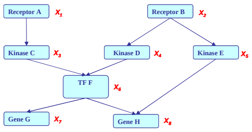
School of Computer Science
Carnegie Mellon

Representation of directed GM

Probabilistic Graphical Models (10-708)

Lecture 1, Sep 12, 2007



Eric Xing

Reading: MJ-Chap 2, KF-Chap. 3

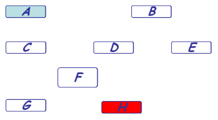
- Recitation?
- Exam dates, poster dates, etc.
- Mailing list
- Questions?

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

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

  - 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?**

- Even in the simplest case where these variables are binary-valued, a joint distribution requires the specification of 2^n numbers — the probabilities of the 2^n different assignments of values $x_1, \ldots, x_n$

- Today's lecture is about …

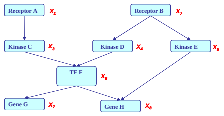
  - how independence properties in the distribution can be used to represent such high-dimensional distributions much more compactly.

  - how a combinatorial data structure — a directed acyclic graph — can provide us with a general-purpose modeling language for exploiting this type of structure in our representation.

Two types of GMs

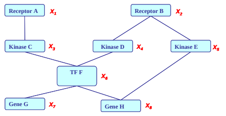
- Directed edges give causality relationships (**Bayesian Network** or **Directed Graphical Model**):

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



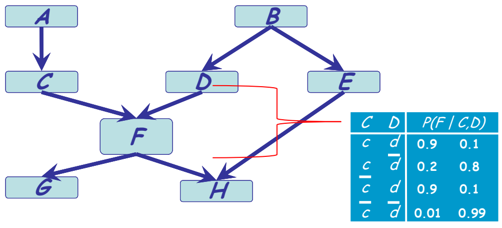
- Undirected edges simply give correlations between variables (**Markov Random Field** or **Undirected Graphical model**):

$$P(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8)$$
$$= 1/Z\ \exp\{E(X_1)+E(X_2)+E(X_3, X_1)+E(X_4, X_2)+E(X_5, X_2) + E(X_6, X_3, X_4)+E(X_7, X_6)+E(X_8, X_5, X_6)\}$$



Specification of a directed GM

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



C	D	P(F / C,D)	
c	d	0.9	0.1
c	$\bar{d}$	0.2	0.8
$\bar{c}$	d	0.9	0.1
$\bar{c}$	$\bar{d}$	0.01	0.99

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.

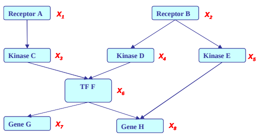
Bayesian Network: Factorization Theorem

- **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”:

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

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



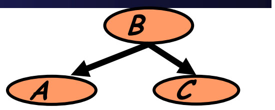
$$P(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8)$$

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

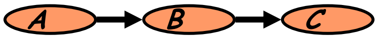
Qualitative Specification

- 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)
  - …

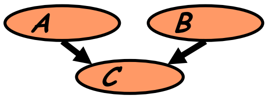
Local Structures & Independencies



- Common parent
  - Fixing B decouples A and C
    "given the level of gene B, the levels of A and C are independent"



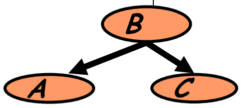
- Cascade
  - Knowing B decouples A and C
    "given the level of gene B, the level gene A provides no extra prediction value for the level of gene C"



- 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

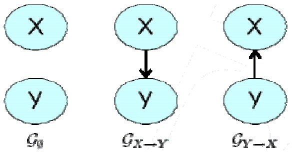
- **Defn (3.2.2):** Let P be a distribution over $\boldsymbol{X}$. We define I(P) to be the set of independence assertions of the form $(X \perp Y \mid Z)$ that hold in P (however how we set the parameter-values).
- **Defn (3.2.3):** Let K be *any graph object* associated with a set of independencies I(K). We say that K is an ***I-map*** for a set of independencies I, I(K) $\subset$ 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

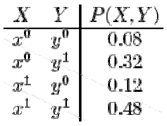
- For G to be an I-map of P, it is necessary that G does not mislead us regarding independencies in P:

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

- Example:

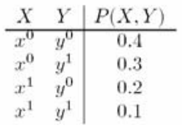


P_1



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 $X_1, \ldots, X_n$.

local Markov assumptions

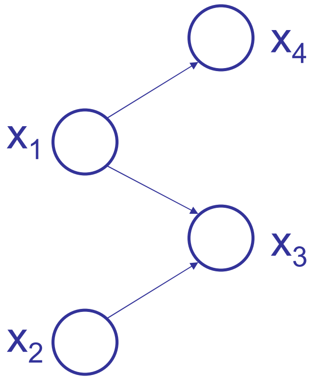
- **Defn (3.2.1):**

  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 ***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.

Example

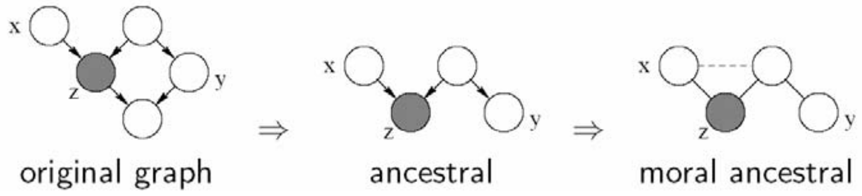


Graph separation criterion

- 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:



Active trail

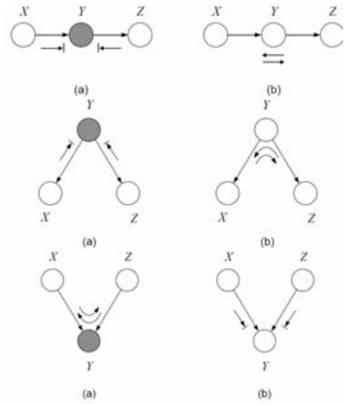
- **Causal trail** X → Z → Y **:** active if and only if Z is not observed.
- **Evidential trail** X ← Z ← Y **:** active if and only if Z is not observed.
- **Common cause** X ← Z → Y **:** active if and only if Z is not observed.
- **Common effect** X → Z ← Y **:** active if and only if either Z or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

Definition (3.3.2): Let $\boldsymbol{X}$, $\boldsymbol{Y}$, $\boldsymbol{Z}$ be three **sets** of nodes in *G*. We say that $\boldsymbol{X}$ and $\boldsymbol{Y}$ are *d-separated given* $\boldsymbol{Z}$, denoted *d-sep*$_G(\boldsymbol{X};\boldsymbol{Y} \mid \boldsymbol{Z})$, if there is **no** active trail between any node $X \in \boldsymbol{X}$ and $Y \in \boldsymbol{Y}$ given $\boldsymbol{Z}$.

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 bellow (and plus some boundary conditions):

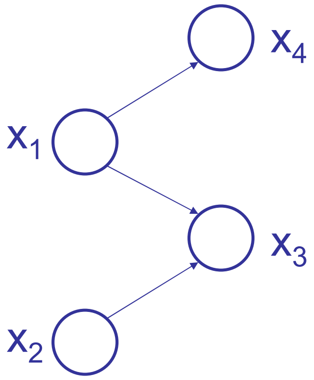


- Defn: *I*(*G*)=all independence properties that correspond to d-separation:

$$I(G) = \left\{ X \perp Z \middle| Y : \mathrm{dsep}_G(X;Z|Y) \right\}$$

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

Example:



- Complete the I(G) of this graph:

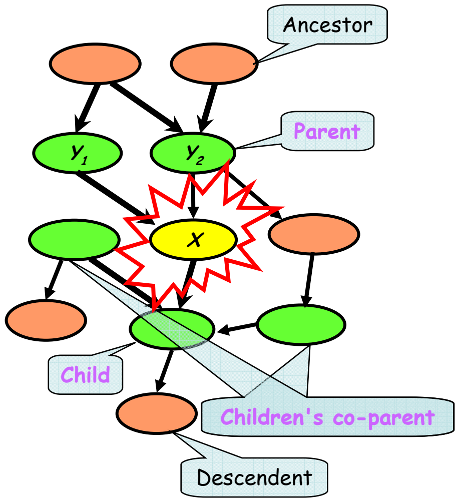
Summary: Conditional Independence Semantics in an BN

Structure: ***DAG***

- Meaning: a node is **conditionally independent** of every other node in the network outside its **Markov blanket**

- Local conditional distributions (**CPD**) and the **DAG** completely determine the **joint** dist.

- Give **causality** relationships, and facilitate a **generative** process



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,

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

  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

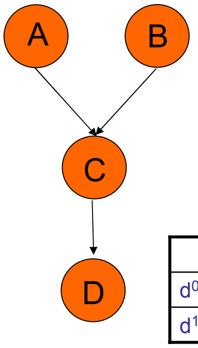
---

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)



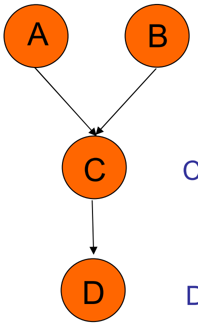
	a^0b^0	a^0b^1	a^1b^0	a^1b^1
c^0	0.45	1	0.9	0.7
c^1	0.55	0	0.1	0.3

	c^0	c^1
d^0	0.3	0.5
d^1	07	0.5

Conditional probability density func. (CPDs)

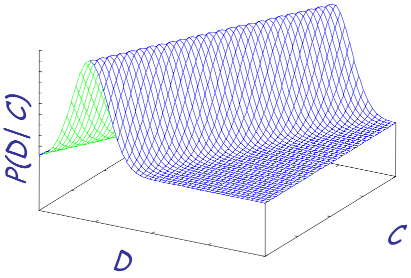
$A \sim N(\mu_a, \Sigma_a)$ $B \sim N(\mu_b, \Sigma_b)$

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



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

$D \sim N(\mu_a+C, \Sigma_a)$



Summary of BN semantics

- **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 CPDs associated with G's nodes.
  - Conditional independencies imply factorization
  - Factorization according to G implies the associated conditional independencies.
  - Are there **other independences** 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?

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->B, for actually independent A and B (the independence can be captured by some subtle way of parameterization)

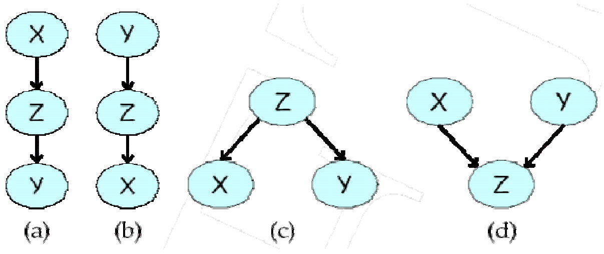
A	b^0	b^1
a^0	0.4	0.6
a^1	0.4	0.6

- **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 3.3.6:** 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

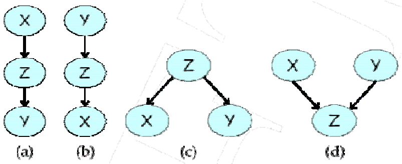
- Very different BN graphs can actually be equivalent, in that they encode precisely the same set of conditional independence assertions.



$(X \perp Y \mid Z)$.

I-equivalence

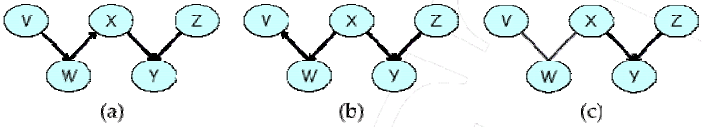
- **Defn (3.3.9):** Two BN graphs G1 and G2 over $\boldsymbol{X}$ are *I-equivalent* if I(G1) = I(G2).
  - The set of all graphs over $\boldsymbol{X}$ is partitioned into a set of mutually exclusive and exhaustive *I-equivalence classes*, which are the set of equivalence classes induced by the I-equivalence 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 (3.3.10):** The *skeleton* of a Bayesian network graph G over $\boldsymbol{V}$ is an undirected graph over $\boldsymbol{V}$ that contains an edge $\{X, Y\}$ for every edge (X, Y) in G.



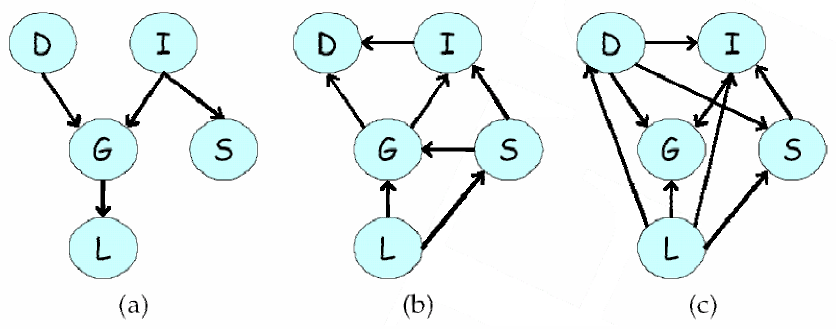
- **Thm (3.3.11):** Let G_1 and G_2 be two graphs over $\boldsymbol{V}$. If G_1 and G_2 have the same skeleton and the same set of v-structures then they are I-equivalent.

  - 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 3.4.1:** 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

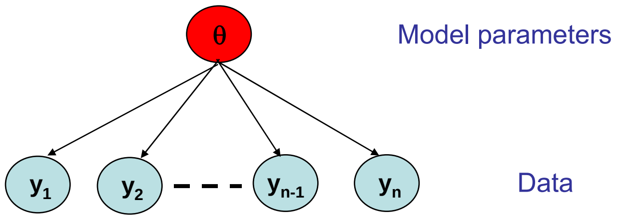


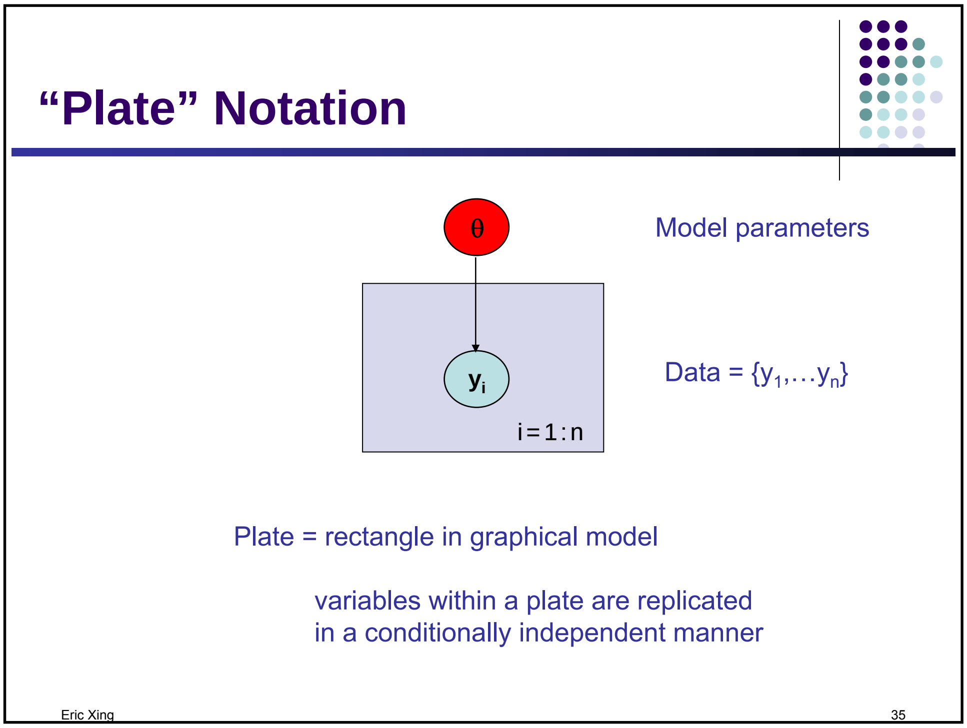
(a) (b) (c)

Perfect Map

- **Defn (3.4.3):** We say that a graph object G is a *perfect map (P-map)* for a set of independencies I if we have that I(G) = I. We say that G is a perfect map for P if I(G) = I(P).
  - The fact that G is a minimal I-map for P is far from a guarantee that G captures the independence structure in P
  - Not all P has a perfect map as DAG!
  - The P-map of a distribution *is* unique up to I-equivalence between networks. That is, a distribution P can have many P-maps, but all of them are I-equivalent.

Conditionally Independent Observations





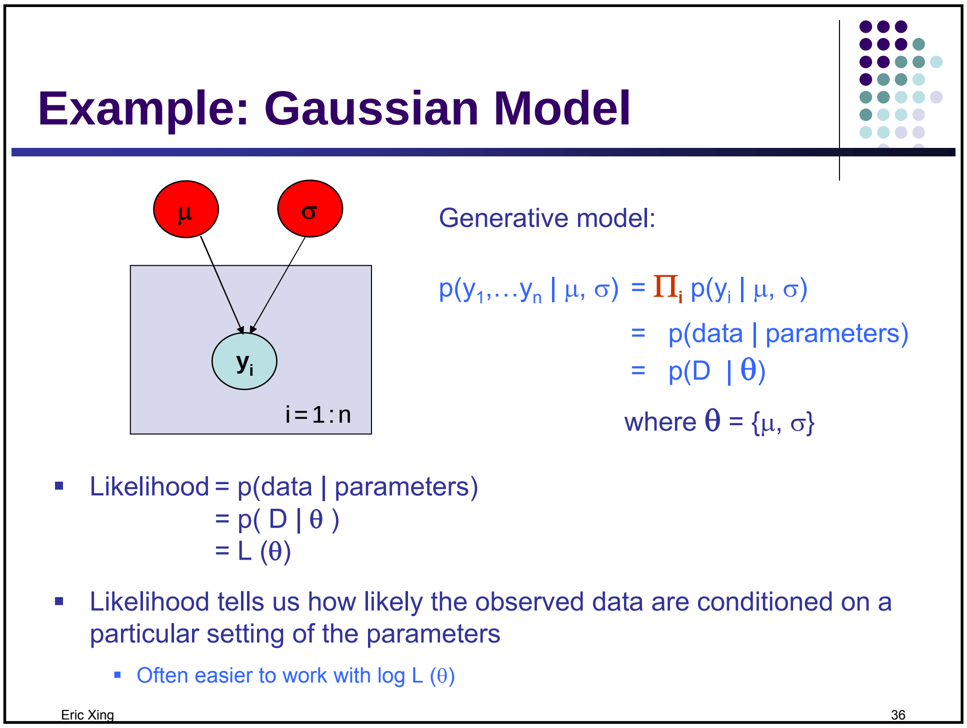
“Plate” Notation

Model parameters

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

Plate = rectangle in graphical model

variables within a plate are replicated
in a conditionally independent manner



Example: Gaussian Model

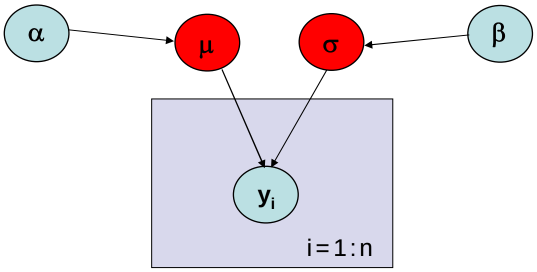
Generative model:

$$p(y_1,\ldots y_n \mid \mu, \sigma) = \Pi_i \, p(y_i \mid \mu, \sigma)$$
$$= p(\text{data} \mid \text{parameters})$$
$$= p(D \mid \theta)$$

where $\theta = \{\mu, \sigma\}$

- Likelihood = p(data | parameters)
  = p(D | θ)
  = L (θ)
- Likelihood tells us how likely the observed data are conditioned on a particular setting of the parameters
  - Often easier to work with log L (θ)

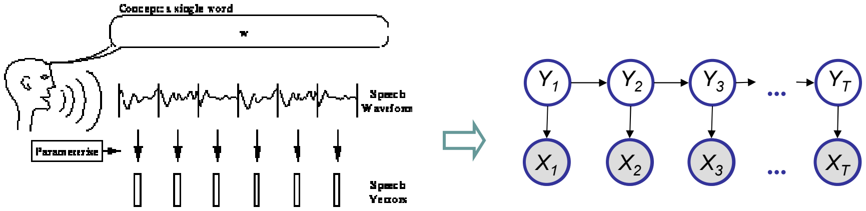
Example: Bayesian Gaussian Model



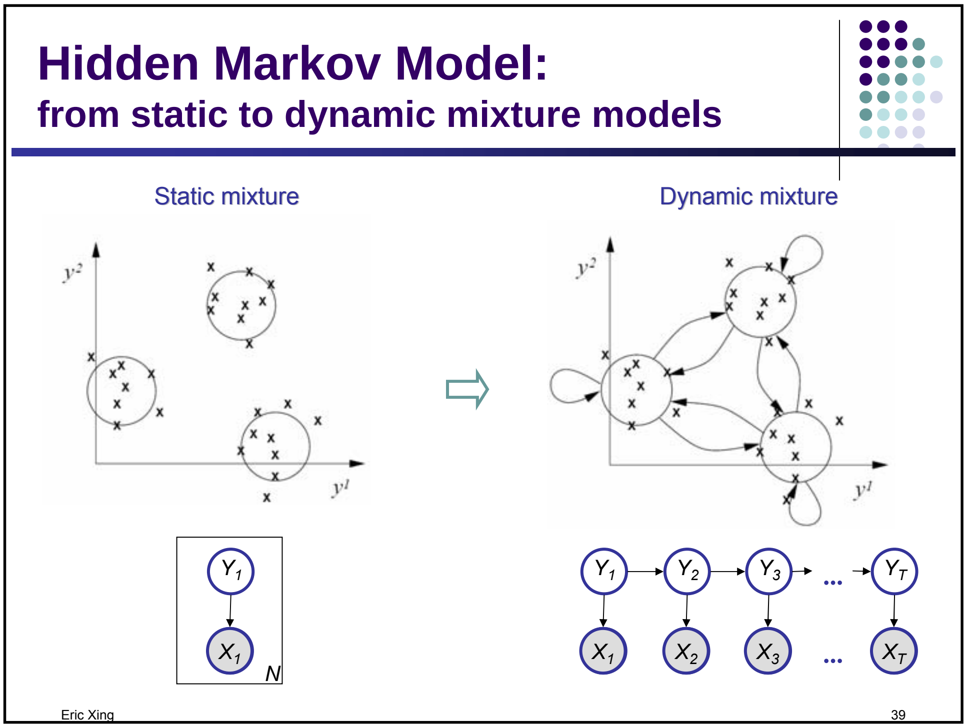
Note: priors and parameters are assumed independent here

Example

- Speech recognition



Hidden Markov Model

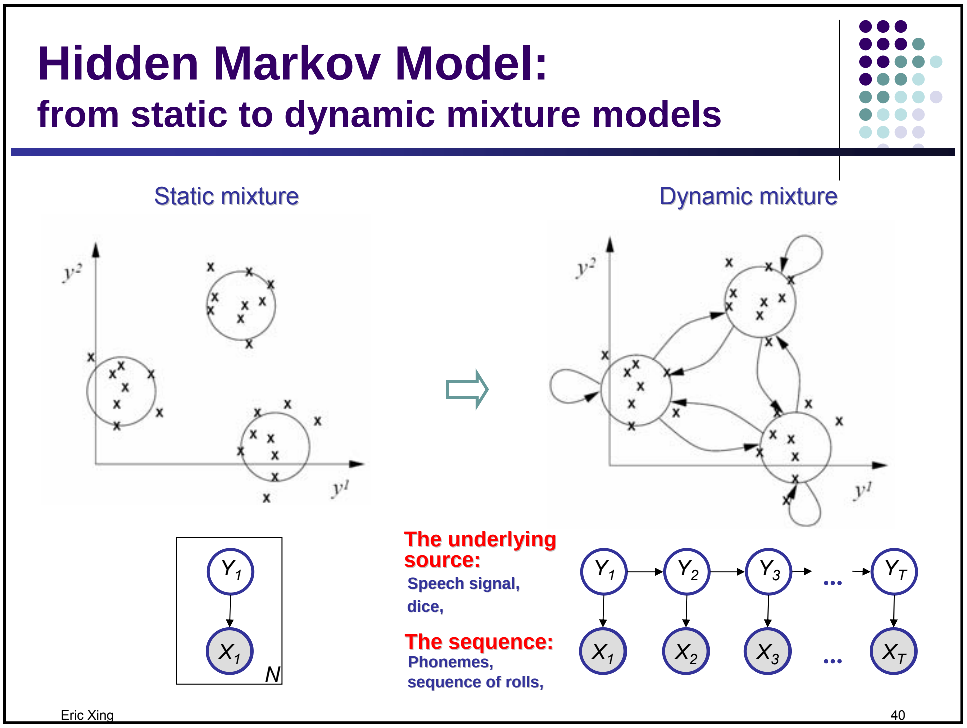


Hidden Markov Model:
from static to dynamic mixture models

Static mixture

Dynamic mixture

Eric Xing



Hidden Markov Model:
from static to dynamic mixture models

Static mixture

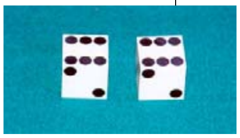
Dynamic mixture

The underlying source:
Speech signal,
dice,

The sequence:
Phonemes,
sequence of rolls,

Eric Xing

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

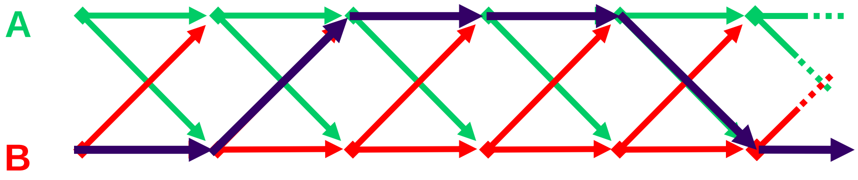
Game:

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

A stochastic generative model

- Observed sequence:

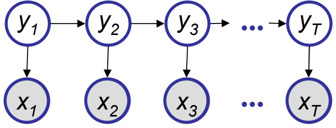
1 → 4 → 3 → 6 → 6 → 4 →



- Hidden sequence (a parse or segmentation):

B → B → A → A → A → B →

Definition (of HMM)



- Observation space

  Alphabetic set: $\mathbb{C} = \{c_1, c_2, \cdots, c_K\}$

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

- Index set of hidden states

  $\mathbb{I} = \{1, 2, \cdots, M\}$

- Transition probabilities between any two states

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

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

- Start probabilities

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

- Emission probabilities associated with each state

  $p(x_t \mid y_t^i = 1) \sim \text{Multinomial}(b_{i,1}, b_{i,1}, \ldots, b_{i,K}), \forall i \in \mathbb{I}.$

  or in general:

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

Puzzles regarding the dishonest casino

GIVEN: A sequence of rolls by the casino player

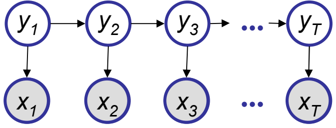
1245526462146146136136661664661636616366163616515615115146123562344

QUESTION

- How likely is this sequence, given our model of how the casino works?
  - This is the **EVALUATION** problem in HMMs
- What portion of the sequence was generated with the fair die, and what portion with the loaded die?
  - This is the **DECODING** question in HMMs
- 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 in HMMs

Probability of a parse

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



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

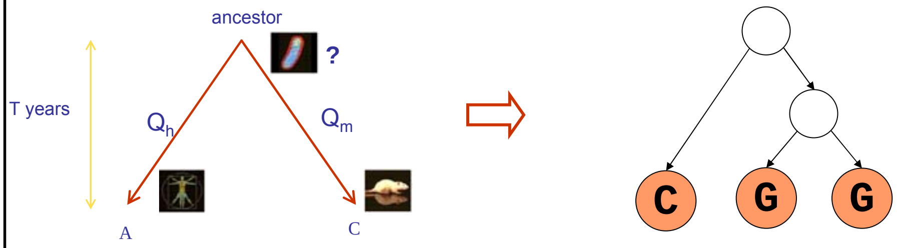
Let $\pi_{y_1} \overset{\text{def}}{=} \prod_{i=1}^{M} [\pi_i]^{y_1^i}$, $\quad a_{y_t, y_{t+1}} \overset{\text{def}}{=} \prod_{i,j=1}^{M} [a_{ij}]^{y_t^i y_{t+1}^j}$, $\quad$ and $\quad b_{y_t, x_t} \overset{\text{def}}{=} \prod_{i=1}^{M} \prod_{k=1}^{K} [b_{ik}]^{y_t^i x_t^k}$,

$$= \pi_{y_1} a_{y_1, y_2} \cdots a_{y_{T-1}, y_T} \quad b_{y_1, x_1} \cdots b_{y_T, x_T}$$

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

Example, con'd

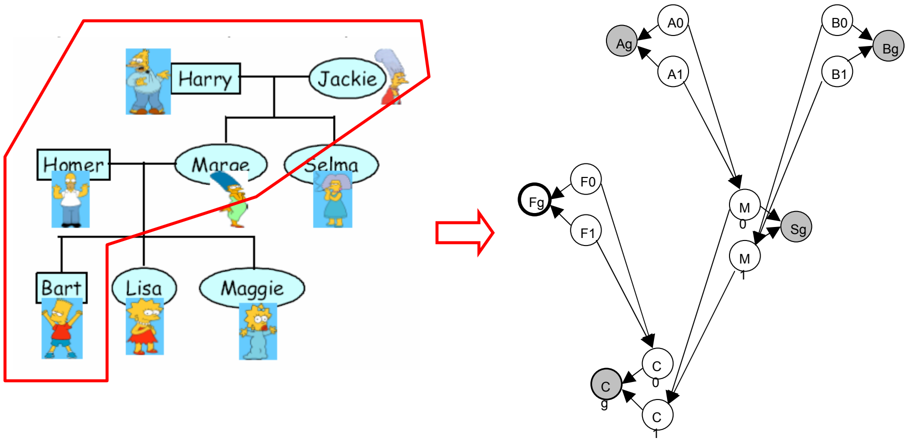
- Evolution



Tree Model

Example, con'd

- Genetic Pedigree



Summary of BN semantics

- **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 CPDs associated with G's nodes.

Knowledge Engineering

- Picking variables
  - Observed
  - Hidden

- Picking structure
  - CAUSAL
  - Generative

- Picking Probabilities
  - Zero probabilities
  - Orders of magnitudes
  - Relative values