

# CS559 Machine Learning

## Probabilistic Graphical Model, Bayesian Network

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Week 11

# Outline

- Introduction to Graphical Model
- Bayesian Network

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# Probabilistic Graphical Models

- A simple way to **visualize** the structure of a probabilistic model

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- **Insight** into the properties of the model
- Complex computations can be expressed in terms of **graphical manipulations**
- Two types:
  - **Directed** graphical models: Bayesian Networks, latent Variable Model, etc
  - **Undirected** graphical models: Markov network (Markov Random Field), Energy-based Model etc

# Graphical Models

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# Graphical Models

- Graphical models are graph-based representations of various factorization assumptions of distributions
- These factorizations are typically equivalent to *conditional independence* statement amongst (sets of) variables in the distributions.

## Directed graphical model for joint probability

- The product rule of probability over three variables  $a$ ,  $b$ ,  $c$ :  
(different ordering has different factorization)

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- A directed graphical model representing the joint probability distribution over  $a, b, c$ :

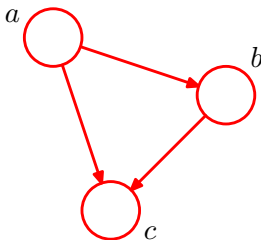


Figure: [C. Bishop, PRML]

## Definitions

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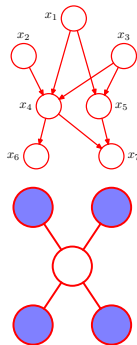
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- Graphs can be represented using: the edge list, the adjacency matrix.

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$$P(X_i|\mathcal{M})$$

- Learning

- What model is “right” for my data?

$$\mathcal{M} = \arg \max_{\mathcal{M} \in \mathcal{M}} F(D; \mathcal{M})$$

## Basic Probability Concepts

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  - Do we get any scientific insight?
- **Inference**: If not all variables are observable, how to compute the conditional distribution of latent variables given evidence?
- **Learning**: where do we get all this probabilities?
  - Maximal-likelihood estimation? but how many data do we need?
  - Are there other est. principles?
  - Where do we put domain knowledge in terms of plausible relationships between variables, and plausible values of the probabilities?

## Two Important Rules

1. **Chain rule or Product rule:** Let  $S_1, S_2, \dots, S_n$  be events, and  $p(S_i) > 0$ , then:

$$p(S_1, S_2, \dots, S_n) = p(S_1)p(S_2|S_1) \cdots p(S_n|S_{n-1}, \dots, S_1)$$

Let  $X, Y$  be two variables, then

$$p(X, Y) = p(X|Y)p(Y)$$

2. **Sum rule:** Let  $X, Y$  be two variables, then:

$$p(X) = \sum_Y p(X, Y)$$

## Marginalization

- Suppose  $X$  and  $Y$  are random variables with distribution  $p(X, Y)$   
 $X$ : Intelligence,  $\text{Val}(X) = \{\text{"Very High"}, \text{"High"}\}$   
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- $p(Y = a) = ?$  0.85
- More generally, suppose we have a joint distribution  $p(X_1, \dots, X_n)$ . Then,

$$p(X_i = x_i) = \sum_{x_1} \sum_{x_2} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_n} p(x_1, \dots, x_n)$$



## Conditioning

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- Can compute the conditional probability:

$$\begin{aligned}
 p(Y = a | X = vh) &= \frac{p(Y = a, X = vh)}{p(X = vh)} \\
 &= \frac{p(Y = a, X = vh)}{p(Y = a, X = vh) + p(Y = b, X = vh)} \\
 &= \frac{0.7}{0.7 + 0.1} = 0.875
 \end{aligned}$$

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- One famous model, Quick Medical Reference (QMR-DT), has 600 diseases and 4000 findings.

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- How many outcomes are there in QMR-DT?  $2^{4600}$
- Estimation of joint distribution would require a huge amount of data
- Inference of conditional probabilities, e.g.  
 $p(\text{common cold} = 1 | \text{cough} = 1, \text{fever} = 1, \text{vomiting} = 0)$   
would require summing over exponentially many variables' values

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- However, this is not a very useful model—observing a variable  $X_i$  cannot influence our predictions of  $X_j$
- If  $X_1, \dots, X_n$  are conditionally independent given  $Y$ , denoted as  $X_i \perp X_{-i} | Y$  then:

$$\begin{aligned} p(y, x_1, \dots, x_n) &= p(y)p(x_1|y) \prod_{i=2}^n p(x_i|x_1, \dots, x_{i-1}, y) \\ &= p(y)p(x_1|y) \prod_{i=2}^n p(x_i|y) \end{aligned}$$

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- Simple, yet powerful

## Example: naive Bayes

- Suppose that the features are conditionally independent given class label  $Y$ . Then

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- Estimate** the model with maximum likelihood. **Predict** with:

$$p(Y = 1|x_1, \dots, x_n) = \frac{p(Y = 1) \prod_{i=1}^n p(x_i|Y = 1)}{\sum_{y=\{0,1\}} p(Y = y) \prod_{i=1}^n p(x_i|Y = y)}$$

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- Are the independence assumptions made here reasonable?
- Philosophy: Nearly all probabilistic models are “wrong”, but many are nonetheless useful

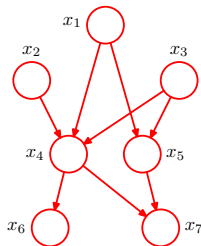
# Bayesian Network

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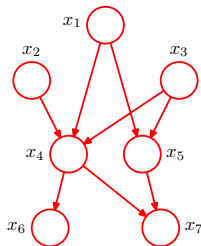
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- $$p(x_1, x_2, x_3, x_4, x_5, x_6, x_7) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3)p(x_5|x_1, x_3)p(x_6|x_4)p(x_7|x_4, x_5)$$

## Bayesian Networks

- A graph with  $K$  nodes, the joint distribution is given by:

$$p(\mathbf{x}) = \prod_{k=1}^K p(x_k | pa_k)$$

where  $pa_k$  denotes the set of parents of  $x_k$  and  
 $\mathbf{x} = \{x_1, \dots, x_K\}$

- This key equation expresses the *factorization* properties of the joint distribution for a directed graphical model.



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- Has she been Burgled (B), or was the alarm triggered by an Earthquake (E)?
- She turns the car Radio (R) on for news of earthquakes
- Without loss of generality, we can write:

$$\begin{aligned} p(A, R, E, B) &= p(A|R, E, B)P(R, E, B) \\ &= p(A|R, E, B)p(R|E, B)p(E, B) \\ &= p(A|R, E, B)p(R|E, B)p(E|B)p(B) \end{aligned}$$

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### Assumptions

- The alarm is not directly influenced by any report on the radio  
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 $p(R|E, B) = p(R|E)$

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- Therefore, we have:

$$p(A, R, E, B) = p(A|E, B)p(R|E)p(E)p(B)$$

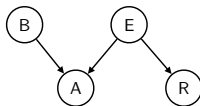


## Alarm Example - probability table

- DAG for  $p(A, R, E, B) = p(A|E, B)p(R|E)p(E)p(B)$

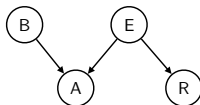
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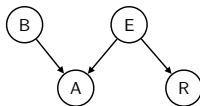


- Probability table for  $p(A|B, E)$ :

Alarm = 1	Burglar	Earthquake
0.9999	1	1
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0.99	0	1
0.0001	0	0

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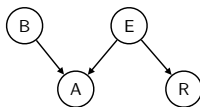
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1	1
0	0

- $p(B = 1) = 0.01$  and  $p(E = 1) = 0.000001$

## Alarm Example - probability table

- Initial evidence: the alarm is sounding

$$\begin{aligned}
 p(B = 1|A = 1) &= \frac{\sum_{E,R} p(B = 1, E, A = 1, R)}{\sum_{B,E,R} P(B, E, A = 1, R)} \\
 &= \frac{\sum_{E,R} p(A = 1|B = 1, E)p(B = 1)p(R|E)p(E)}{\sum_{B,E,R} p(A = 1|B, E)p(B)p(E)p(R|E)} \\
 &\approx 0.99
 \end{aligned}$$

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- Initially, because the alarm sounds, Sally thinks that she's been burgled. However, this probability drops dramatically when she hears that there has been an earthquake.

## Alarm Example - inference

- Additional evidence: the radio broadcasts an earthquake warning
- A similar calculation gives:  $p(B = 1|A = 1, R = 1) \approx 0.01$
- Initially, because the alarm sounds, Sally thinks that she's been burgled. However, this probability drops dramatically when she hears that there has been an earthquake.
- The earthquake "explains away" to an extent the fact that the alarm is ringing

## Wet grass example

- One morning Tracey leaves her house and realizes that her grass is wet (T).

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- One morning Tracey leaves her house and realizes that her grass is wet (T).
- Is it due to overnight Rain (R) or did she forget to turn off the sprinkler (S) last night?
- Next she notices that the grass of her neighbor, Jack, is also wet (J). This explains away to some extent the possibility that her sprinkler was left on, and she concludes therefore that it has probably been raining.

## Wet grass example (cont)

- $R \in \{0, 1\}$ ,  $R = 1$  means that it has been raining, and 0 otherwise

## Wet grass example (cont)

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## Wet grass example (cont)

- $R \in \{0, 1\}$ ,  $R = 1$  means that it has been raining, and 0 otherwise
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- $J \in \{0, 1\}$ ,  $J = 1$  means that Jack's grass is wet, and 0 otherwise



## Wet grass example (cont)

- $R \in \{0, 1\}$ ,  $R = 1$  means that it has been raining, and 0 otherwise
- $S \in \{0, 1\}$ ,  $S = 1$  means that Tracey has forgotten to turn off the sprinkler, and 0 otherwise
- $J \in \{0, 1\}$ ,  $J = 1$  means that Jack's grass is wet, and 0 otherwise
- Joint probability

$$\begin{aligned}
 p(T, J, R, S) &= p(T|J, R, S)p(J, R, S) \\
 &= p(T|J, R, S)p(J|R, S)p(R, S) \\
 &= p(T|J, R, S)p(J|R, S)p(R|S)p(S)
 \end{aligned}$$

## Wet grass example (cont)

- The number of values that need to be specified in general scales exponentially with the number of variables in the model. This is impractical in general and motivates simplifications

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- Conditional independence:
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## Wet grass example (cont)

- The number of values that need to be specified in general scales exponentially with the number of variables in the model. This is impractical in general and motivates simplifications
- Conditional independence:
  - $p(T|J, R, S) = p(T|R, S)$
  - $p(J|R, S) = p(J|R)$
  - $p(R|S) = p(R)$

## Wet grass example (cont)

- Original equation:

$$\begin{aligned}p(T, J, R, S) &= p(T|J, R, S)p(J, R, S) \\&= p(T|J, R, S)p(J|R, S)p(R, S) \\&= p(T|J, R, S)p(J|R, S)p(R|S)p(S)\end{aligned}$$

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- Now it becomes:

$$p(T, J, R, S) = p(T|R, S)p(J|R)p(R)p(S)$$

## Wet grass example - probability table

- $p(R = 1) = 0.2$  and  $p(S = 1) = 0.1$



## Wet grass example - probability table

- $p(R = 1) = 0.2$  and  $p(S = 1) = 0.1$
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## Wet grass example - probability table

- $p(R = 1) = 0.2$  and  $p(S = 1) = 0.1$
- $p(J = 1|R = 1) = 1$ ,  $p(J = 1|R = 0) = 0.2$
- Probability table for  $p(T|R, S)$ :

T = 1	R	S
1	1	0
1	1	1
0.9	0	1
0	0	0

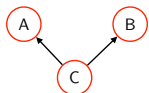
## Wet grass example - inference

$$\begin{aligned}
 p(S = 1|T = 1) &= \frac{p(S = 1, T = 1)}{p(T = 1)} = \frac{\sum_{J,R} p(T = 1, J, R, S = 1)}{\sum_{J,R,S} p(T = 1, J, R, S)} \\
 &= \frac{\sum_{J,R} p(T = 1|R, S = 1)p(J|R)p(R)p(S = 1)}{\sum_{J,R,S} p(T = 1|R, S)p(J|R)p(R)p(S)} \\
 &= \frac{\sum_R p(T = 1|R, S = 1)p(R)p(S = 1)}{\sum_{R,S} p(T = 1|R, S)p(R)p(S)} \\
 &= \frac{0.9 \cdot 0.8 \cdot 0.1 + 0.2 \cdot 0.1}{0.9 \cdot 0.8 \cdot 0.1 + 1 \cdot 0.2 \cdot 0.1 + 0 \cdot 0.8 \cdot 0.9 + 1 \cdot 0.2 \cdot 0.9} \approx 0.3382
 \end{aligned}$$

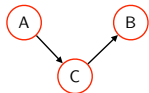
## Wet grass example - inference

$$\begin{aligned}
 p(S = 1|T = 1, J = 1) &= \frac{p(S = 1, T = 1, J = 1)}{p(T = 1, J = 1)} \\
 &= \frac{\sum_R p(T = 1, J = 1, R, S = 1)}{\sum_{R,S} p(T = 1, J = 1, R, S)} \\
 &= \frac{\sum_R p(J = 1|R)p(T = 1|R, S = 1)p(R)p(S = 1)}{\sum_{R,S} p(J = 1|R)p(T = 1|R, S)p(R)p(S)} \\
 &= \frac{0.0344}{0.2144} \approx 0.1604
 \end{aligned}$$

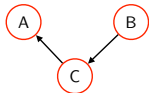
# Independence in Bayesian Network - Marginal independence



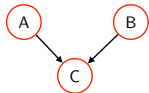
A,B are **marginally dependent**:  $A \not\perp B$   
 $p(A, B) = \sum_C p(A|C)P(B|C)P(C) \neq p(A)p(B)$



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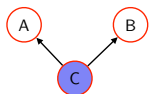


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A,B are **marginally independent**:  $A \perp B$   
 $p(A, B, C) = p(A)p(B)p(C|A, B) \rightarrow p(A, B) = p(A)p(B)$

# Independence in Bayesian Network - Conditional independence

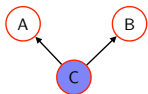


A,B are **conditionally independent** given C

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

Node C is said to be *tail-to-tail*.

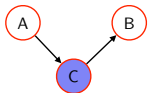
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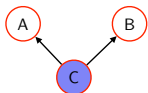


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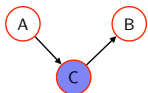
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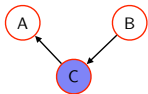
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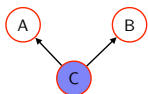


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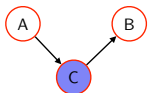
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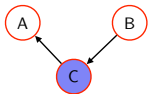
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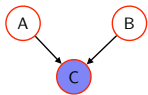
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A,B are **conditionally dependent** given C

$$p(A, B|C) \propto p(C|A, B)p(A)p(B) \neq p(A|C)p(B|C)$$

Node C is said to be *head-to-head*.

## Example: Fuel system on the car

- $B \in \{0, 1\}$ : representing the state of a battery that is either charged ( $B = 1$ ) or flat ( $B = 0$ ).
- $F \in \{0, 1\}$ : representing the state of the fuel tank that is either full of fuel ( $F = 1$ ) or empty ( $F = 0$ ).
- $G \in \{0, 1\}$ : representing the state of an electric fuel gauge and which indicates either full ( $G = 1$ ) or empty ( $G = 0$ ).

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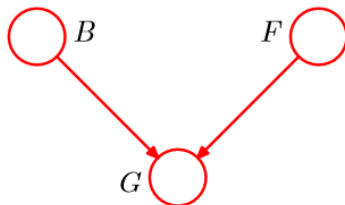


Figure: [C. Bishop, PRML]

## Example: Fuel system on the car

Probability table:  $p(G, B, F) = p(B)p(F)p(G|B, F)$

$$p(B = 1) = 0.9$$

$$p(F = 1) = 0.9$$

G = 1	B	F
0.8	1	1
0.2	1	0
0.2	0	1
0.1	0	0

## Example: Fuel system on the car

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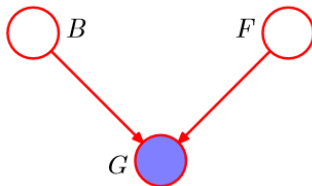


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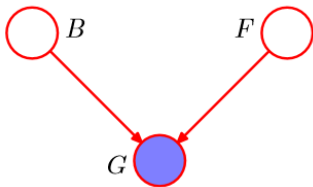


Figure: [C. Bishop, PRML]

- $p(F = 0|G = 0) > p(F = 0)$  observing that the gauge reads empty makes it more likely that the tank is indeed empty.

$$p(F = 0|G = 0) = \frac{p(G = 0|F = 0)p(F = 0)}{p(G = 0)} \approx 0.257$$

## Example: Fuel system on the car

- Now observed the states of both the fuel gauge and the battery:

$$p(F = 0 | G = 0, B = 0) \approx 0.111$$

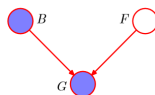


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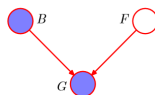


Figure: [C. Bishop, PRML]

- The probability that the tank is empty has *decreased* (from 0.257 to 0.111) as a result of the observation of the state of the battery. Finding out that the battery is flat *explains away* the observation that the fuel gauge reads empty.

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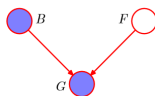


Figure: [C. Bishop, PRML]

- The probability that the tank is empty has *decreased* (from 0.257 to 0.111) as a result of the observation of the state of the battery. Finding out that the battery is flat *explains away* the observation that the fuel gauge reads empty.
- The state of the fuel tank (F) and that of the battery (B) have indeed become dependent on each other as a result of observing the reading on the fuel gauge (G).

## D-separation ( “directed separated” ) in Bayesian networks

- Algorithm to find out whether  $A \perp B | C$  is implied by a given directed acyclic graph.

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- Look at all possible paths from A to B, any such path is said to be **blocked** if it includes a node such that either
  1. the arrows on the path meet either **head-to-tail** or **tail-to-tail** at the node, and the node is in the set C
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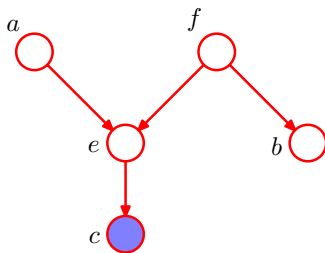
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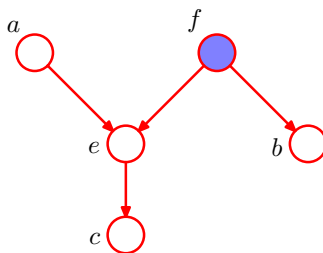
## D-separation (“directed separated”) in Bayesian networks

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- If all such paths are blocked, then  $A$  is said to be *d-separated* from  $B$  by  $C$ . And the joint distribution for all variables in the graph will satisfy  $A \perp B | C$ .
- d-separation reduces statistical independencies (hard) to connectivity in graphs (easy)
- Important because it allows us to quickly prune the Bayesian network, finding just the relevant variables for answering a query

# D-separation examples



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



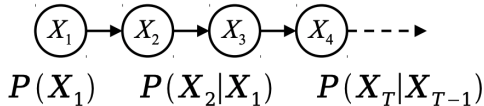
(b)  $a \perp b | f$

# Some frequently used graphical models



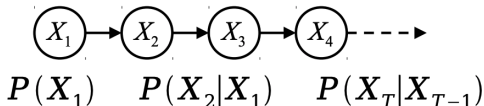
## Markov Models

- A Markov model is a chain-structured BN
  - Each node is identically distributed (stationarity)
  - Value of  $X$  at a given time is called the state
  - As a BN:



- Parameters: called transition probabilities or dynamics, specify how the state evolves over time (also, initial probs)

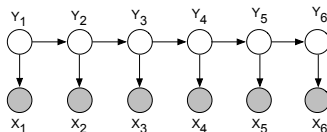
## Markov Models - Conditional Independence



- Basic conditional independence
  - Past and future independent of the present
  - Each time step only depends on the previous
  - This is called the (first order) Markov property
- Note that the chain is just a (growing) BN
  - We can always use generic BN reasoning on it (if we truncate the chain)

## Hidden Markov models

- Markov chains not so useful for most agents
  - Eventually you don't know anything anymore
  - Prediction needs previous observations.
- Hidden Markov Models



- Frequently used for speech recognition and video modelling
- Underlying Markov chain over states  $S$
- Joint distribution factors as:

$$p(\mathbf{y}, \mathbf{x}) = p(y_1)p(x_1|y_1) \prod_{t=2}^T p(y_t|y_{t-1})p(x_t|y_t)$$

## Hidden Markov models

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$$p(\mathbf{y}, \mathbf{x}) = p(y_1)p(x_1|y_1) \prod_{t=2}^T p(y_t|y_{t-1})p(x_t|y_t)$$

- $p(y_1)$  is the distribution for the starting state
  - $p(y_t|y_{t-1})$  is the transition probability between any two states
  - $p(x_t|y_t)$  is the emission probability
- What are the conditional independencies here? e.g.  
 $Y_1 \perp \{Y_3, \dots, Y_6\} | Y_2$
- Markov assumptions:
  - The current state is conditionally independent of all the past states given the states in the previous time step.
  - The current evidence is only dependent on the current state.

# Acknowledgement and Further Reading

Slides are adapted from Dr. Y. Ning's Spring 19 offering of CS-559.

Further Reading:

Chapter 8.1 8.2 of *Pattern Recognition and Machine Learning* by C. Bishop.