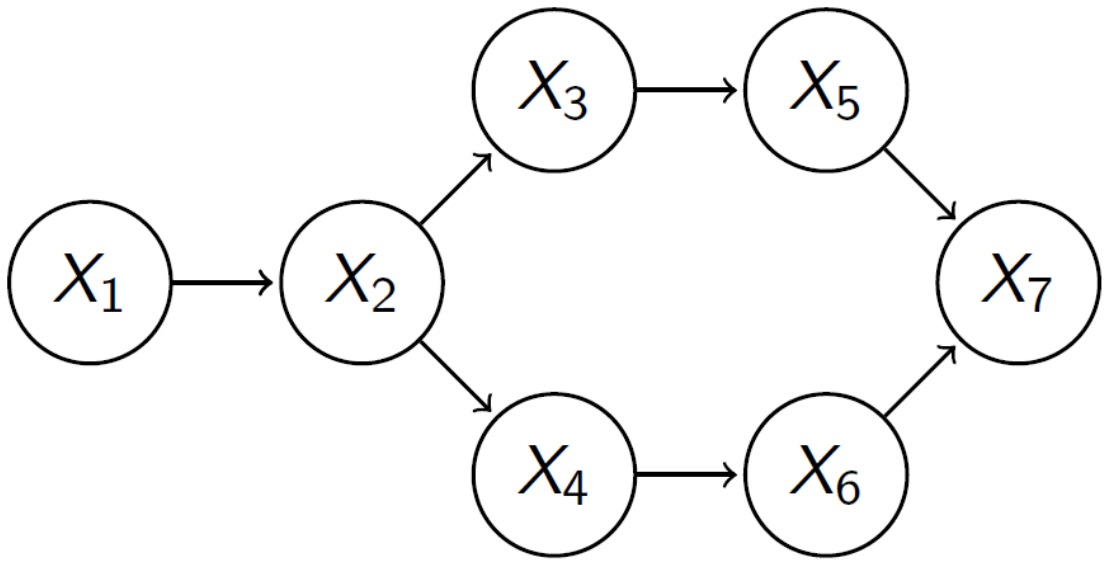
COMP562 - Lecture 10

Plan for today:

- Conditional Independence
- Bayesian Networks
- Learning Parameters of Networks

Bayesian networks

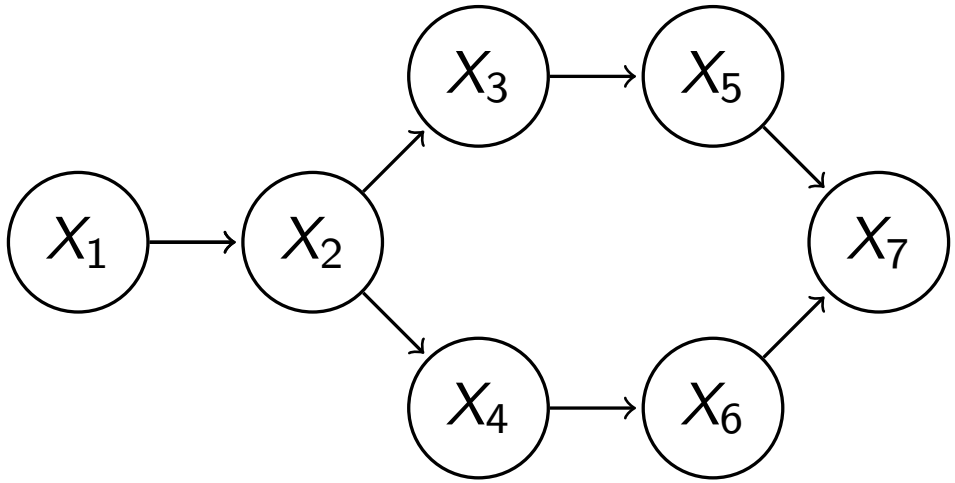
A directed graphical model is a graphical model whose graph is a directed acyclic graph (DAG). Also known as Bayesian network or belief network or causal network.



In DAGs the nodes can be ordered such that parents come before children. This is called a **topological ordering**.

Specifying a graphical model

Each of these nodes corresponds to a random variable.



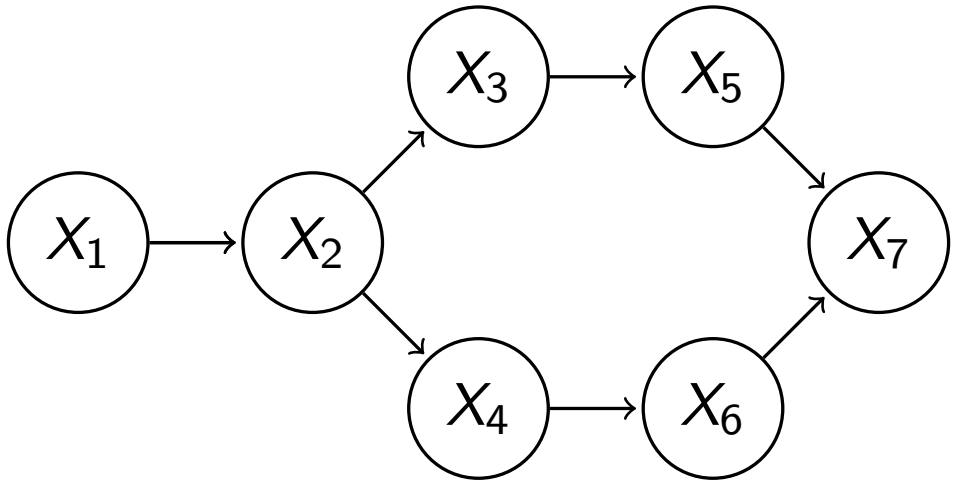
and each node has a conditional probability associated with it

$$p(X_j|X_{\mathbf{pa}(j)})$$

where $\mathbf{pa}(j)$ is a list of parent nodes of node j, e.g.

$$p(X_7|X_5, X_6)$$

Specifying a graphical model



This graphical model specifies a joint distribution

$$
\begin{aligned}
p(X_1, X_2, X_3, X_4, X_5, X_6, X_7) &= \prod_i p(X_i | X_{\mathbf{pa}(i)}) \\
&= p(X_1)
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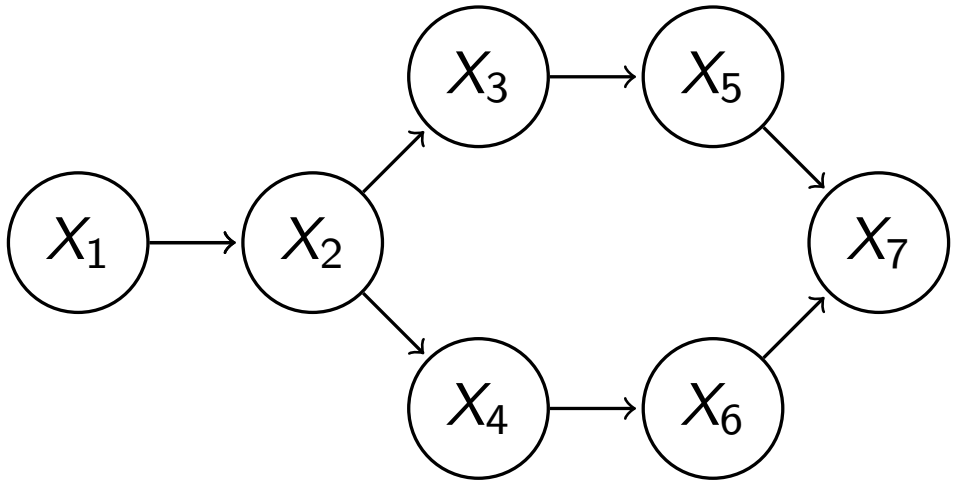

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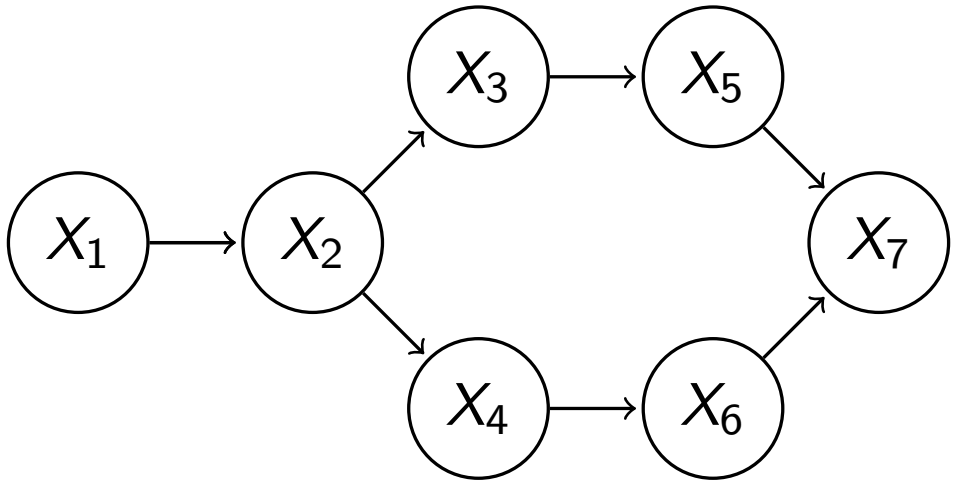

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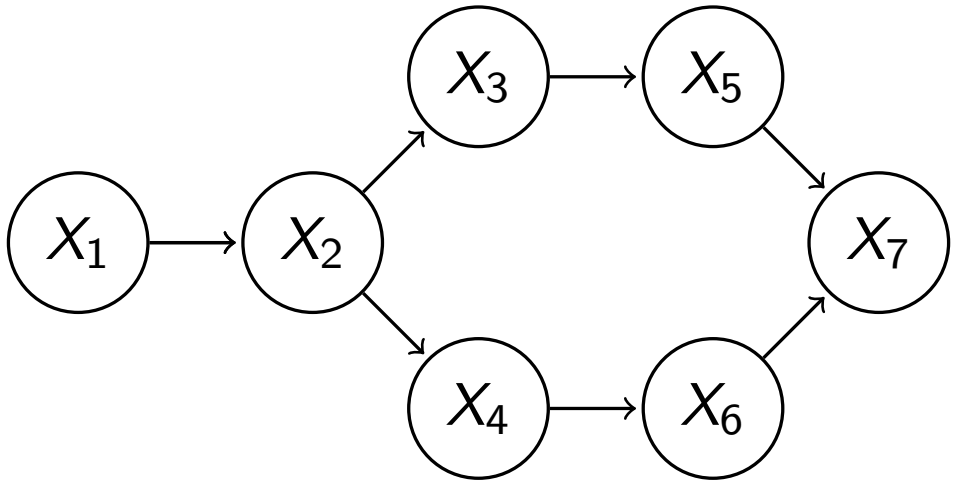

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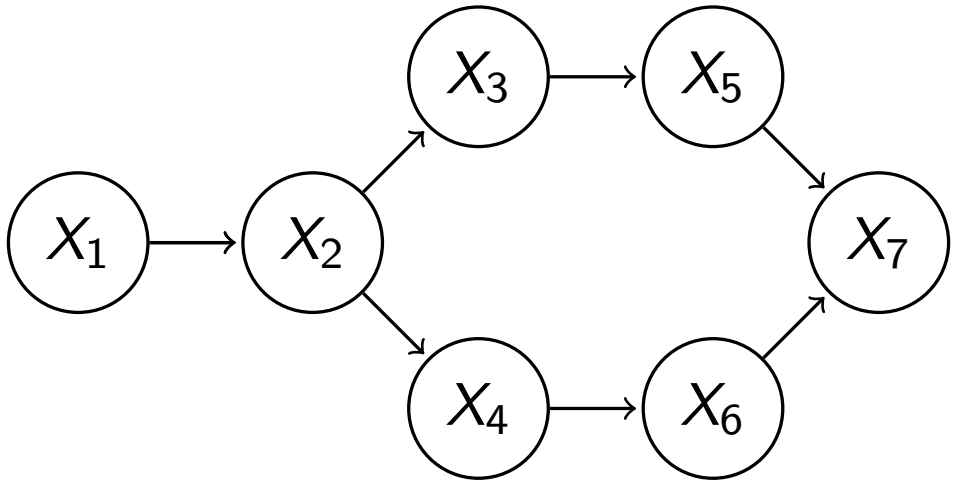

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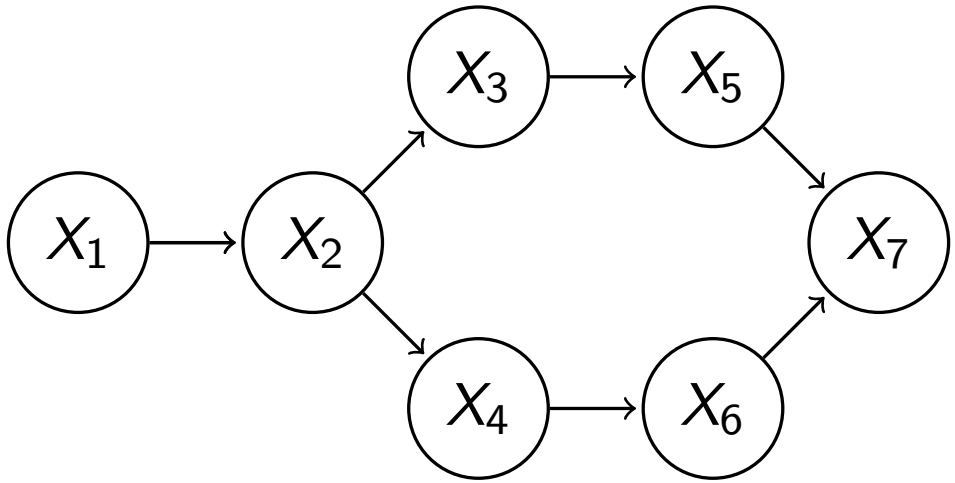

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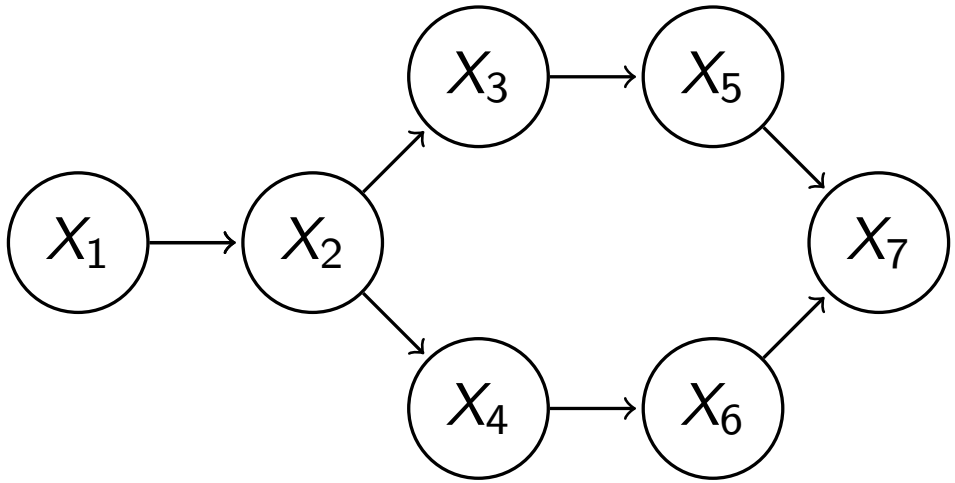

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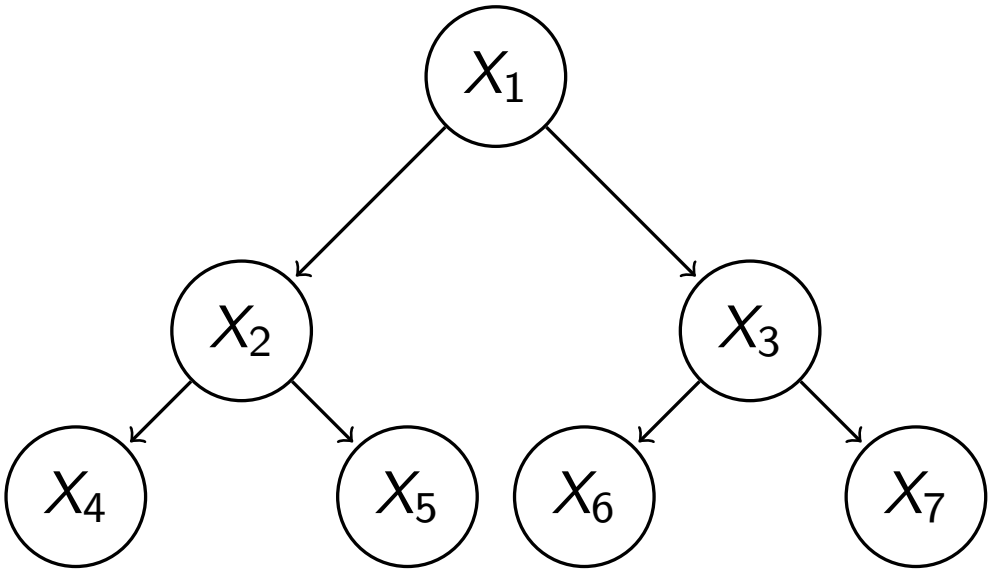
These are basic conditional independence relationships.

Obtaining basic conditional independencies



A topological order:
$X_1, X_2, X_3, X_4, X_5, X_6, X_7$

$$X_1 \perp \emptyset \mid \emptyset$$

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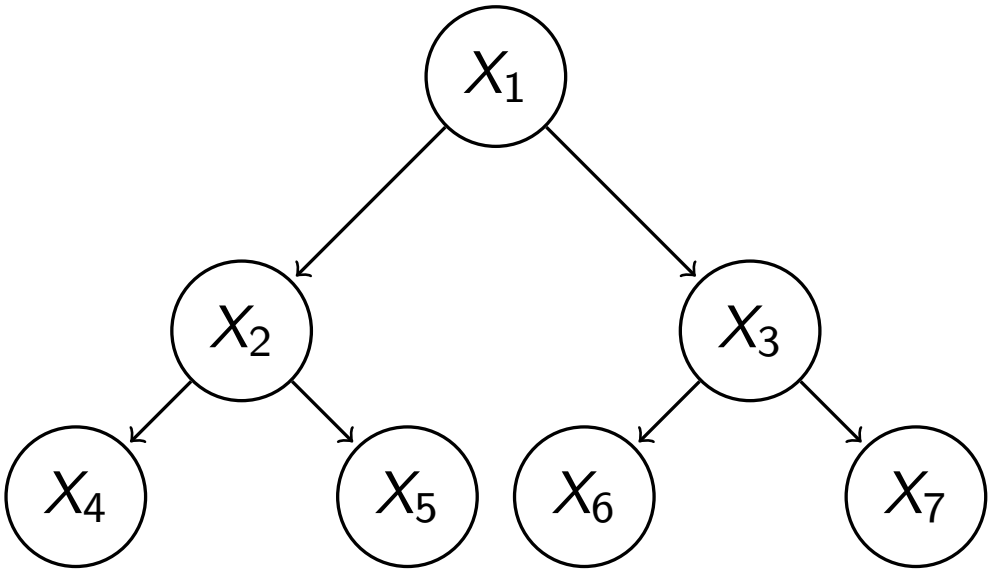

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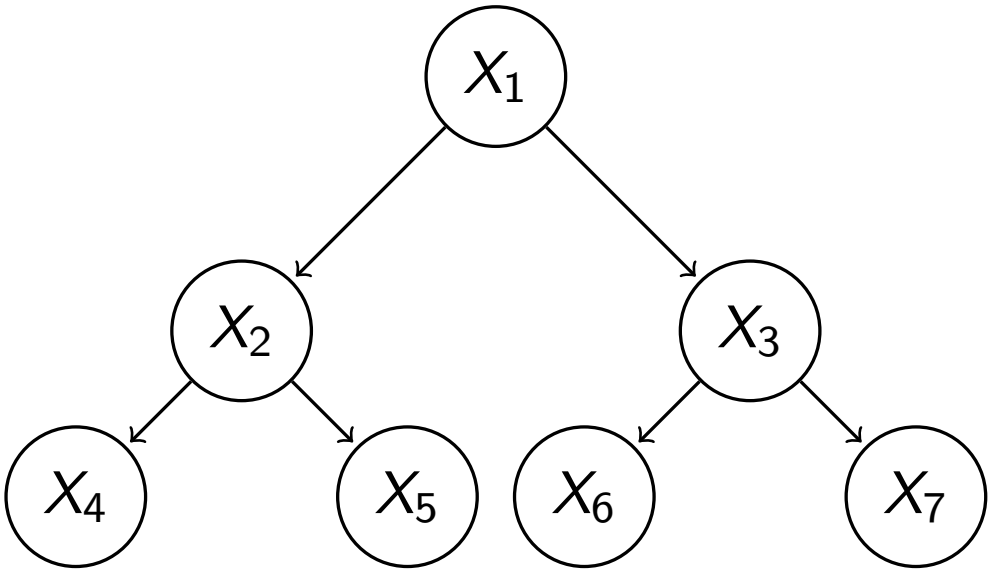

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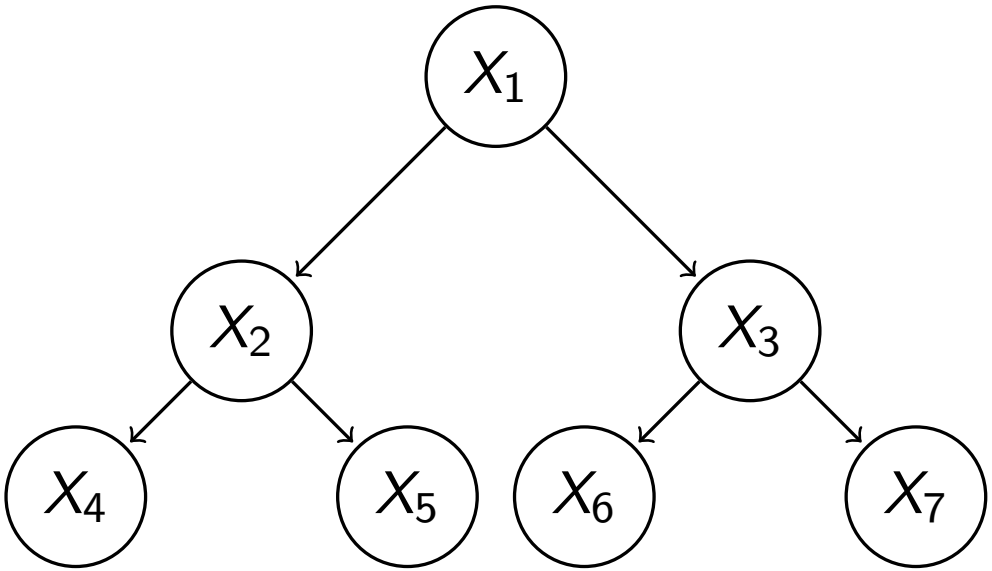

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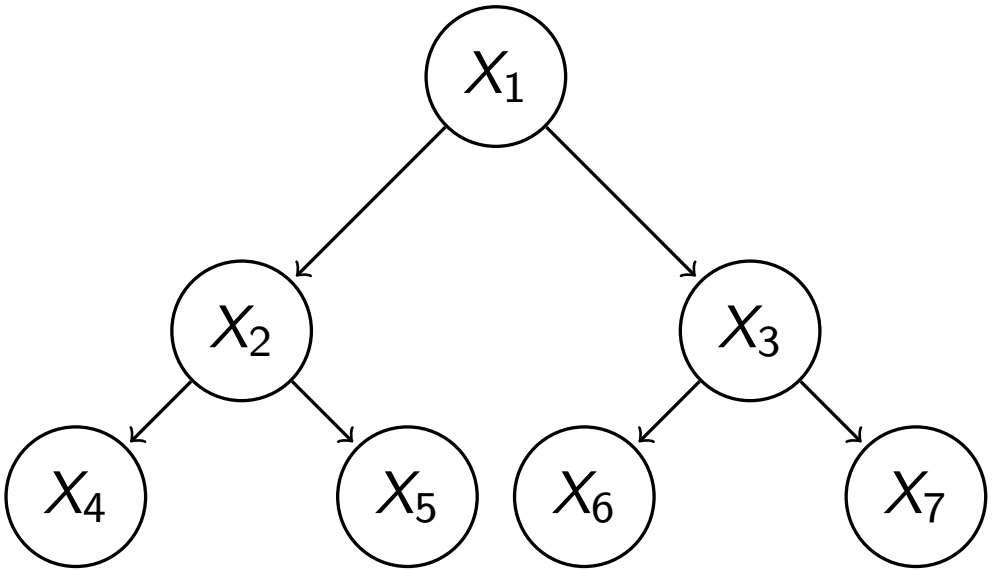

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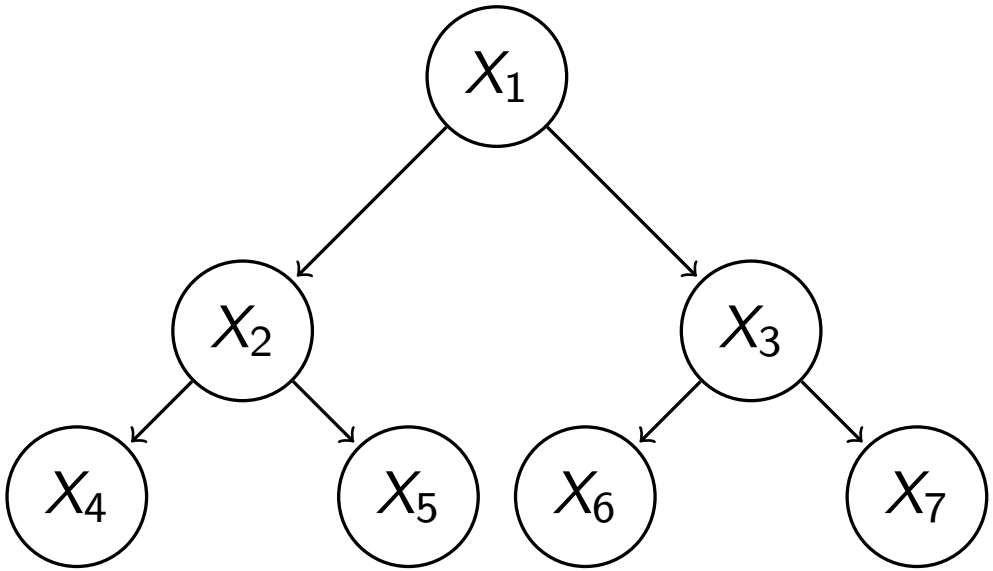

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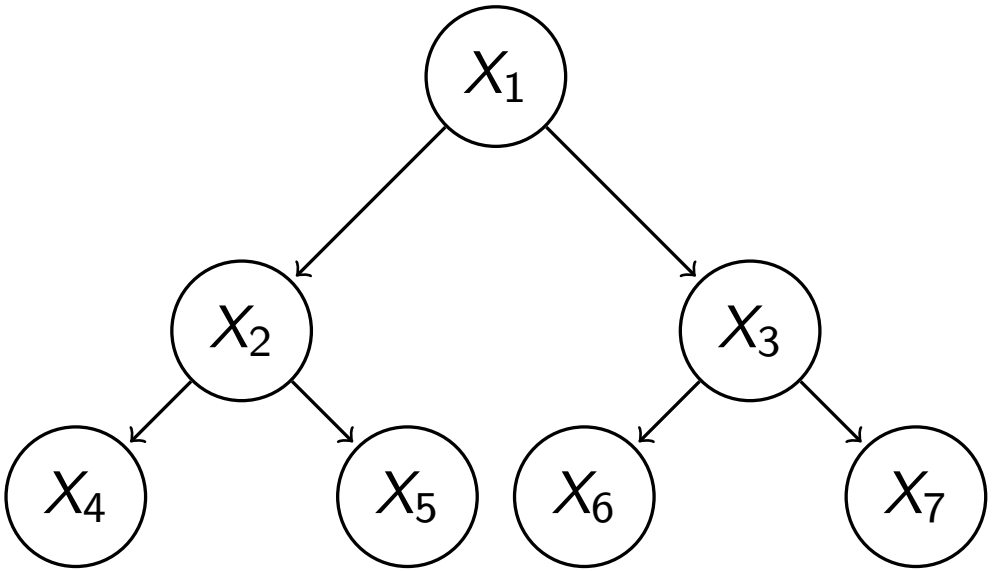

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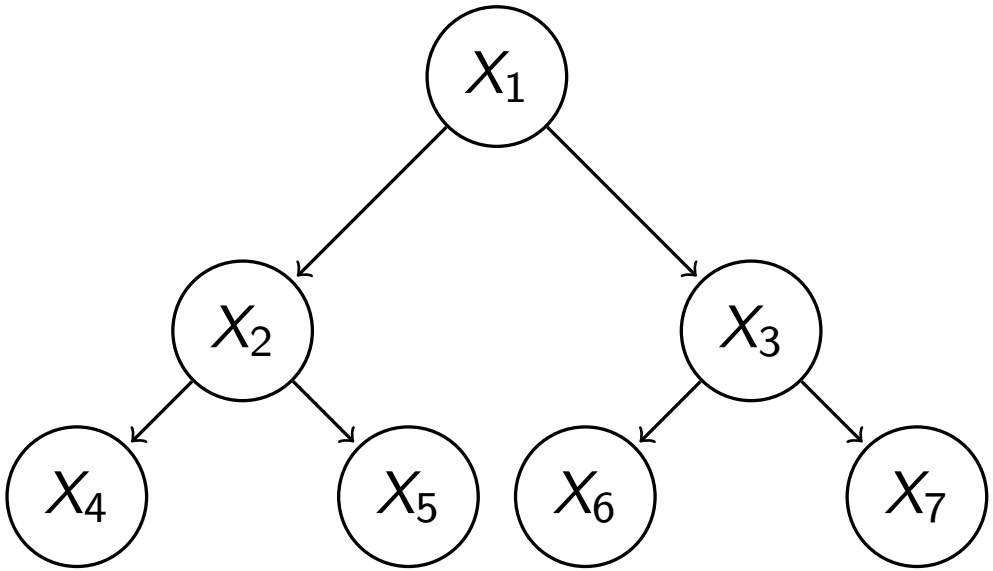

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And we are going to verify one of these because it highlights the distributive property that is crucial for message passing algorithm derivations.

Verifying a conditional independence

We want to show

$$p(X_3|X_2, X_1) = \frac{p(X_3, X_2, X_1)}{p(X_2, X_1)} = p(X_3|X_1)$$

Marginal $p(X_3, X_2, X_1)$

$$p(X_1, X_2, X_3) =$$

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$$p(X_1)p(X_2|X_1)p(X_3|X_1)\sum_{X_4} p(X_4|X_2)\sum_{X_5} p(X_5|X_2)\sum_{X_6} p(X_6|X_3) =$$

$$p(X_1)p(X_2|X_1)p(X_3|X_1)\sum_{X_4} p(X_4|X_2)\sum_{X_5} p(X_5|X_2) =$$

$$p(X_1)p(X_2|X_1)p(X_3|X_1)\sum_{X_4} p(X_4|X_2) = p(X_1)p(X_2|X_1)p(X_3|X_1)$$

Verifying a conditional independence

We want to show

$$p(X_3|X_2,X_1) = \frac{p(X_3,X_2,X_1)}{p(X_2,X_1)} = p(X_3|X_1)$$

Marginals are

$$\begin{aligned} p(X_3,X_2,X_1) &= p(X_1)p(X_2|X_1)p(X_3|X_1) \\ p(X_2,X_1) &= p(X_1)p(X_2|X_1) \end{aligned}$$

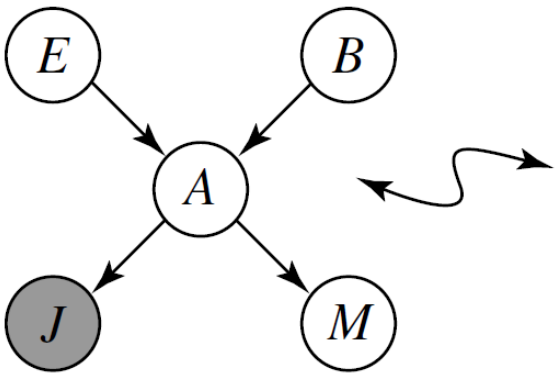
plugging them in we get

$$p(X_3|X_2,X_1) = \frac{p(X_3,X_2,X_1)}{p(X_2,X_1)} = \frac{p(X_1)p(X_2|X_1)p(X_3|X_1)}{p(X_1)p(X_2|X_1)} = p(X_3|X_1)$$

and this confirms $X_3 \perp X_2|X_1$

Representing evidence in Bayesian networks

- When we condition on some of the variables, the result is a conditional density that can have different independence properties.
- When we condition on a variable, we shade the corresponding node in the Bayes net.



$$p_{EBAM|J} = \frac{p_E \times p_B \times p_{A|EB} \times p_{J|A} \times p_{M|A}}{\sum_e \sum_b \sum_a \sum_m p_E \times p_B \times p_{A|EB} \times p_{J|A} \times p_{M|A}}$$

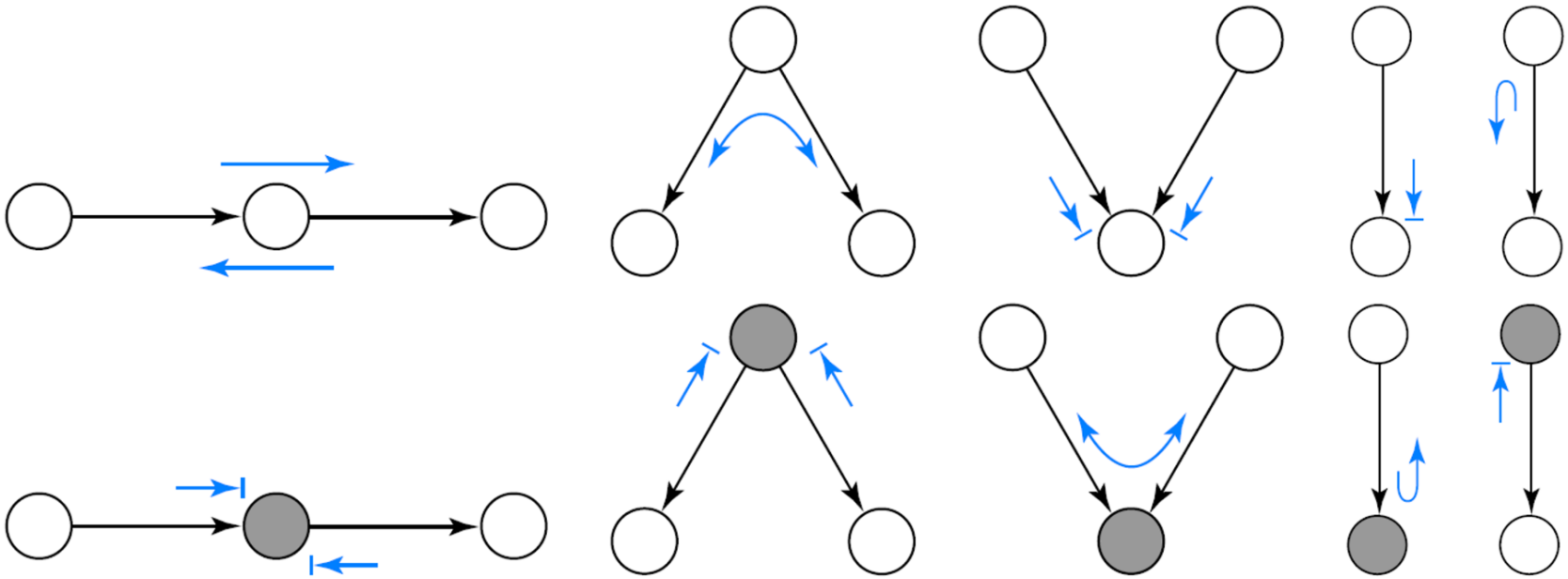
Encoding conditional independence via d-separation

- Bayesian networks encode the independence properties of a density.
- We can determine if a conditional independence $X \perp Y | \mathcal{Z}$ holds by appealing to a graph separation criterion called *d-separation* (*direction-dependent separation*).
- X and Y are d-separated if there is no active path between them.
- The formal definition of active paths is somewhat involved. The *Bayes Ball Algorithm* gives a nice graphical definition.

Bayes Ball Algorithm

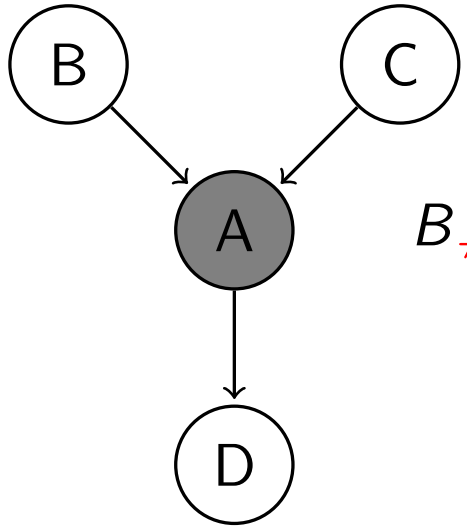
- You want to check if $X \perp Y | \mathcal{Z}$. Imagine passing a " from a node to a node, if the ball can make it from X to Y they are dependent. Shade the nodes in $\mathcal{Z}$ and apply following rules:

An Undirected path P is active if a Bayes ball travelling along it never encounters the "stop" symbol



P Contains a Chain | **P Contains a fork** | **P Contains a V-structure** | **Boundary Conditions**

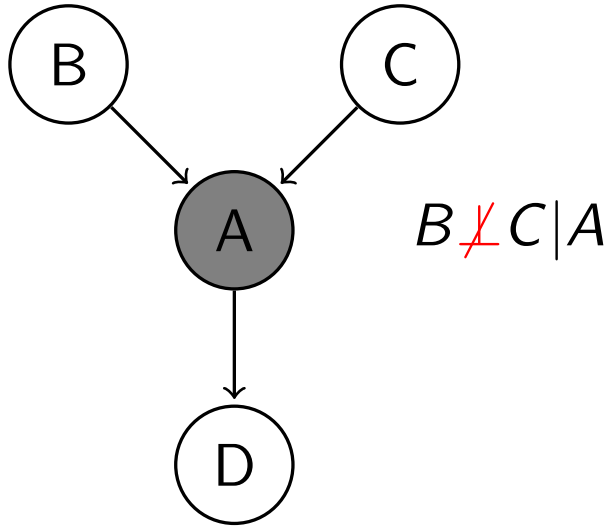
V-structure with a hanging unobserved variable



$B \not\perp C|A$

$$p(B, C|A) = \frac{p(A, B, C)}{p(A)} \quad =$$

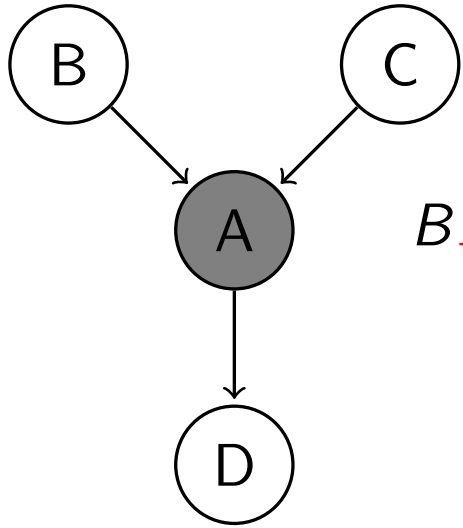
V-structure with a hanging unobserved variable



$$p(B, C|A) = \frac{p(A, B, C)}{p(A)} = \frac{\sum_D p(B)p(C)p(A|B, C)p(D|A)}{\sum_B \sum_C \sum_D p(B)p(C)p(A|B, C)p(D|A)}$$

$$=$$

V-structure with a hanging unobserved variable

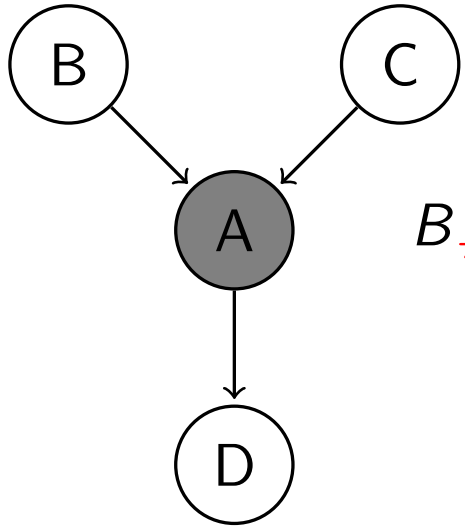


$B \not\perp C|A$

$$p(B,C|A) = \frac{p(A,B,C)}{p(A)} = \frac{\sum_D p(B)p(C)p(A|B,C)p(D|A)}{\sum_B \sum_C \sum_D p(B)p(C)p(A|B,C)p(D|A)}$$

$$= \frac{p(B)p(C)p(A|B,C)\sum_D p(D|A)}{\sum_B \sum_C p(B)p(C)p(A|B,C)\sum_D p(D|A)}$$

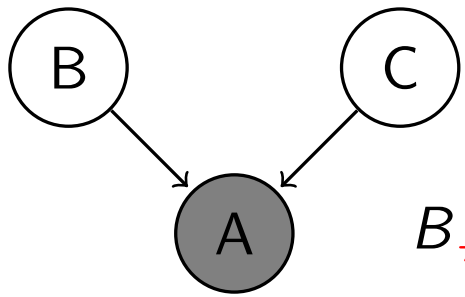
V-structure with a hanging unobserved variable



$B \not\perp C|A$

$$p(B,C|A) = \frac{p(A,B,C)}{p(A)} = \frac{\sum_D p(B)p(C)p(A|B,C)p(D|A)}{\sum_B \sum_C \sum_D p(B)p(C)p(A|B,C)p(D|A)}$$

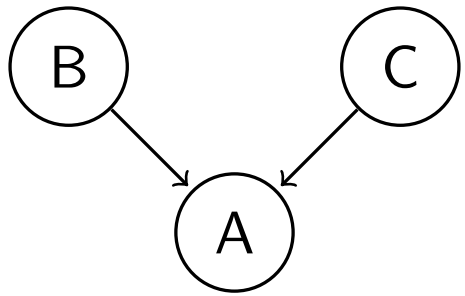
$$= \frac{p(B)p(C)p(A|B,C)\sum_D p(D|A)}{\sum_B \sum_C p(B)p(C)p(A|B,C)\sum_D p(D|A)}$$



$B \not\perp C|A$

V-structures and explaining away

Suppose we know of two competing explanations of an outcome.

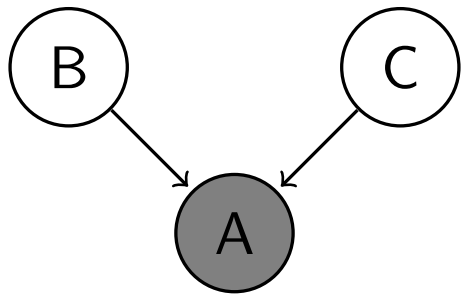


variables B and C are independent

$$\begin{aligned} p(B,C) &= \sum_A p(A|B,C)p(B)p(C) = p(B)p(C)\sum_A p(A|B,C) \\ &= p(B)p(C) \end{aligned}$$

V-structures and explaining away

But as soon as we observe A the variables B and C become dependent



$$
\begin{aligned}
p(B, C|A = a) &= \frac{p(A = a|B, C)p(B)p(C)}{\sum_B \sum_C p(A = a|B, C)p(B)p(C)} \\
&\neq p(B)p(C)
\end{aligned}
$$

Examples of explaining away

Outcome	Explanation 1	Explanation 2
wet grass	sprinkler	rain

Examples of explaining away

Outcome	Explanation 1	Explanation 2
wet grass	sprinkler	rain
student admitted	student brainy	student athletic

Examples of explaining away

Outcome	Explanation 1	Explanation 2
wet grass	sprinkler	rain
student admitted	student brainy	student athletic
house jumps	truck hits house	earthquake

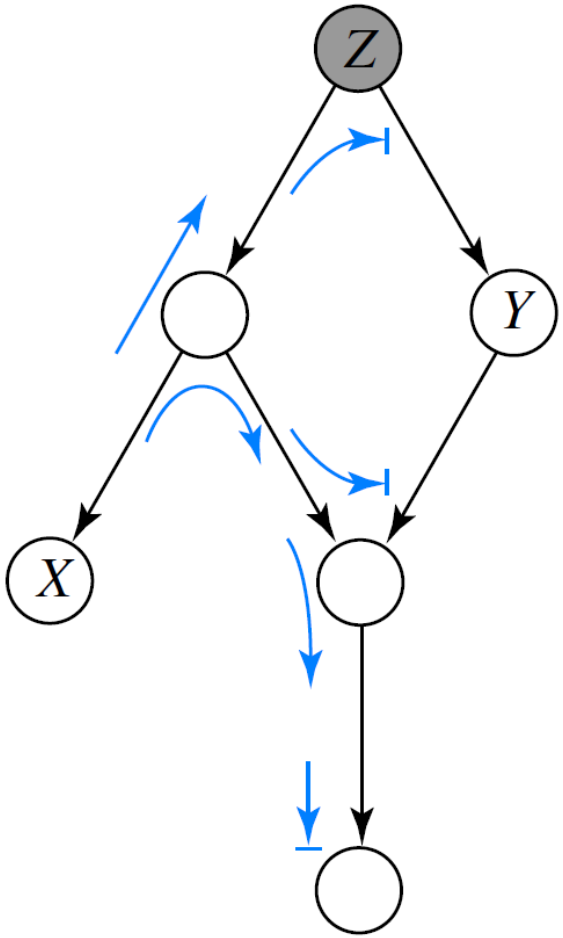
Examples of explaining away

Outcome	Explanation 1	Explanation 2
wet grass	sprinkler	rain
student admitted	student brainy	student athletic
house jumps	truck hits house	earthquake

Explaining away: Given outcome two causes are not independent.

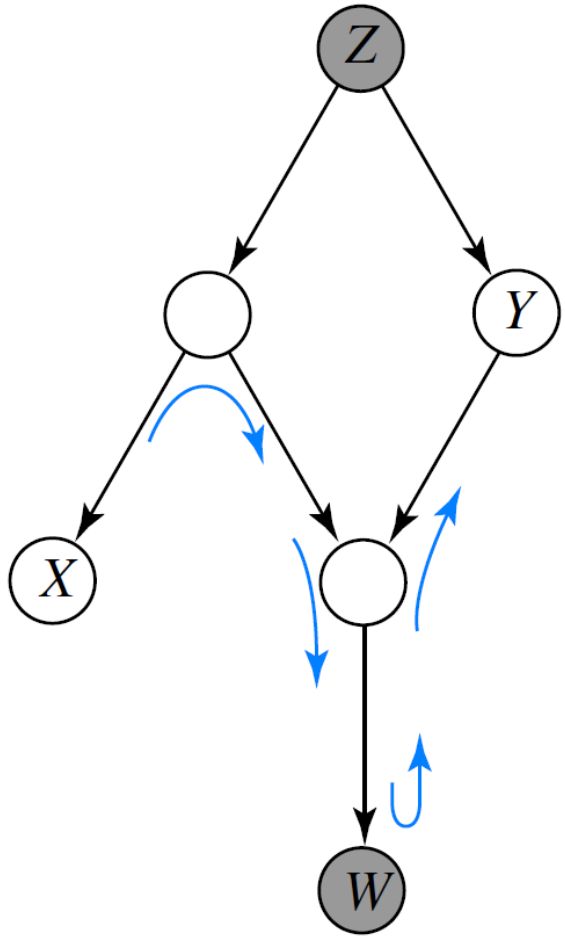
This is also called Berkson's paradox.

A double-header: two games of Bayes Ball



no active paths

$X \perp\!\!\!\perp Y \mid Z$

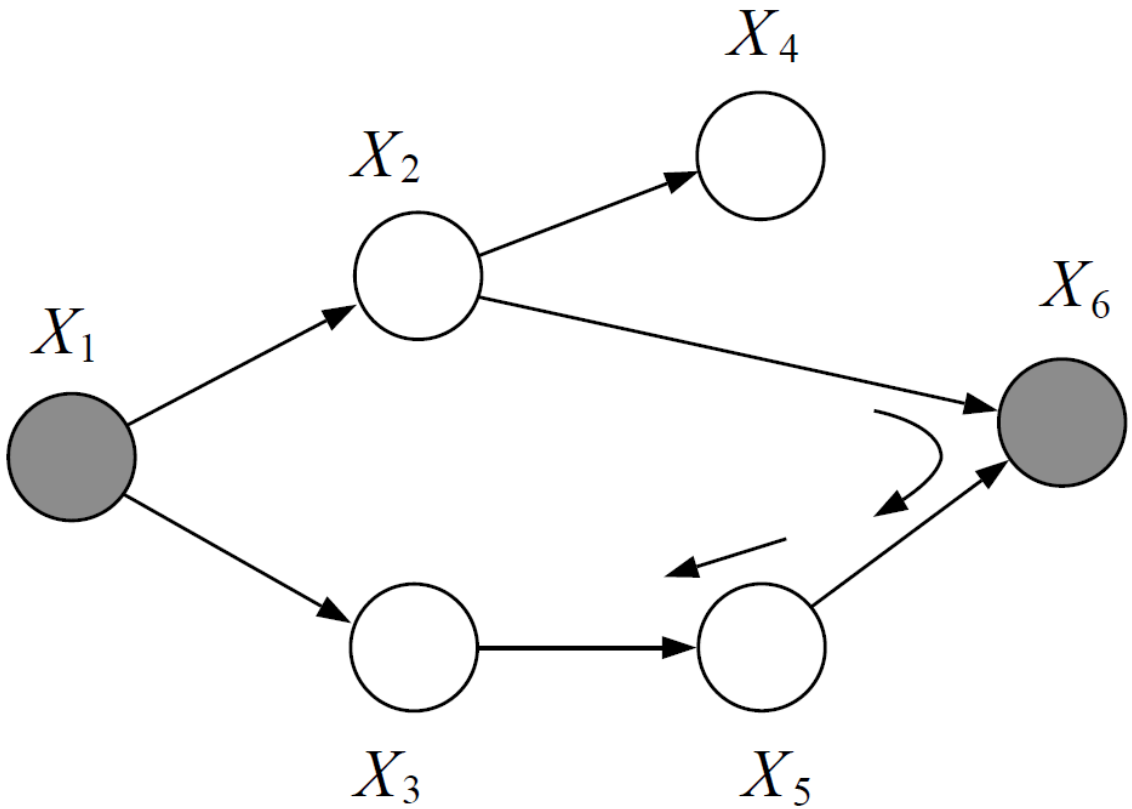


one active path

$X \not\perp\!\!\!\perp Y \mid \{W, Z\}$

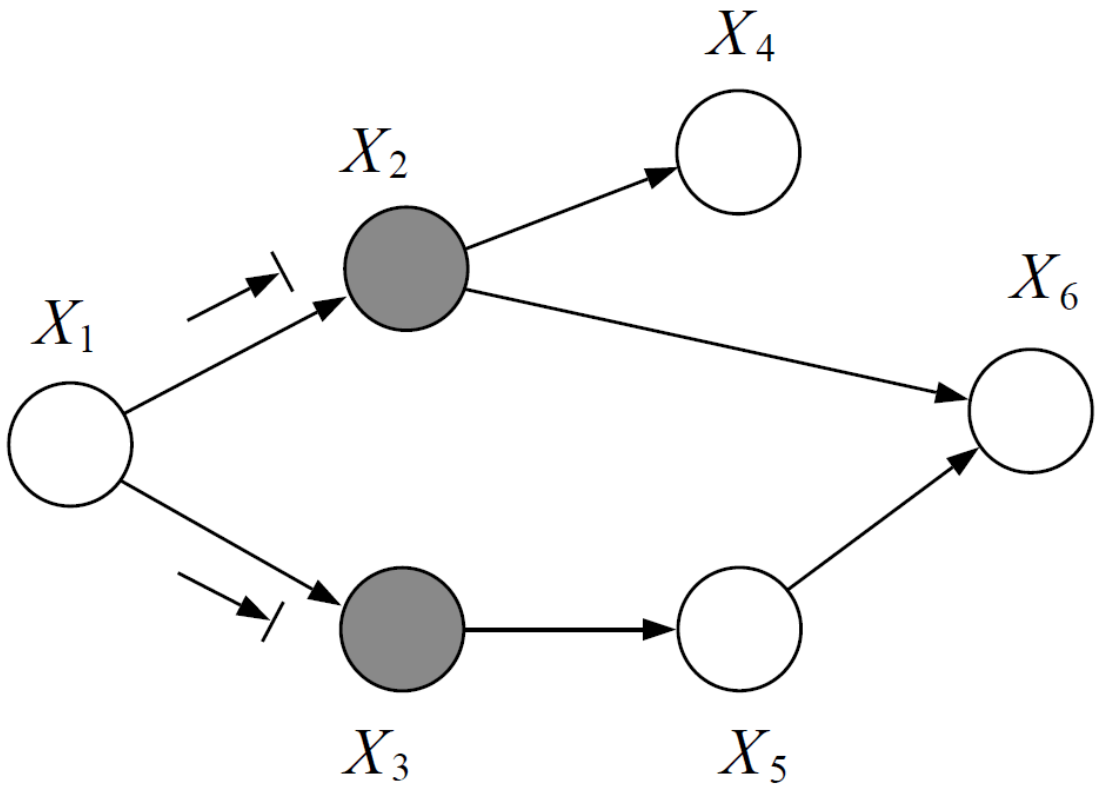
Examples of Bayes-Ball Algorithm

$$\mathbf{x}_2 \perp \mathbf{x}_3 | \{\mathbf{x}_1, \mathbf{x}_6\} \quad ?$$



Examples of Bayes-Ball Algorithm

$$\mathbf{x}_1 \perp \mathbf{x}_6 | \{\mathbf{x}_2, \mathbf{x}_3\} \quad ?$$



Learning Bayesian Networks

Learning a Bayesian Network requires us to determine

- network's structure
- network's parameters

You will implement both of these in your HW2.

Learning a BayesNet

Probability of a state of all n variables $\mathbf{x}$

$$p(X_1 = x_1, ..., X_n = x_n) = \prod_{j=1}^{n} p(X_j = x_j | X_{\mathbf{pa}(j)} = x_{\mathbf{pa}(j)}, \theta_j)$$

Learning a BayesNet

Probability of a state of all n variables $\mathbf{x}$

$$p(X_1 = x_1, ..., X_n = x_n) = \prod_{j=1}^{n} p(X_j = x_j | X_{\mathbf{pa}(j)} = x_{\mathbf{pa}(j)}, \theta_j)$$

Our goal is to learn parameters $\Theta = (\theta_1, ...\theta_n)$ from multiple samples of the state of the Bayes net.

Example

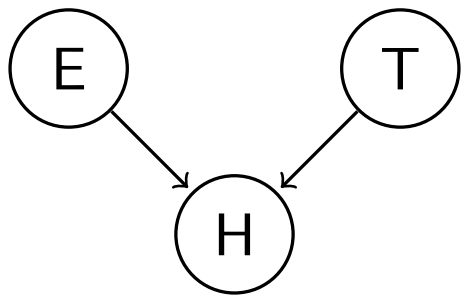
Data:

Sample \ Variable	Earthquake	Truck	House moved
1	1	0	1
2	0	0	0
⋮	⋮	⋮	⋮
S	0	1	0

Example

Data:

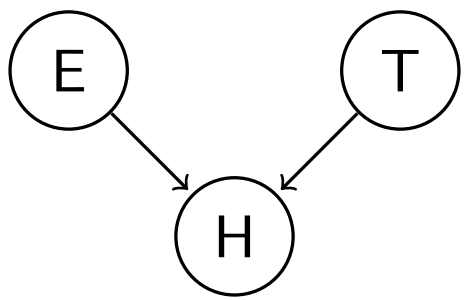
Variable / Sample	Earthquake	Truck	House moved
1	1	0	1
2	0	0	0
⋮	⋮	⋮	⋮
S	0	1	0



Example

Data:

Sample \ Variable	Earthquake	Truck	House moved
1	1	0	1
2	0	0	0
⋮	⋮	⋮	⋮
S	0	1	0



Conditional distributions and their parameters

- $p(E = 1|\theta_E) = \theta_E$, where $\theta_E \in [0, 1]$
- $p(T = 1|\theta_T) = \theta_T$, where $\theta_R \in [0, 1]$
- $p(H = 1|E = e, T = t, \theta_H) = \theta_{H,e,t}$, where $\theta_{H,e,t} \in [0, 1]$

Learning a BayesNet – likelihood

Data S instances of Bayes net's state; $x_{i,j}$ state of variable X_j in i^{th} sample.

$$L(\Theta) = \underbrace{\prod_{i=1}^{S}}_{\text{samples}} \underbrace{\prod_{j=1}^{n}}_{\text{variables}} p(X_j = x_{i,j} | X_{\mathbf{pa}(j)} = x_{i,\mathbf{pa}(j)}, \theta_j)$$

Likelihood Example

Data:

Sample \ Variable	Earthquake	Truck	House moved
1	1	0	1
2	0	0	0
⋮	⋮	⋮	⋮
S	0	1	0

$$
\begin{aligned}
L(\Theta) \quad = \quad & p(E=1|\theta_E)p(T=0|\theta_T)p(H=1|E=1,T=0,\theta_H) \\
& p(E=0|\theta_E)p(T=0|\theta_T)p(H=0|E=0,T=0,\theta_H) \\
& \vdots \\
& p(E=0|\theta_E)p(T=1|\theta_T)p(H=0|E=0,T=1,\theta_H)
\end{aligned}
$$

Likelihood Example – continued

$$
\begin{aligned}
L(\Theta) &= p(E=1|\theta_E)p(T=0|\theta_T)p(H=1|E=1,T=0,\theta_H) \\
&\times p(E=0|\theta_E)p(T=0|\theta_T)p(H=0|E=0,T=0,\theta_H) \\
&\times \vdots \\
&\times p(E=0|\theta_E)p(T=1|\theta_T)p(H=0|E=0,T=1,\theta_H)
\end{aligned}
$$

In terms of parameters

$$
\begin{aligned}
L(\Theta) &= \theta_E & (1-\theta_T) & \theta_{H,1,0} \\
&\times (1-\theta_E) & (1-\theta_T) & (1-\theta_{H,0,0}) \\
&\times \vdots & & \\
&\times (1-\theta_E) & \theta_T & (1-\theta_{H,1,0})
\end{aligned}
$$

Learning a BayesNet – log-likelihood

Log-likelihood is given by

$$\mathrm{LL}(\Theta) = \underbrace{\sum_{i=1}^{S}}_{\text{samples}} \underbrace{\sum_{j=1}^{n}}_{\text{variables}} \log p(X_j = x_{i,j} | X_{\mathbf{pa}(j)} = x_{i,\mathbf{pa}(j)}, \theta_j)$$

Crucial observation:

$$\mathrm{LL}(\Theta) = \underbrace{\sum_{j=1}^{n}}_{\text{variables}} \underbrace{\sum_{i=1}^{S}}_{\text{samples}} \log p(X_j = x_{i,j} | X_{\mathbf{pa}(j)} = x_{i,\mathbf{pa}(j)}, \theta_j)$$

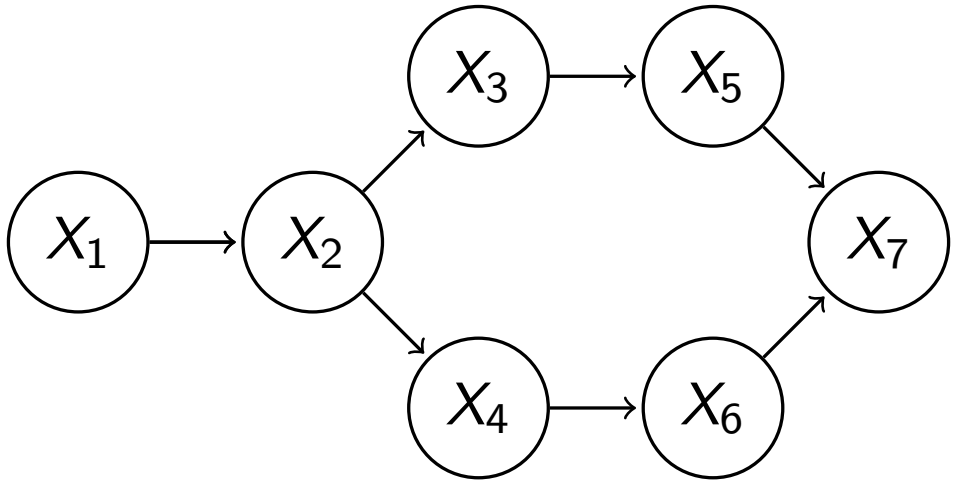
Learning a BayesNet – maximizing log-likelihood

$$\begin{aligned}
\underset{\theta_j}{\operatorname{argmax}}\, \mathrm{LL}(\Theta) &= \underset{\theta_j}{\operatorname{argmax}} \sum_{j=1}^{n} \sum_{i=1}^{S} \log p(X_j = x_{i,j} | X_{\mathbf{pa}(j)} = x_{i,\mathbf{pa}(j)}, \theta_j) \\
&= \underset{\theta_j}{\operatorname{argmax}} \sum_{i=1}^{S} \log p(X_j = x_{i,j} | X_{\mathbf{pa}(j)} = x_{i,\mathbf{pa}(j)}, \theta_j)
\end{aligned}$$

To learn parameters θ_j we only need states of node j and its parents.

Further, we do not need to concern ourselves with the rest of the graph.

For example



Learning $p(X_3|X_2)$ uses only states for X_2 and X_3

Sample \ Variable	X_1	X_2	X_3	X_4	X_5	X_6	X_7
1		0	1				
⋮		⋮	⋮				
S		1	0				

Learning BayesNets – structure learning

If we assume that BayesNet is a tree – each variable has a single parent – we can derive an algorithm to discover the optimal structure.
Given an empirical distribution of the data f we wish to find optimal distribution with factorization

$$p(X_1, ..., X_n) = \prod_{j=1}^{n} p(X_j | X_{\mathbf{pa}(j)})$$

where $\mathbf{pa}(j)$ has at most one element for all j.
Under this assumption, we can define edge set

$$\text{Edges} = \{(j, \mathbf{pa}(j)) | j = 1, ..., n\}$$

Learning BayesNets – structure learning

Writing out log-likelihood

$$\mathrm{LL}(\Theta) = \sum_{i=1}^{S} \sum_{j} \log p(x_{i,j} | x_{i,\mathbf{pa}(j)})$$

Learning BayesNets – structure learning

Writing out log-likelihood

$$\begin{aligned} \mathrm{LL}(\Theta) &= \sum_{i=1}^{S} \sum_{j} \log p(x_{i,j} | x_{i,\mathbf{pa}(j)}) \\ &= \sum_{i=1}^{S} \sum_{j=1}^{n} \sum_{k=1}^{n} [(j,k) \in \mathrm{Edges}] \log p(x_{i,j} | x_{i,k}) \end{aligned}$$

Learning BayesNets – structure learning

Writing out log-likelihood

$$
\begin{aligned}
\mathrm{LL}(\Theta) &= \sum_{i=1}^{S} \sum_{j} \log p(x_{i,j} | x_{i,\mathbf{pa}(j)}) \\
&= \sum_{i=1}^{S} \sum_{j=1}^{n} \sum_{k=1}^{n} [(j,k) \in \mathrm{Edges}] \log p(x_{i,j} | x_{i,k}) \\
&= \sum_{j=1}^{n} \sum_{k=1}^{n} [(j,k) \in \mathrm{Edges}] \left(\sum_{i=1}^{S} \log p(x_{i,j} | x_{i,k}) \right)
\end{aligned}
$$

Learning BayesNets – structure learning

Writing out log-likelihood

$$
\begin{aligned}
\mathrm{LL}(\Theta) &= \sum_{i=1}^{S} \sum_{j} \log p(x_{i,j} | x_{i,\mathbf{pa}(j)}) \\
&= \sum_{i=1}^{S} \sum_{j=1}^{n} \sum_{k=1}^{n} [(j,k) \in \mathrm{Edges}] \log p(x_{i,j} | x_{i,k}) \\
&= \sum_{j=1}^{n} \sum_{k=1}^{n} [(j,k) \in \mathrm{Edges}] \left(\sum_{i=1}^{S} \log p(x_{i,j} | x_{i,k}) \right) \\
&= \sum_{(j,k) \in \mathrm{Edges}} \left(\sum_{i=1}^{S} \log p(x_{i,j} | x_{i,k}) \right)
\end{aligned}
$$

Learning BayesNets – structure learning

$$\mathrm{LL}(\Theta) = \sum_{(j,k)\in \mathrm{Edges}} \left(\sum_{i=1}^{S} \log p(x_{i,j}|x_{i,k}) \right)$$

We observed that we can learn optimal $p(X_j|X_k, \theta_j)$ independently of the graph structure.

$$\theta_j^* = \operatorname*{argmax}_{\theta_j} \sum_{i=1}^{S} \log p(x_{i,j}|x_{i,k}, \theta_j)$$

Learning BayesNets – structure learning

$$\mathrm{LL}(\Theta) \sum_{(j,k)\in \mathrm{Edges}} \underbrace{\sum_{i=1}^{S} \log p(x_{i,j}|x_{i,k},\theta_j^*)}_{\text{weight of edge (j,k)}}$$

Hence, we wish to find a tree with maximum weight, where each edge's weight is

$$w_{j,k} = \sum_{i=1}^{S} \log p(X_j = x_{i,j}|X_k = x_{i,k},\theta_j^*)$$

Chow-Liu tree learning algorithm

Observe that

$$\sum_{i=1}^{S} \log p(X_j = x_{i,j} | X_k = x_{i,k}) = I(X_j, X_k) - H(X_j)$$

and since $H(X_j)$ does not depend on the edges we can rewrite the problem as

$$\underset{\text{Edges}}{\operatorname{argmax}} \sum_{(j,k) \in Edges} I(X_j, X_k) - H(X_j) = \underset{\text{Edges}}{\operatorname{argmax}} \sum_{(j,k) \in Edges} I(X_j, X_k)$$

Note that this is an example of **maximum spanning tree** problem which can be solved efficiently – HW2.

Chow-Liu tree learning algorithm – details

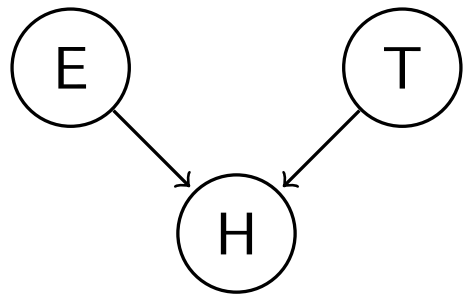
Mutual information $I(X_j, X_k)$ is computed on the empirical distribution

$$
\begin{aligned}
f_{j,k}(a,b) &= \frac{\sum_{i=1}^{S}[X_j = a, X_k = b]}{S} \\
f_l(a) &= \frac{\sum_{i=1}^{S}[X_l = a]}{S} \\
I(X_j, X_k) &= \sum_a \sum_b f_{j,k}(a,b) \log \frac{f_{j,k}(a,b)}{f_j(a) f_k(b)}
\end{aligned}
$$

Chow-Liu tree – downsides

Single parent assumptions can be restrictive.

The tree models do not permit explaining away.



Tree structured Bayes nets are step above independent models.

On the upside, they are extremely easy to learn.

Today

- Bayesian Networks
- Learning Bayesian Networks