Bayesian Networks

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Probabilistic Reasoning

• Represent system of interest by a set of random variables

$$(X_1,\ldots,X_d)$$
.

• Suppose by research or machine learning, we get a joint probability distribution

$$p(x_1,\ldots,x_d).$$

- We'd like to be able to do **inference** on this model essentially, answer queries:
 - **1** What is the most likely of value X_1 ?
 - 2 What is the most likely of value X_1 , given we've observed $X_2 = 1$?
 - Solution of (X_1, X_2) given observation of $(X_3 = x_3, \dots, X_d = x_d)$?

Example: Medical Diagnosis

- Variables for each symptom
 - fever, cough, fast breathing, shaking, nausea, vomiting
- Variables for each disease
 - pneumonia, flu, common cold, bronchitis, tuberculosis
- Diagnosis is performed by **inference** in the model:

p(pneumonia = 1 | cough = 1, fever = 1, vomiting = 0)

- The QMR-DT (Quick Medical Reference Decision Theoretic) has
 - 600 diseases
 - 4000 symptoms

Example from David Sontag's Inference and Representation, Lecture 1.

Some Notation

- This lecture we'll only be considering discrete random variables.
- Capital letters X_1, \ldots, X_d, Y , etc. denote random variables.
- Lower case letters x_1, \ldots, x_n, y denote the values taken.
- Probability that $X_1 = x_1$ and $X_2 = x_2$ will be denoted

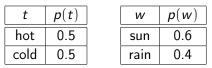
$$\mathbb{P}(X_1 = x_1, X_2 = x_2).$$

• We'll generally write things in terms of the probability mass function:

$$p(x_1, x_2, \dots, x_d) := \mathbb{P}(X_1 = x_1, X_2 = x_2, \dots, X_d = x_d)$$

Representing Probability Distributions

- Let's consider the case of discrete random variables.
- Conceptually, everything can be represented with probability tables.
- Variables
 - Temperature $T \in \{hot, cold\}$
 - Weather $W \in \{sun, rain\}$



- These are the marginal probability distributions.
- To do reasoning, we need the joint probability distribution.

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Based on David Sontag's DS-GA 1003 Lectures, Spring 2014, Lecture 10.

Joint Probability Distributions

• A joint probability distribution for T and W is given by

t	W	p(t,w)
hot	sun	0.4
hot	rain	0.1
cold	sun	0.2
cold	rain	0.3

- A valid probability distribution if
 - $\forall t, w: p(t, w) \ge 0$
 - $\sum_{t,w} p(t,w) = 1.$

Based on David Sontag's DS-GA 1003 Lectures, Spring 2014, Lecture 10.

Conditional Distributions From the Joint Distribution

• We observe T = hot. What's the conditional distribution of W?

$$p(w \mid T = hot) =?$$

Method:

① Find entries in joint distribution table where T = hot.

t	W	p(t,w)
hot	sun	0.4
hot	rain	0.1

2 Renormalize to get conditional probability.

t	W	p(t, w)	$p(w \mid T = hot)$
hot	sun	0.4	0.4/0.5 = 0.8
hot	rain	0.1	0.1/0.5 = 0.2

Conditional Distributions From the Joint Distribution

Definition

The conditional probability for w given t is

$$p(w \mid t) = \frac{p(w, t)}{p(t)}.$$

t	W	p(t,w)	$p(w \mid T = hot)$
hot	sun	0.4	0.4/0.5 = 0.8
hot	rain	0.1	0.1/0.5 = 0.2

Representing Joint Distributions

- Consider random variables $X_1, \ldots, X_d \in \{0, 1\}$.
- How many parameters do we need to represent the joint distribution?
- Joint probability table has 2^d rows.
- For QMR-DT, that's $2^{4600} > 10^{1000}$ rows.
- That's not going to happen.
- Having exponentially many parameters is a problem for
 - storage
 - computation (inference is summing over exponentially many rows)
 - statistical estimation / learning
 - (Estimating 10¹⁰⁰⁰ parameters? Nope.)

How to Restrict the Complexity?

- Restrict the space of probability distributions
- We will make various independence assumptions.
- Extreme assumption: X_1, \ldots, X_d are **mutually independent**.

Definition

Discrete random variables X_1, \ldots, X_d are **mutually independent** if their joint probability mass function (PMF) factorizes as

$$p(x_1, x_2, \ldots, x_d) = p(x_1)p(x_2)\cdots p(x_d).$$

- Note: We usually just write independent for "mutually independent".
- How many parameters to represent the joint distribution, assuming independence?

Assume Full Independence

- How many parameters to represent the joint distribution?
- Say $p(X_i = 1) = \theta_i$, for i = 1, ..., d.
- Clever representation: Since $x_i \in \{0, 1\}$, we can write

$$\mathbb{P}(X_i=x_i)=\theta_i^{x_i}\left(1-\theta_i\right)^{1-x_i}.$$

• Then by independence,

$$p(x_1,\ldots,x_d) = \prod_{i=1}^d \theta_i^{x_i} (1-\theta_i)^{1-x_i}$$

- How many parameters?
- *d* parameters needed to represent the joint.

Conditional Interpretation of Independence

• Suppose X and Y are independent, then

$$p(x \mid y) = p(x).$$

Proof:

$$p(x \mid y) = \frac{p(x, y)}{p(y)}$$
$$= \frac{p(x)p(y)}{p(y)} = p(x).$$

- With full independence, we have no relationships among variables.
- Information about one variable says nothing about any other variable.
 - Would mean diseases don't have symptoms.

Conditional Independence

- Consider 3 events:
 - $W = \{\text{The grass is wet}\}$
 - 2 $S = \{\text{The road is slippery}\}$
 - $R = \{ It's raining \}$
- These events are certainly not independent.
 - Raining $(R) \implies$ Grass is wet AND The road is slippery $(W \cap S)$
 - Grass is wet $(W) \implies$ More likely that the road is slippery (S)
- Suppose we know that it's raining.
 - Then, we learn that the grass is wet.
 - Does this tell us anything new about whether the road is slippery?
- Once we know R, then W and S become independent.
- This is called conditional independence, and we'll denote it as

$$W \perp S \mid R.$$

Conditional Independence

Definition

We say W and S are conditionally independent given R, denoted

 $W \perp S \mid R$,

if the conditional joint factorizes as

$$p(w,s \mid r) = p(w \mid r)p(s \mid r).$$

Also holds when W, S, and R represent sets of random variables.

Example: Rainy, Slippery, Wet

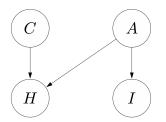
- Consider 3 events:
 - $W = \{\text{The grass is wet}\}$
 - 2 $S = \{\text{The road is slippery}\}$
 - 3 $R = \{$ It's raining $\}$
- Represent joint distribution as

$$p(w, s, r) = p(w, s | r)p(r)$$
(no assumptions so far)
= $p(w | r)p(s | r)p(r)$ (assuming $W \perp S | R$)

- How many parameters to specify the joint?
 - p(w | r) requires two parameters: one for r = 1 and one for r = 0.
 - p(s | r) requires two.
 - p(r) requires one parameter,
- Full joint: 7 parameters. Conditional independence: 5 parameters. Full independence: 3 parameters.

Bayesian Networks: Introduction

- Bayesian Networks are
 - used to specify joint probability distributions that
 - have a particular factorization.



$$p(c, h, a, i) = p(c)p(a)$$
$$\times p(h \mid c, a)p(i \mid a)$$

• With practice, one can read conditional independence relationships directly from the graph.

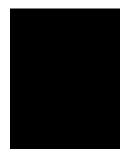
From Percy Liang's "Lecture 14: Bayesian networks II" slides from Stanford's CS221, Autumn 2014.

Directed Graphs

A directed graph is a pair $G = (\mathcal{V}, \mathcal{E})$, where

•
$$\mathcal{V} = \{1, \dots, d\}$$
 is a set of **nodes** and

•
$$\mathcal{E} = \{(s, t) \mid s, t \in \mathcal{V}\}$$
 is a set of **directed edges**.



- $\mathsf{Parents}(5) \ = \ \{3\}$
- $\mathsf{Parents}(4) = \{2,3\}$
- $Children(3) = \{4, 5\}$
- $\mathsf{Descendants}(1) = \{2, 3, 4, 5\}$

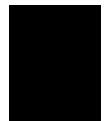
 $NonDescendants(3) = \{1,2\}$

KPM Figure 10.2(a).

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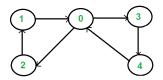
Directed Acyclic Graphs (DAGs)

A DAG is a directed graph with no directed cycles.



DAG

Not a DAG



Every DAG has a **topological ordering**, in which parents have lower numbers than their children.

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http://www.geeksforgeeks.org/wp-content/uploads/SCC1.png and KPM Figure 10.2(a).

Bayesian Networks

Definition

A Bayesian network is a

• DAG $G = (\mathcal{V}, \mathcal{E})$, where $\mathcal{V} = \{1, \dots, d\}$, and

• a corresponding set of random variables $X = \{X_1, \dots, X_d\}$ where

• the joint probability distribution over X factorizes as

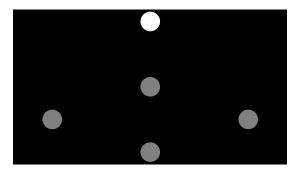
$$p(x_1,\ldots,x_d) = \prod_{i=1}^d p(x_i \mid x_{\mathsf{Parents}(i)}).$$

Bayesian networks are also known as

- directed graphical models, and
- belief networks.

Bayesian Networks: Example

Consider the Bayesian network depicted below:



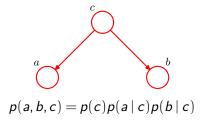
It implies the following factorization for the joint probability distribution:

 $p(x_1, x_2, x_3, x_4, y) = p(y)p(x_1 \mid y)p(x_2 \mid x_1, y)p(x_3 \mid x_1, y)p(x_4 \mid x_3, y)$

KPM Figure 10.2(b).

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Bayesian Networks: "A Common Cause"



Are a and b independent? (c=Rain, a=Slippery, b=Wet?)

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

which in general will not be equal to p(a)p(b).

From Bishop's Pattern recognition and machine learning, Figure 8.15.

Bayesian Networks: "A Common Cause"

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

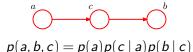
Are a and b independent, conditioned on observing c? (c=Rain, a=Slippery, b=Wet?)

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

So $a \perp b \mid c$.

From Bishop's Pattern recognition and machine learning, Figure 8.16.

Bayesian Networks: "An Indirect Effect"



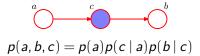
Are *a* and *b* independent? (Note: This is a **Markov chain**) (e.g. a=raining, c=wet ground, b=mud on shoes)

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

So doesn't factorize, thus not independent, in general.

From Bishop's Pattern recognition and machine learning, Figure 8.17.

Bayesian Networks: "An Indirect Effect"



Are *a* and *b* independent after observing *c*? (e.g. a=raining, c=wet ground, b=mud on shoes)

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

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

So $a \perp b \mid c$.

From Bishop's Pattern recognition and machine learning, Figure 8.18.

Bayesian Networks: "A Common Effect"

$$p(a, b, c) = p(a)p(b)p(c \mid a, b)$$
Are *a* and *b* independent? (a=course difficulty, b=knowledge, c= grade)
$$p(a, b) = \sum_{c} p(a)p(b)p(c \mid a, b)$$

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

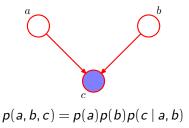
$$= p(a)p(b)$$

So $a \perp b$.

From Bishop's Pattern recognition and machine learning, Figure 8.19.

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Bayesian Networks: "A Common Effect" or "V-Structure"



Are a and b independent, given observation of c? (a=course difficulty, b=knowledge, c= grade) p(a,b | c) = p(a)p(b)p(c | a, b)/p(c)

which does not factorize into p(a | c)p(b | c), in general.

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From Bishop's Pattern recognition and machine learning, Figure 8.20.

Conditional Independence from Graph Structure

- In general, given 3 sets of nodes A, B, and C
- How can we determine whether

$A \perp B \mid C?$

- There is a purely graph-theoretic notion of "d-separation" that is equivalent to conditional independence.
- Suppose we have observed C and we want to do inference on A.
- We could ignore any evidence collected about *B*, where $A \perp B \mid C$.
- See KPM Section 10.5.1 for details.

Markov Blanket

- Suppose we have a very large Bayesian network.
- We're interested in a single variable A, which we cannot observe.
- To get maximal information about *A*, do we have to observe all other variables?
- No! We only need to observe the Markov blanket of A:

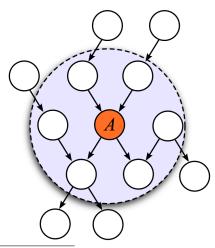
p(A | all other nodes) = p(A | MarkovBlanket(A)).

- In a Bayesian network, the Markov blanket of A consists of
 - the parents of A
 - the children of A
 - the "co-parents" of A, i.e. the parents of the children of A

(See KPM Sec. 10.5.3 for details.)

Markov Blanket

Markov Blanket of A in a Bayesian Network:



 $\label{eq:From http://en.wikipedia.org/wiki/Markov_blanket: "Diagram of a Markov blanket" by Laughsinthestocks - Licensed under CC0 via Wikimedia Commons$

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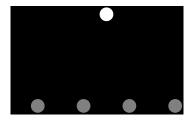
Bayesian Networks

- Bayesian Networks are great when
 - you know something about the relationships between your variables, or
 - you will routinely need to make inferences with incomplete data.
- Challenges:
 - The naive approach to inference doesn't work beyond small scale.
 - Need more sophisticated algorithm:
 - exact inference
 - approximate inference

Naive Bayes: A Generative Model for Classification

•
$$\mathfrak{X} = \left\{ \left(X_1, X_2, X_3, X_4 \right) \in \{0, 1\}^4 \right) \right\}$$
 $\mathfrak{Y} = \{0, 1\}$ be a class label.

• Consider the Bayesian network depicted below:



• BN structure implies joint distribution factors as:

 $p(x_1, x_2, x_3, x_4, y) = p(y)p(x_1 \mid y)p(x_2 \mid y)p(x_3 \mid y)p(x_4 \mid y)$

• Features X_1, \ldots, X_4 are independent given the class label Y.

KPM Figure 10.2(a).

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Parameters for Naive Bayes

- Generalize to *d* features.
- Knowing the joint distribution means we need to know

$$p(y), p(x_1 | y), \dots p(x_d | y).$$

• We could parameterize as:

$$\mathbb{P}(Y = 1) = \theta_{y}$$
$$\mathbb{P}(X_{i} = 1 \mid Y = 1) = \theta_{i1}$$
$$\mathbb{P}(X_{i} = 1 \mid Y = 0) = \theta_{i0}$$

 \implies 1+2d parameters to characterize the joint distribution

Parameterized Expression for Joint

• Parameters:

$$\mathbb{P}(Y=1) = \theta_y$$
 $\mathbb{P}(X_i = 1 | Y = 1) = \theta_{i1}$ $\mathbb{P}(X_i = 1 | Y = 0) = \theta_{i0}$

• Joint distribution is

$$p(x_1, \dots, x_d, y) = p(y) \prod_{i=1}^n p(x_i \mid y)$$

= $(\theta_y)^y (1 - \theta_y)^{1-y}$
 $\times \prod_{i=1}^n (\theta_{i1})^{yx_i} (1 - \theta_{i1})^{y(1-x_i)} (\theta_{i0})^{(1-y)x_i} (1 - \theta_{i0})^{(1-y)(1-x_i)}$

Naive Bayes

• Suppose we know all conditional distributions:

$$p(y), p(x_1 | y), \dots p(x_d | y)$$

- We observe $X = (X_1, ..., X_d)$. What's the prediction for Y?
- We have a full probability model

$$p(y, x_1, ..., x_d) = p(y)p(x_1, ..., x_d | y)$$
 (no assumptions)
= $p(y)\prod_{i=1}^d p(x_i | y)$ (conditional independence)

We can use Bayes rule to compute anything we want...

Posterior Class Probability

• Let
$$x = (x_1, \dots, x_d)$$
, and apply Bayes rule:

$$p(y \mid x) = \frac{p(y, x)}{p(x)} = \frac{p(y) \prod_{i=1}^{d} p(x_i \mid y)}{p(x)}$$

- We know everything except p(x).
- We can compute it explicitly:

$$p(x) = \sum_{y \in \{0,1\}} p(x,y) = \sum_{y \in \{0,1\}} p(x|y)p(y)$$

• So final predicted probability distribution is

$$p(y \mid x) = \frac{p(y) \prod_{i=1}^{d} p(x_i \mid y)}{\sum_{y \in \{0,1\}} p(x \mid y) p(y)}$$

Dropping Normalization Constant

• Consider p(y | x) as a distribution over y, for fixed x.

$$p(y \mid x) = p(y, x) / p(x).$$

• With x fixed, p(x) is a constant – let's write it as k to make it clear:

$$p(y \mid x) = k^{-1}p(y,x)$$
$$\implies p(y \mid x) \propto p(y,x)$$

• How to recover value of k? p(y | x) must be a distribution on y:

$$\sum_{y \in \{0,1\}} p(y \mid x) = k^{-1} \sum_{y \in \{0,1\}} p(y,x) = 1$$
$$\implies k = \sum_{y \in \{0,1\}} p(y,x)$$

So we can always recover the normalizing constant whenever we want.
Often no need to keep track of it.

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Naive Bayes and Logistic Regression

• Recall the logistic regression prediction function is of the form

$$x \mapsto p(Y=1 \mid x) = \frac{1}{1 + \exp\left(-w^T x\right)},$$

for some parameter vector $w \in \mathbf{R}^d$.

Theorem

If p(y,x) is any Naive Bayes model with binary x and y, the prediction function

$$x \mapsto p(Y=1 \mid x)$$

corresponds to logistic regression, for some $w \in \mathbf{R}^d$.

Proof: Homework.

Naive Bayes vs Logistic Regression

• Naive Bayes is a model for the joint distribution p(y, x).

- We can sample (x, y) pairs from this distribution.
- Models of the joint distribution are called generative models.
- Logistic regression is directly modeling the conditional distribution

$$p(y \mid x).$$

- No model for the features $x = (x_1, \ldots, x_d)$.
- Conditional probability models are called discriminative models.
- Logistic regression is a specialist in the conditional distribution.
- Naive Bayes is doing more!

Naive Bayes vs Logistic Regression

- Missing data is no problem for Naive Bayes.
- Suppose we're missing X₁ and X₂ from the input vector.
- Just predict with

$$\mathbb{P}(y \mid x_3, \dots, x_d) \propto p(y, x_3, \dots, x_d)$$
$$= \sum_{x_1, x_2 \in \{0, 1\}} p(y, x)$$

 For logistic regression? No natural way to predict with missing features.

Naive Bayes vs Logistic Regression

- Logistic regression handles binary or continuous features seamlessly.
- For naive Bayes, you need a different family of conditional distributions, e.g.

$$\boldsymbol{p}(x_i \mid y) = \mathcal{N}\left(x_i \mid \boldsymbol{\mu}_{iy}, \sigma_{iy}^2\right)$$

- Wasted effort to model all features if you only care about p(y | x)?
- Suppose we're missing X_1 and X_2 from the input vector.
- Just predict with

$$\mathbb{P}(y \mid x_3, \dots, x_d) \propto p(y, x_3, \dots, x_d)$$
$$= \sum_{x_1, x_2 \in \{0, 1\}} p(y, x)$$

• No natural method for missing features with logistic regression.

Easy Estimators for Naive Bayes

- Training set $\mathcal{D} = \{(x^1, y^1), \dots, (x^n, y^n)\}.$
- There are obvious "plug-in" estimators for the Naive Bayes model:

$$\mathbb{P}(Y=1) \approx \hat{\theta}_{y} = \frac{1}{n} \sum_{i=1}^{n} 1(y^{i} = 1)$$
$$\mathbb{P}(X_{i} = 1 \mid Y = 1) \approx \hat{\theta}_{i1} = \frac{\sum_{j=1}^{n} 1(y^{j} = 1 \text{ and } x_{i}^{j} = 1)}{\sum_{j=1}^{n} 1(y^{j} = 1)}$$
$$\mathbb{P}(X_{i} = 1 \mid Y = 0) = \hat{\theta}_{i0} = \frac{\sum_{j=1}^{n} 1(y^{j} = 0 \text{ and } x_{i}^{j} = 1)}{\sum_{j=1}^{n} 1(y^{j} = 0)}$$

Naive Bayes

Maximum Likelihood Estimation for Naive Bayes

- Training set $\mathcal{D} = \{(x^1, y^1), \dots, (x^n, y^n)\}.$
- More principled: find the MLE for the Naive Bayes model.
- The log-likelihood objective function is

$$J(\theta) = \sum_{i=1}^{n} \log p(y^{i}, x^{i}),$$

where we found the likelihood for a single point (x, y) is

$$p(x,y) = (\theta_{y})^{y} (1-\theta_{y})^{1-y} \\ \times \prod_{i=1}^{n} (\theta_{i1})^{yx_{i}} (1-\theta_{i1})^{y(1-x_{i})} \\ \times \prod_{i=1}^{n} (\theta_{i0})^{(1-y)x_{i}} (1-\theta_{i0})^{(1-y)(1-x_{i})}$$

• Theorem: MLE is exactly the plug-in estimator.

• Proof: Optional Homework.

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Class Prediction

• If we want to predict a single class, we would use

$$y^* = \arg\max_{y} p(y \mid x).$$

• One approach to this is to write

$$\frac{p(Y=1 \mid x)}{p(Y=0 \mid x)} = \frac{p(Y=1,x)/p(x)}{p(Y=0,x)/p(x)} = \frac{p(Y=1,x)}{p(Y=0,x)}$$
$$= \frac{p(Y=1)\prod_{i=1}^{d} p(x_i \mid Y=1)}{p(Y=0)\prod_{i=1}^{d} p(x_i \mid Y=0)}$$
$$= \frac{p(Y=1)}{p(Y=0)} \prod_{i=1}^{d} \frac{p(x_i \mid Y=1)}{p(x_i \mid Y=0)}$$

• Compare ratio to 1 to get prediction.

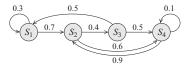
Markov Chain Model

• A Markov chain model has structure:



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

- Conditional distributions $p(x_i | x_{i-1})$ is called the transition model.
- When conditional distribution independent of *i*, called **time-homogeneous**.
- 4-state transition model for $X_i \in \{S_1, S_2, S_3, S_4\}$:

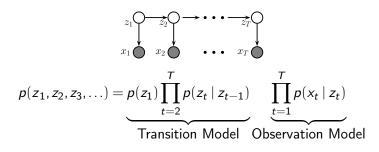


KPM Figure 10.3(a) and Koller and Friedman's Probabilistic Graphical Models Figure 6.04.

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Hidden Markov Model

• A hidden Markov model (HMM) has structure:



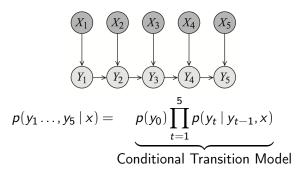
- At deployment time, we typically only observe X_1, \ldots, X_T .
- Want to infer Z_1, \ldots, Z_T .
- e.g. Want to most likely sequence (Z_1, \ldots, Z_T) . (Use Viterbi algorithm.)

KPM Figure 10.4

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Maximum Entropy Markov Model

• A maximum entropy Markov model (MEMM) has structure:



- At deployment time, we only observe X_1, \ldots, X_T .
- This is a conditional model. (And not a generative model).

Koller and Friedman's Probabilistic Graphical Models Figure 20.A.1.

Maximum Entropy Markov Model

• The MEMM transition model takes the following form:

$$p(y_i|y_{i-1},x) \propto \exp\left(\sum_k \lambda_k f_k(y_{i-1},y_i) + \sum_r \mu_r g_r(y_i,x)\right)$$

- The functions f_k and g_r are feature functions.
- Suppose Y's represent parts-of-speech; X's represent words.
 Could have

$$g_r(y_i, x) = \begin{cases} 1 & \text{if } y_i = \text{"NOUN" and } x_i = \text{"apple"} \\ 0 & \text{otherwise} \end{cases}$$

• For the "transition features", typical would be

$$f_k(y_{i-1}, y_i) = \begin{cases} 1 & \text{if } (y_{i-1}, y_i) = (\text{ADJ}, \text{NOUN}) \\ 0 & \text{otherwise.} \end{cases}$$