

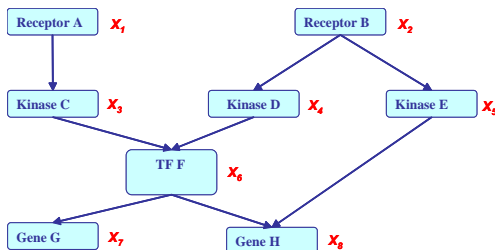
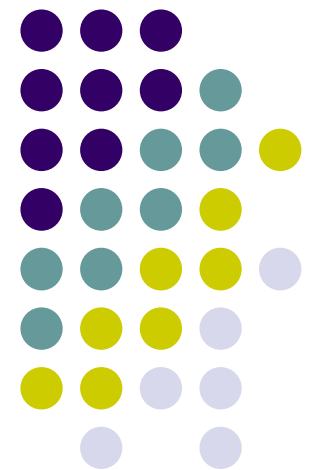


# Probabilistic Graphical Models

## Directed GMs: Bayesian Networks

Eric Xing

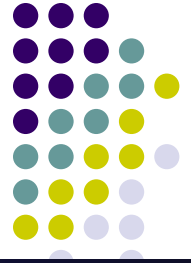
Lecture 2, January 15, 2014



Reading: see class homepage

# Questions ?

---



- Scribes ?
- Waiting list
- Reading: required vs suggested

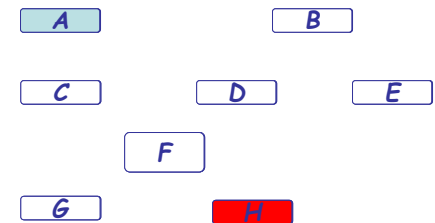


# Representing Multivariate Distribution

- Representation: what is the joint probability dist. on multiple variables?

$$P(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8,)$$

- How many state configurations in total? ---  $2^8$
- Are they all needed to be represented?
- Do we get any scientific/medical insight?



- Factored representation: the chain-rule

$$\begin{aligned}
 &P(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8) \\
 &= P(X_1)P(X_2 | X_1)P(X_3 | X_1, X_2)P(X_4 | X_1, X_2, X_3)P(X_5 | X_1, X_2, X_3, X_4)P(X_6 | X_1, X_2, X_3, X_4, X_5) \\
 &P(X_7 | X_1, X_2, X_3, X_4, X_5, X_6)P(X_8 | X_1, X_2, X_3, X_4, X_5, X_6, X_7)
 \end{aligned}$$

- This factorization is true for any distribution and any variable ordering
- Do we save any parameterization cost?

- If  $X_i$ 's are **independent**: ( $P(X_i|\cdot) = P(X_i)$ )

$$\begin{aligned}
 &P(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8) \\
 &= P(X_1)P(X_2)P(X_3)P(X_4)P(X_5)P(X_6)P(X_7)P(X_8) = \prod_i P(X_i)
 \end{aligned}$$

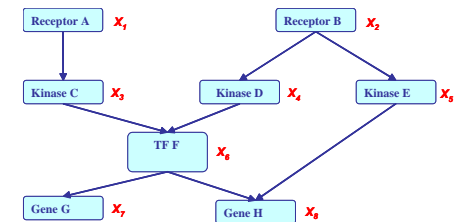
- What do we gain?
- What do we lose?



# Two types of GMs

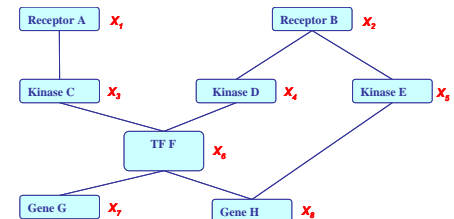
- **Directed edges** give **causality** relationships (Bayesian Network or Directed Graphical Model):

$$\begin{aligned}
 &P(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8) \\
 &= P(X_1) P(X_2) P(X_3/X_1) P(X_4/X_2) P(X_5/X_2) \\
 &\quad P(X_6/X_3, X_4) P(X_7/X_6) P(X_8/X_5, X_6)
 \end{aligned}$$



- **Undirected edges** simply give **correlations** between variables (Markov Random Field or Undirected Graphical model):

$$\begin{aligned}
 &P(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8) \\
 &= \frac{1}{Z} \exp\{E(X_1)+E(X_2)+E(X_3, X_1)+E(X_4, X_2)+E(X_5, X_2) \\
 &\quad + E(X_6, X_3, X_4)+E(X_7, X_6)+E(X_8, X_5, X_6)\}
 \end{aligned}$$





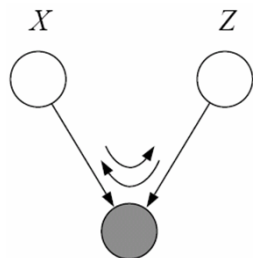
# Notation

---

- Variable, value and index
- Random variable
- Random vector
- Random matrix
- Parameters



- Representation of directed GM





# Example: The Dishonest Casino

A casino has two dice:

- Fair die

$$P(1) = P(2) = P(3) = P(5) = P(6) = 1/6$$

- Loaded die

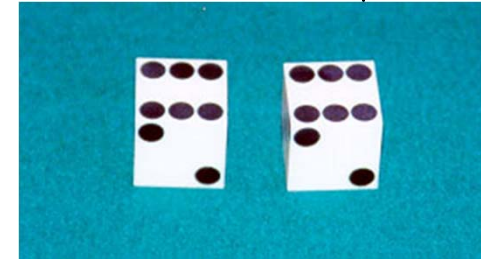
$$P(1) = P(2) = P(3) = P(5) = 1/10$$

$$P(6) = 1/2$$

Casino player switches back-&-forth  
between fair and loaded die once every  
20 turns

## Game:

1. You bet \$1
2. You roll (always with a fair die)
3. Casino player rolls (maybe with fair die, maybe with loaded die)
4. Highest number wins \$2



# Puzzles regarding the dishonest casino



**GIVEN:** A sequence of rolls by the casino player

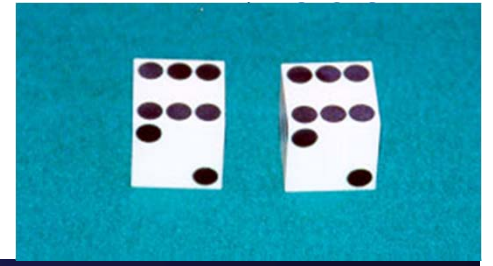
1245526462146146136136661664661636616366163616515615115146123562344

## QUESTION

- How likely is this sequence, given our model of how the casino works?
  - This is the **EVALUATION** problem
- What portion of the sequence was generated with the fair die, and what portion with the loaded die?
  - This is the **DECODING** question
- How “loaded” is the loaded die? How “fair” is the fair die? How often does the casino player change from fair to loaded, and back?
  - This is the **LEARNING** question



# Knowledge Engineering



- **Picking variables**
  - Observed
  - Hidden
  
- **Picking structure**
  - CAUSAL
  - Generative
  - Coupling
  
- **Picking Probabilities**
  - Zero probabilities
  - Orders of magnitudes
  - Relative values



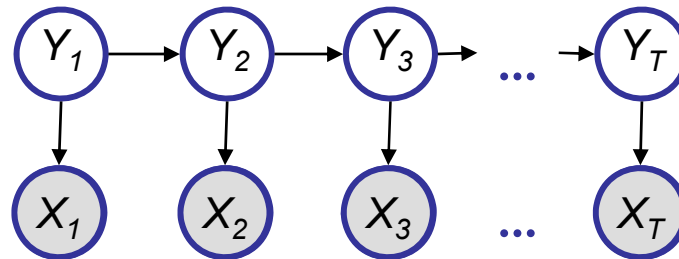
# Hidden Markov Model

## The underlying source:

Speech signal  
genome function  
dice

## The sequence:

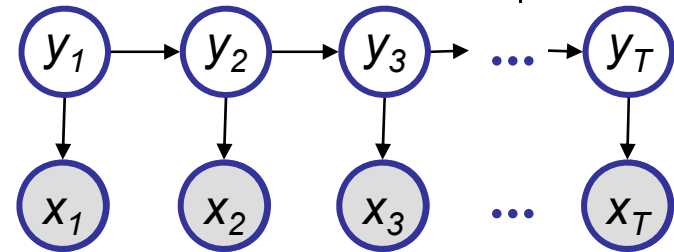
Phonemes  
DNA sequence  
sequence of rolls





# Probability of a parse

- Given a sequence  $\mathbf{x} = x_1 \dots x_T$  and a parse  $\mathbf{y} = y_1, \dots, y_T$ ,
- To find how likely is the parse: (given our HMM and the sequence)



$$\begin{aligned} p(\mathbf{x}, \mathbf{y}) &= p(x_1 \dots x_T, y_1, \dots, y_T) && \text{(Joint probability)} \\ &= p(y_1) p(x_1 | y_1) p(y_2 | y_1) p(x_2 | y_2) \dots p(y_T | y_{T-1}) p(x_T | y_T) \\ &= p(y_1) P(y_2 | y_1) \dots p(y_T | y_{T-1}) \times p(x_1 | y_1) p(x_2 | y_2) \dots p(x_T | y_T) \\ &= p(y_1, \dots, y_T) p(x_1 \dots x_T | y_1, \dots, y_T) \end{aligned}$$

- Marginal probability:  $p(\mathbf{x}) = \sum_{\mathbf{y}} p(\mathbf{x}, \mathbf{y}) = \sum_{y_1} \sum_{y_2} \dots \sum_{y_N} \pi_{y_1} \prod_{t=2}^T a_{y_{t-1}, y_t} \prod_{t=1}^T p(x_t | y_t)$
- Posterior probability:  $p(\mathbf{y} | \mathbf{x}) = p(\mathbf{x}, \mathbf{y}) / p(\mathbf{x})$

- We will learn how to do this explicitly (polynomial time)



# Bayesian Network:

---

- A BN is a directed graph whose nodes represent the random variables and whose edges represent direct influence of one variable on another.
- It is a data structure that provides the skeleton for representing a **joint distribution** compactly in a **factorized** way;
- It offers a compact representation for **a set of conditional independence assumptions** about a distribution;
- We can view the graph as encoding a **generative sampling process** executed by nature, where the value for each variable is selected by nature using a distribution that depends only on its parents. In other words, each variable is a stochastic function of its parents.



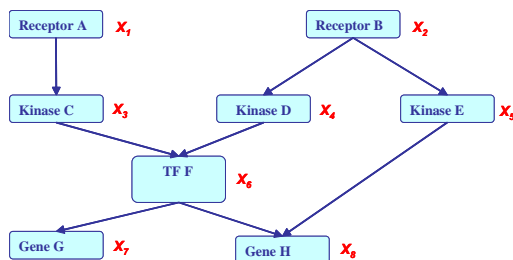
# Bayesian Network: Factorization Theorem

- **Theorem:**

Given a DAG, The most general form of the probability distribution that is **consistent with** the graph factors according to “node given its parents”:

$$P(\mathbf{X}) = \prod_{i=1:d} P(X_i | \mathbf{X}_{\pi_i})$$

where  $\mathbf{X}_{\pi_i}$  is the set of parents of  $X_i$ ,  $d$  is the number of nodes (variables) in the graph.

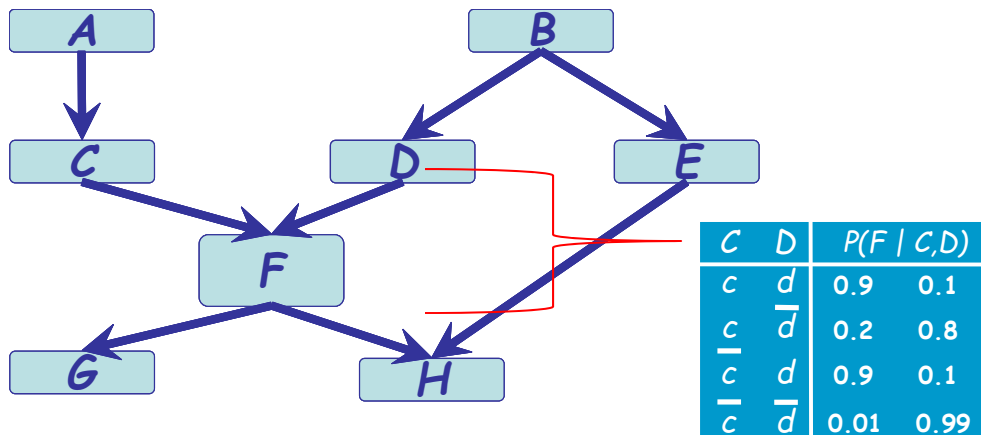


$$\begin{aligned} & P(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8) \\ &= P(X_1) P(X_2) P(X_3 | X_1) P(X_4 | X_2) P(X_5 | X_2) \\ & \quad P(X_6 | X_3, X_4) P(X_7 | X_6) P(X_8 | X_5, X_6) \end{aligned}$$



# Specification of a directed GM

- There are two components to any GM:
  - the *qualitative* specification
  - the *quantitative* specification



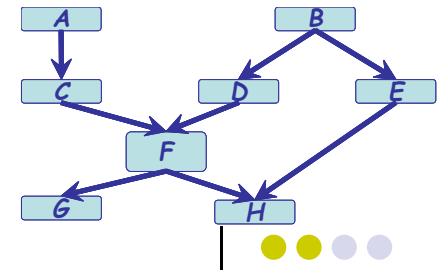
# Qualitative Specification

---



- Where does the qualitative specification come from?
  - Prior knowledge of causal relationships
  - Prior knowledge of modular relationships
  - Assessment from experts
  - Learning from data
  - We simply link a certain architecture (e.g. a layered graph)
  - ...

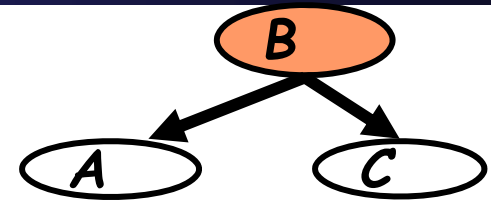
# Local Structures & Independencies



- Common parent

- Fixing B decouples A and C

"given the level of gene B, the levels of A and C are independent"



- Cascade

- Knowing B decouples A and C

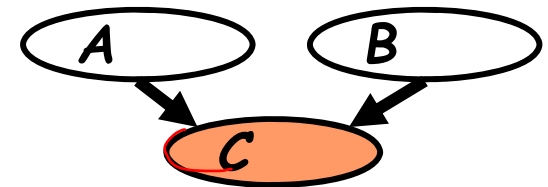
"given the level of gene B, the level gene A provides no extra prediction value for the level of gene C"



- V-structure

- Knowing C couples A and B because A can "explain away" B w.r.t. C

"If A correlates to C, then chance for B to also correlate to B will decrease"

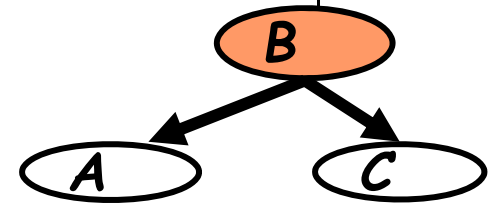


- The language is compact, the concepts are rich!



# A simple justification

---



# I-maps



- **Defn** : Let  $P$  be a distribution over  $X$ . We define  $I(P)$  to be the set of independence assertions of the form  $(X \perp Y \mid Z)$  that hold in  $P$  (however how we set the parameter-values).
- **Defn** : Let  $K$  be *any graph object* associated with a set of independencies  $I(K)$ . We say that  $K$  is an *I-map* for a set of independencies  $I$ , if  $I(K) \subseteq I$ .
- We now say that  $G$  is an I-map for  $P$  if  $G$  is an I-map for  $I(P)$ , where we use  $I(G)$  as the set of independencies associated.

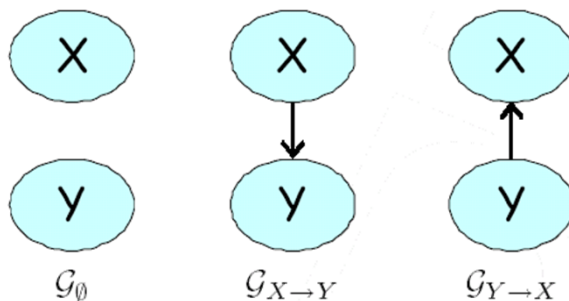


# Facts about I-map

- For  $G$  to be an I-map of  $P$ , it is necessary that  $G$  does not mislead us regarding independencies in  $P$ :

any independence that  $G$  asserts must also hold in  $P$ . Conversely,  $P$  may have additional independencies that are not reflected in  $G$

- Example:



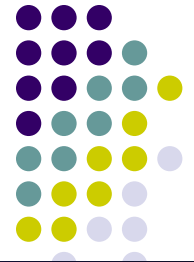
$P_1$

| $X$   | $Y$   | $P(X, Y)$ |
|-------|-------|-----------|
| $x^0$ | $y^0$ | 0.08      |
| $x^0$ | $y^1$ | 0.32      |
| $x^1$ | $y^0$ | 0.12      |
| $x^1$ | $y^1$ | 0.48      |

$P_2$

| $X$   | $Y$   | $P(X, Y)$ |
|-------|-------|-----------|
| $x^0$ | $y^0$ | 0.4       |
| $x^0$ | $y^1$ | 0.3       |
| $x^1$ | $y^0$ | 0.2       |
| $x^1$ | $y^1$ | 0.1       |

# What is in $I(G)$ --- local Markov assumptions of BN



A *Bayesian network structure*  $G$  is a directed acyclic graph whose nodes represent random variables  $X_1, \dots, X_n$ .

## local Markov assumptions

- **Defn :**

Let  $Pa_{X_i}$  denote the parents of  $X_i$  in  $G$ , and  $NonDescendants_{X_i}$  denote the variables in the graph that are not descendants of  $X_i$ . Then  $G$  encodes the following set of **local conditional independence assumptions**  $I_\ell(G)$ :

$$I_\ell(G): \{X_i \perp NonDescendants_{X_i} \mid Pa_{X_i} : \forall i\},$$

In other words, each node  $X_i$  is independent of its nondescendants given its parents.

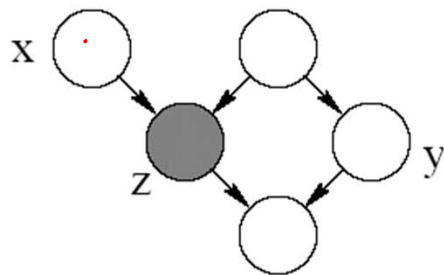


# Graph separation criterion

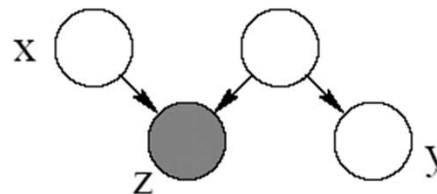
- D-separation criterion for Bayesian networks (D for Directed edges):

**Defn:** variables  $x$  and  $y$  are *D-separated* (conditionally independent) given  $z$  if they are separated in the *moralized* ancestral graph

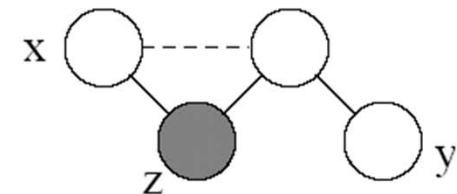
- Example:



original graph



ancestral



moral ancestral



# Active trail

- **Causal trail**  $X \rightarrow Z \rightarrow Y$  : active if and only if  $Z$  is not observed.
- **Evidential trail**  $X \leftarrow Z \leftarrow Y$  : active if and only if  $Z$  is not observed.
- **Common cause**  $X \leftarrow Z \rightarrow Y$  : active if and only if  $Z$  is not observed.
- **Common effect**  $X \rightarrow Z \leftarrow Y$  : active if and only if either  $Z$  or one of  $Z$ 's descendants is observed

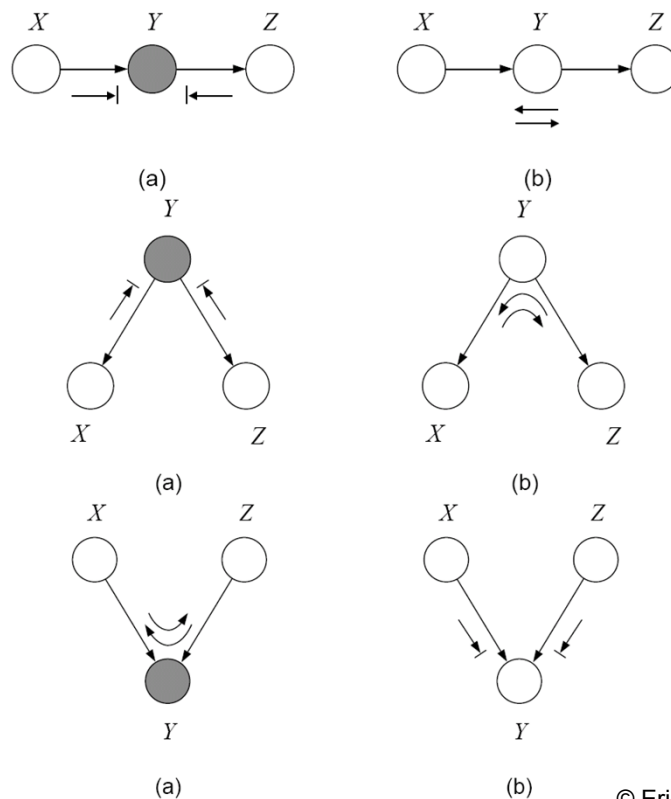
**Definition** : Let  $X, Y, Z$  be three **sets** of nodes in  $G$ . We say that  $X$  and  $Y$  are ***d-separated given  $Z$*** , denoted  ***$d\text{-sep}_G(X;Y | Z)$*** , if there is **no** active trail between any node  $X \in X$  and  $Y \in Y$  given  $Z$ .

# What is in $I(G)$ ---

## Global Markov properties of BN



- $X$  is **d-separated** (directed-separated) from  $Z$  given  $Y$  if we can't send a ball from any node in  $X$  to any node in  $Z$  using the "*Bayes-ball*" algorithm illustrated below (and plus some boundary conditions):



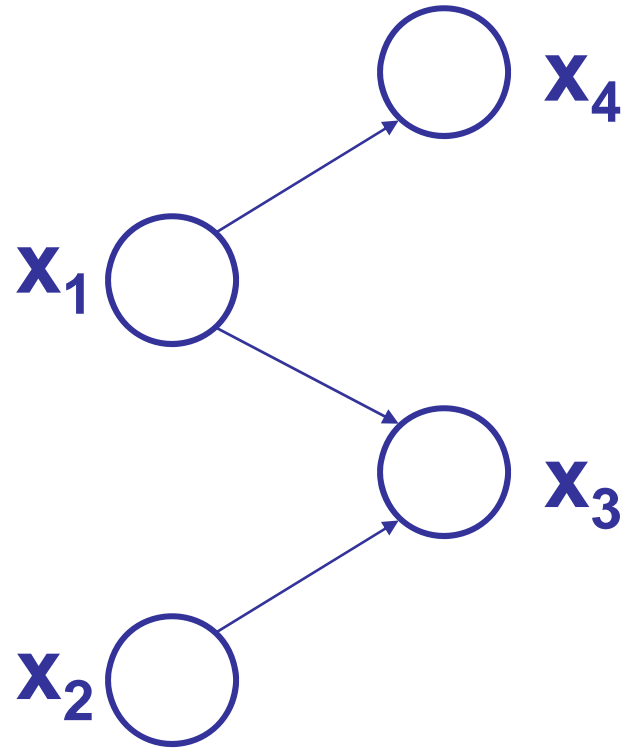
- **Defn:**  $I(G)$  = all independence properties that correspond to d-separation:

$$I(G) = \{X \perp Z | Y : \text{dsep}_G(X; Z | Y)\}$$

- **D-separation is sound and complete** (more details later)



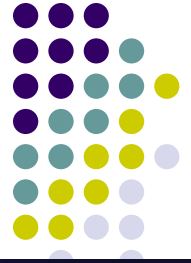
# Example:



- Complete the  $I(G)$  of this graph:



# Toward quantitative specification of probability distribution



- Separation properties in the graph imply independence properties about the associated variables
- **The Equivalence Theorem**

For a graph  $G$ ,

Let  $\mathcal{D}_1$  denote the family of **all distributions** that satisfy  $I(G)$ ,

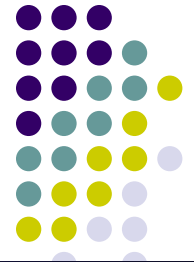
Let  $\mathcal{D}_2$  denote the family of **all distributions** that factor according to  $G$ ,

$$P(\mathbf{X}) = \prod_{i=1:d} P(X_i | \mathbf{X}_{\pi_i})$$

Then  $\mathcal{D}_1 \equiv \mathcal{D}_2$ .

- For the graph to be useful, any conditional independence properties we can derive from the graph should hold for the probability distribution that the graph represents

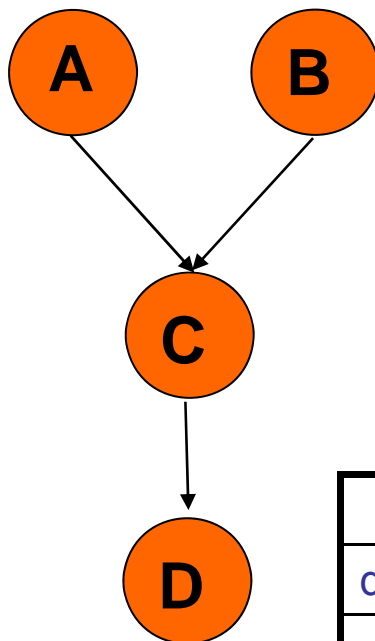
# Conditional probability tables (CPTs)



|       |      |
|-------|------|
| $a^0$ | 0.75 |
| $a^1$ | 0.25 |

|       |      |
|-------|------|
| $b^0$ | 0.33 |
| $b^1$ | 0.67 |

$$P(a,b,c,d) = P(a)P(b)P(c|a,b)P(d|c)$$



|       | $a^0b^0$ | $a^0b^1$ | $a^1b^0$ | $a^1b^1$ |
|-------|----------|----------|----------|----------|
| $c^0$ | 0.45     | 1        | 0.9      | 0.7      |
| $c^1$ | 0.55     | 0        | 0.1      | 0.3      |

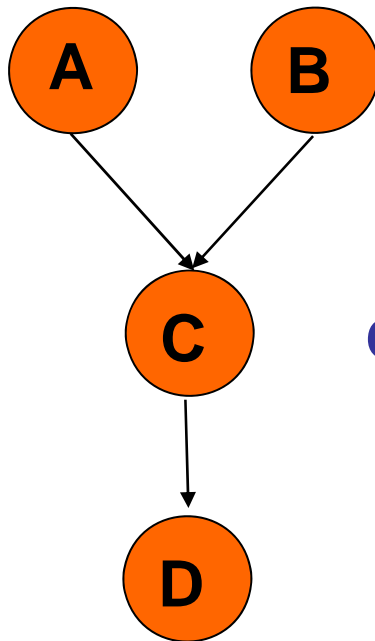
|       | $c^0$ | $c^1$ |
|-------|-------|-------|
| $d^0$ | 0.3   | 0.5   |
| $d^1$ | 0.7   | 0.5   |

# Conditional probability density func. (CPDs)



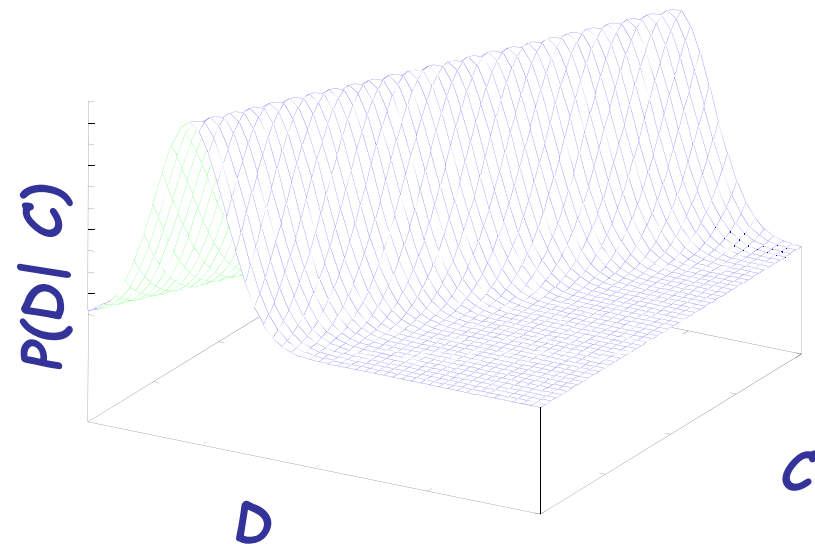
$$A \sim N(\mu_a, \Sigma_a) \quad B \sim N(\mu_b, \Sigma_b)$$

$$P(a,b,c,d) = P(a)P(b)P(c|a,b)P(d|c)$$



$$C \sim N(A+B, \Sigma_c)$$

$$D \sim N(\mu_d + C, \Sigma_d)$$

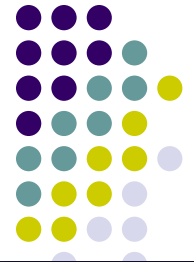


# Summary of BN semantics

---



- **Defn** : A *Bayesian network* is a pair  $(G, P)$  where  $P$  factorizes over  $G$ , and where  $P$  is specified as set of CPDs associated with  $G$ 's nodes.
  - Conditional independencies imply factorization
  - Factorization according to  $G$  implies the associated conditional independencies.
  - Are there **other independencies** that hold for every distribution  $P$  that factorizes over  $G$ ?



# Soundness and completeness

D-separation is sound and "complete" w.r.t. BN factorization law

**Soundness:**

**Theorem:** If a distribution  $P$  factorizes according to  $G$ , then  $I(G) \subseteq I(P)$ .

**"Completeness":**

**"Claim":** For any distribution  $P$  that factorizes over  $G$ , if  $(X \perp Y \mid Z) \in I(P)$  then  $d\text{-sep}_G(X; Y \mid Z)$ .

Contrapositive of the completeness statement

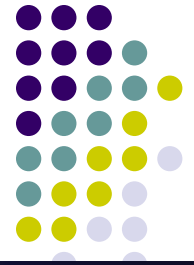
- "If  $X$  and  $Y$  are **not**  $d$ -separated given  $Z$  in  $G$ , then  $X$  and  $Y$  are **dependent in all** distributions  $P$  that factorize over  $G$ ."
- Is this true?

# Distributional equivalence and I-equivalence

---



- All independence in  $I_d(G)$  will be captured in  $I_f(G)$ , is the reverse true?
- Are "not-independence" from  $G$  all honored in  $P_f$  ?



# Soundness and completeness

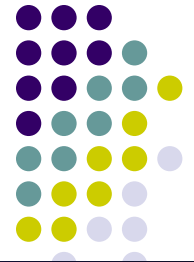
- Contrapositive of the completeness statement
  - "If  $X$  and  $Y$  are **not**  $d$ -separated given  $Z$  in  $G$ , then  $X$  and  $Y$  are **dependent in all** distributions  $P$  that factorize over  $G$ ."
  - Is this true?

- No. Even if a distribution factorizes over  $G$ , it can still contain **additional independencies** that are not reflected in the structure

- Example: graph  $A \rightarrow B$ , for actually independent  $A$  and  $B$  (the independence can be captured by some subtle way of parameterization)

| $A$   | $b^0$ | $b^1$ |
|-------|-------|-------|
| $a^0$ | 0.4   | 0.6   |
| $a^1$ | 0.4   | 0.6   |

- **Thm:** Let  $G$  be a BN graph. If  $X$  and  $Y$  are not  $d$ -separated given  $Z$  in  $G$ , then  $X$  and  $Y$  are **dependent in some** distribution  $P$  that factorizes over  $G$ .



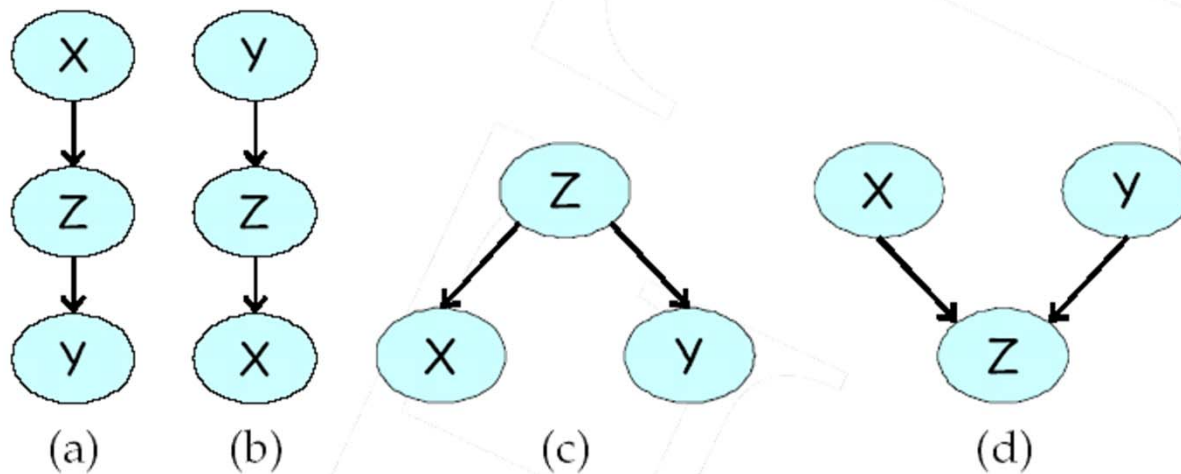
- **Theorem** : For **almost all** distributions  $P$  that factorize over  $G$ , i.e., for all distributions except for a set of "measure zero" in the space of CPD parameterizations, we have that  $I(P) = I(G)$



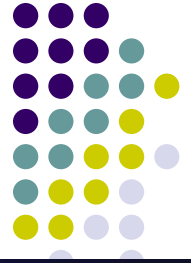


# Uniqueness of BN

- Very different BN graphs can actually be equivalent, in that they encode precisely the same set of conditional independence assertions.

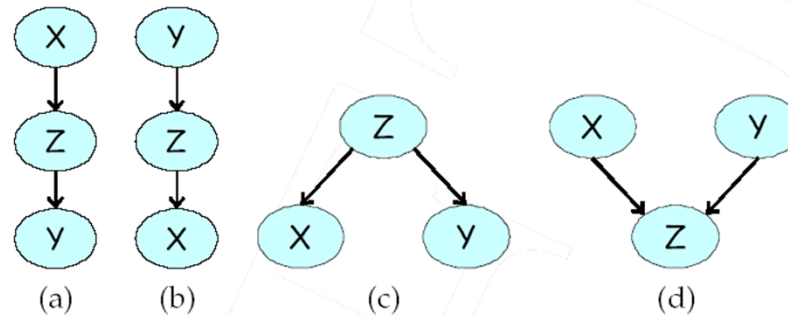


$(X \perp Y | Z)$ .



# I-equivalence

- **Defn** : Two BN graphs  $G1$  and  $G2$  over  $X$  are *I-equivalent* if  $I(G1) = I(G2)$ .
- The set of all graphs over  $X$  is partitioned into a set of mutually exclusive and exhaustive *I-equivalence classes*, which are the set of equivalence classes induced by the I-equivalence relation.

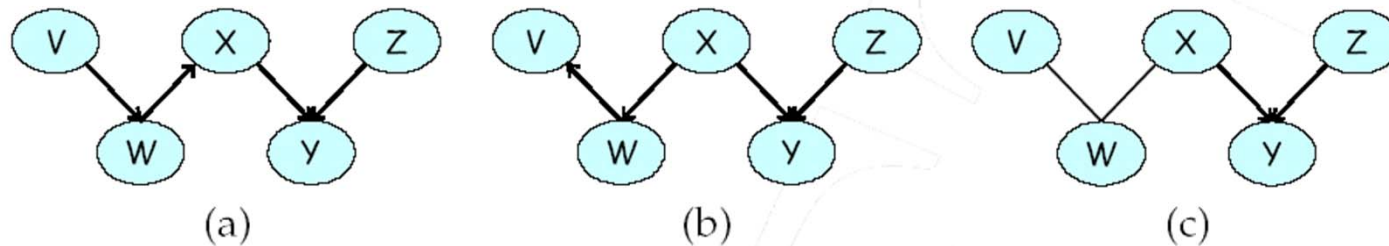


- Any distribution  $P$  that can be factorized over one of these graphs can be factorized over the other.
- Furthermore, there is no intrinsic property of  $P$  that would allow us associate it with one graph rather than an equivalent one.
- This observation has important implications with respect to our ability to determine the directionality of influence.



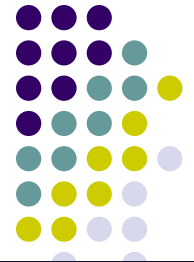
# Detecting I-equivalence

- **Defn** : The *skeleton* of a Bayesian network graph  $G$  over  $V$  is an undirected graph over  $V$  that contains an edge  $\{X, Y\}$  for every edge  $(X, Y)$  in  $G$ .



- **Thm** : Let  $G_1$  and  $G_2$  be two graphs over  $V$ . If  $G_1$  and  $G_2$  have the same skeleton and the same set of v-structures then they are I-equivalent.

- graph equivalence
- Same trail
- But not necessarily active

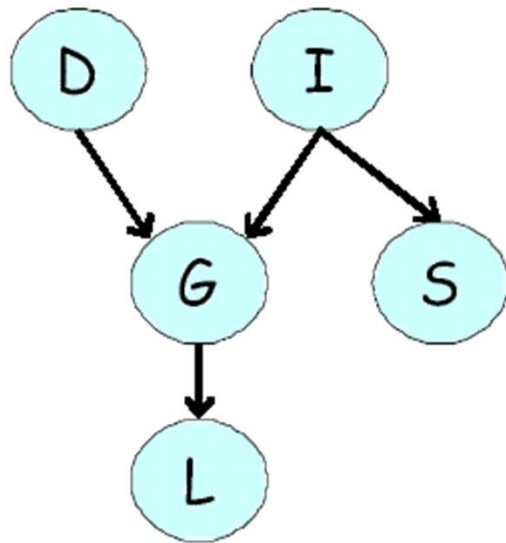


# Minimum I-MAP

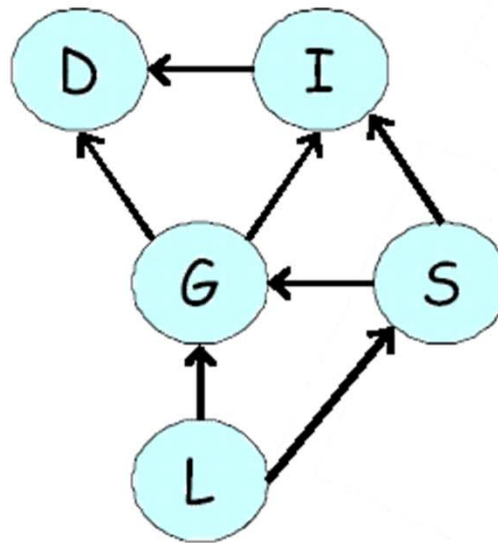
- Complete graph is a (trivial) I-map for any distribution, yet it does not reveal any of the independence structure in the distribution.
  - Meaning that the graph dependence is arbitrary, thus by careful parameterization an dependencies can be captured
  - We want a graph that has the maximum possible  $I(G)$ , yet still  $\subseteq I(P)$
- **Defn** : A graph object  $G$  is a *minimal I-map* for a set of independencies  $I$  if it is an I-map for  $I$ , and if the removal of even a single edge from  $G$  renders it not an I-map.



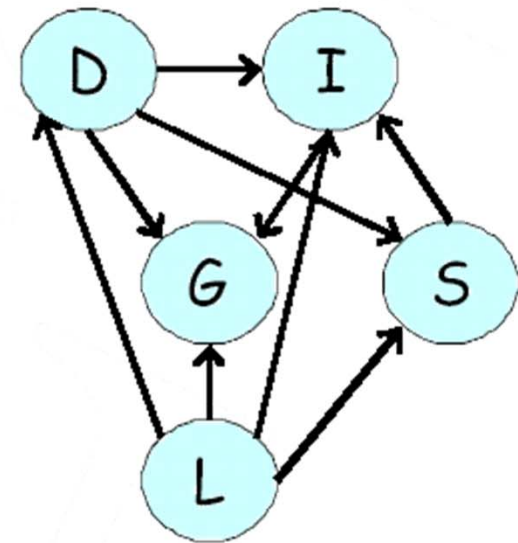
# Minimum I-MAP is not unique



(a)

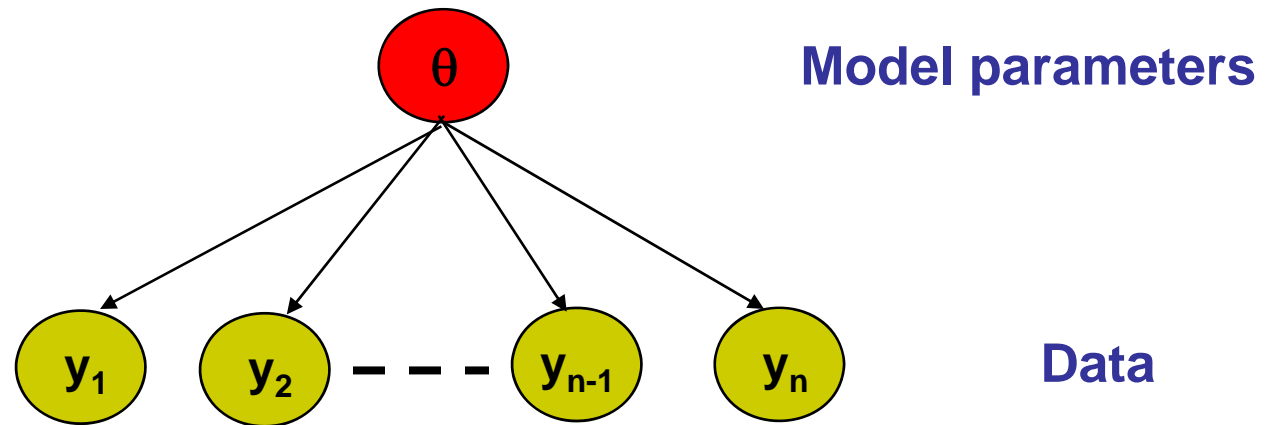


(b)



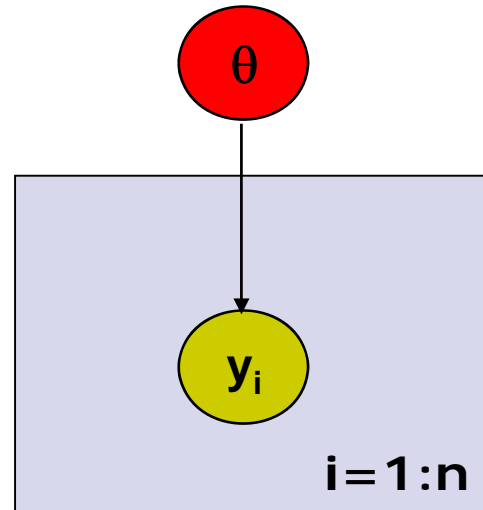
(c)

# Simple BNs: Conditionally Independent Observations





# The “Plate” Micro



Model parameters

Data =  $\{y_1, \dots, y_n\}$

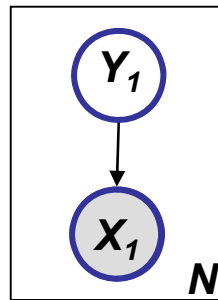
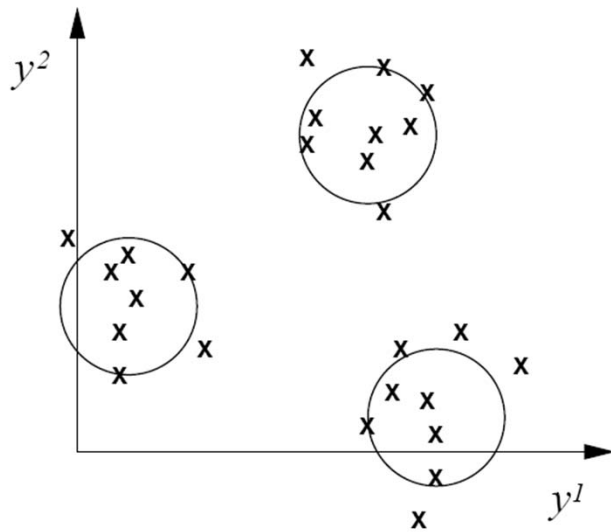
**Plate = rectangle in graphical model**

**variables within a plate are replicated  
in a conditionally independent manner**

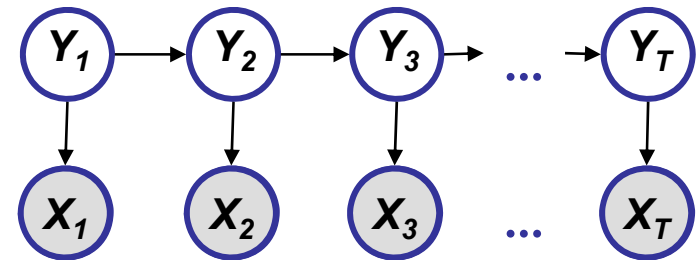
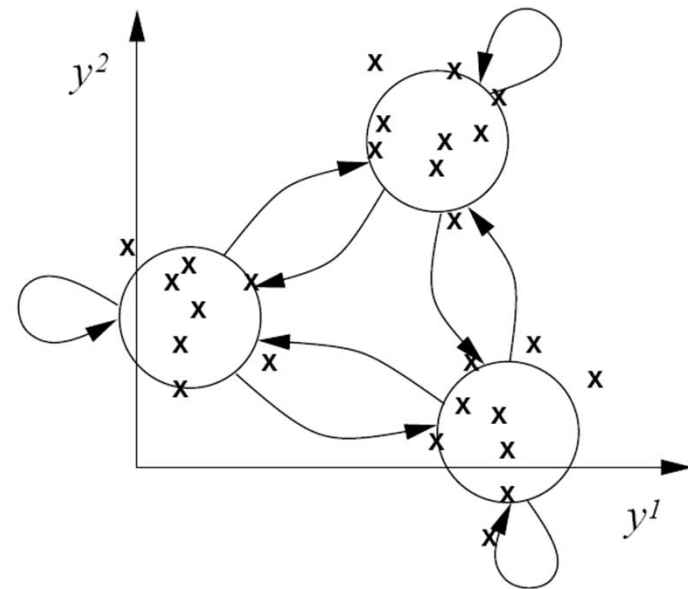
# Hidden Markov Model: from static to dynamic mixture models



Static mixture



Dynamic mixture







# Definition (of HMM)

- **Observation space**

Alphabetic set:  $\mathcal{C} = \{c_1, c_2, \dots, c_K\}$

Euclidean space:  $\mathbb{R}^d$

- **Index set of hidden states**

$$\mathcal{I} = \{1, 2, \dots, M\}$$

- **Transition probabilities** between any two states

$$p(y_t^j = 1 | y_{t-1}^i = 1) = a_{i,j},$$

or  $p(y_t | y_{t-1}^i = 1) \sim \text{Multinomial}(a_{i,1}, a_{i,1}, \dots, a_{i,M}), \forall i \in \mathcal{I}.$

- **Start probabilities**

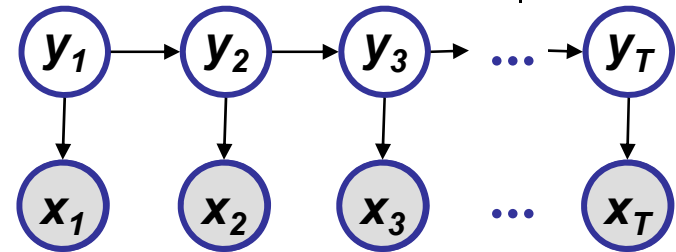
$$p(y_1) \sim \text{Multinomial}(\pi_1, \pi_2, \dots, \pi_M).$$

- **Emission probabilities** associated with each state

$$p(x_t | y_t^i = 1) \sim \text{Multinomial}(b_{i,1}, b_{i,1}, \dots, b_{i,K}), \forall i \in \mathcal{I}.$$

or in general:

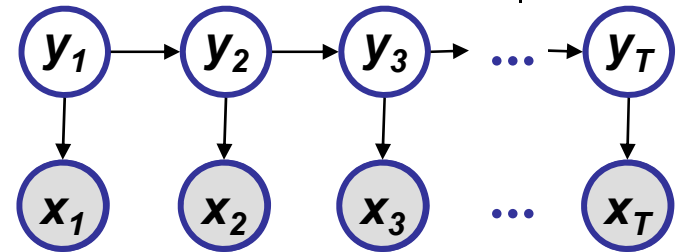
$$p(x_t | y_t^i = 1) \sim f(\cdot | \theta_i), \forall i \in \mathcal{I}.$$





# Probability of a parse

- Given a sequence  $\mathbf{x} = x_1 \dots x_T$  and a parse  $\mathbf{y} = y_1, \dots, y_T$ ,
- To find how likely is the parse:  
(given our HMM and the sequence)



$$\begin{aligned} p(\mathbf{x}, \mathbf{y}) &= p(x_1 \dots x_T, y_1, \dots, y_T) && \text{(Joint probability)} \\ &= p(y_1) p(x_1 | y_1) p(y_2 | y_1) p(x_2 | y_2) \dots p(y_T | y_{T-1}) p(x_T | y_T) \\ &= p(y_1) P(y_2 | y_1) \dots p(y_T | y_{T-1}) \times p(x_1 | y_1) p(x_2 | y_2) \dots p(x_T | y_T) \\ &= p(y_1, \dots, y_T) p(x_1 \dots x_T | y_1, \dots, y_T) \end{aligned}$$



# Summary

---

- **Defn (3.2.5):** A *Bayesian network* is a pair  $(G, P)$  where  $P$  factorizes over  $G$ , and where  $P$  is specified as set of **local conditional probability dist.** CPDs associated with  $G$ 's nodes.
- A BN capture “causality”, “generative schemes”, “asymmetric influences”, etc., between entities
- Local and global independence properties identifiable via d-separation criteria (Bayes ball)
- Computing joint likelihood amounts multiplying CPDs
  - But computing marginal can be difficult
  - Thus inference is in general hard
- Important special cases:
  - Hidden Markov models
  - Tree models