## 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

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

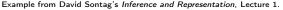
- We'd like to be able to do inference on this model essentially, answer queries:
  - **1** What is the most likely of value  $X_1$ ?
  - ② What is the most likely of value  $X_1$ , given we've observed  $X_2 = 1$ ?
  - 3 Distribution of  $(X_1, X_2)$  given observation of  $(X_3 = x_3, ..., X_d = x_d)$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

## 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



#### Some Notation

- This lecture we'll only be considering discrete random variables.
- Capital letters  $X_1, ..., X_d, Y$ , 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:

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

### Representing Probability Distributions

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

t	p(t)
hot	0.5
cold	0.5

W	p(w)
sun	0.6
rain	0.4

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

#### Joint Probability Distributions

ullet 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
  - $\forall t, w : p(t, w) \geqslant 0$
  - $\bullet \ \sum_{t,w} p(t,w) = 1.$

#### 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

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)	$\rho(w \mid T = hot)$
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<sup>d</sup> 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 10<sup>1000</sup> 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  $X_1, ..., X_d$  are mutually independent if their joint probability mass function (PMF) factorizes as

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

- 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

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

• Then by independence,

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

- 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:

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

- 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:

  - 2  $S = \{\text{The road is slippery}\}\$
- 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:

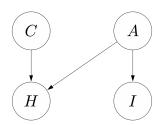
  - 2  $S = \{ \text{The road is slippery} \}$
- Represent joint distribution as

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

- How many parameters to specify the joint?
  - $p(w \mid r)$  requires two parameters: one for r = 1 and one for r = 0.
  - $p(s \mid r)$  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.



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

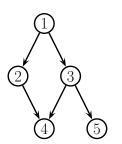
 With practice, one can read conditional independence relationships directly from the graph.

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

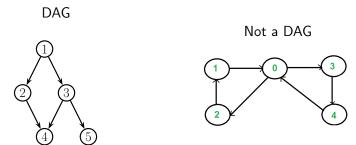
- $\mathcal{V} = \{1, \dots, d\}$  is a set of **nodes** and
- $\mathcal{E} = \{(s, t) \mid s, t \in \mathcal{V}\}$  is a set of **directed edges**.



```
\begin{array}{rcl} {\sf Parents}(5) & = & \{3\} \\ {\sf Parents}(4) & = & \{2,3\} \\ {\sf Children}(3) & = & \{4,5\} \\ {\sf Descendants}(1) & = & \{2,3,4,5\} \\ {\sf NonDescendants}(3) & = & \{1,2\} \end{array}
```

# Directed Acyclic Graphs (DAGs)

A **DAG** is a directed graph with **no directed cycles**.



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

# Bayesian Networks

#### Definition

#### A Bayesian network is a

- DAG  $G = (\mathcal{V}, \mathcal{E})$ , where  $\mathcal{V} = \{1, ..., d\}$ , and
- a corresponding set of random variables  $X = \{X_1, \dots, X_d\}$

#### where

the joint probability distribution over X factorizes as

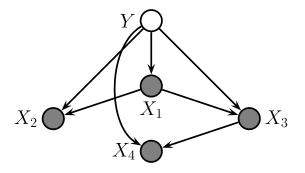
$$p(x_1,\ldots,x_d) = \prod_{i=1}^d p(x_i \mid x_{\mathsf{Parents}(i)}).$$

#### Bayesian networks are also known as

- directed graphical models, and
- belief networks.

## Bayesian Networks: Example

Consider the Bayesian network depicted below:

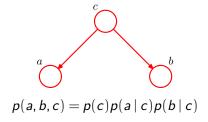


It implies the following factorization for the joint probability distribution:

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

KPM Figure 10.2(b).

#### Bayesian Networks: "A Common Cause"

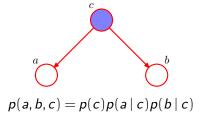


Are a and b independent? (c=Rain, a=Slippery, b=Wet?)

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

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

#### Bayesian Networks: "A Common Cause"



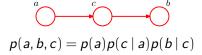
Are a and b independent, conditioned on observing c? (c=Rain, a=Slippery, b=Wet?)

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

So  $a \perp b \mid c$ .

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

#### Bayesian Networks: "An Indirect Effect"

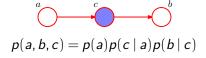


Are a and b independent? (Note: This is a Markov chain) (e.g. a=raining, c=wet ground, b=mud on shoes)

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

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

#### Bayesian Networks: "An Indirect Effect"



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

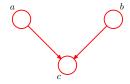
$$p(a,b|c) = p(a,b,c)/p(c)$$

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

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

So  $a \perp b \mid c$ .

## Bayesian Networks: "A Common Effect"



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

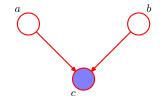
Are a and b independent? (a=course difficulty, b=knowledge, c= grade)

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

So  $a \perp b$ .

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

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



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

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  $p(a \mid c)p(b \mid c)$ , in general.

#### 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*:

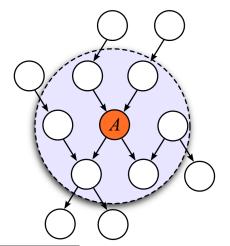
$$p(A \mid \text{all other nodes}) = p(A \mid \text{MarkovBlanket}(A)).$$

- 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:



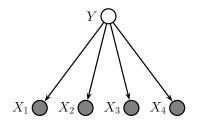
From http://en.wikipedia.org/wiki/Markov\_blanket: "Diagram of a Markov blanket" by Laughsinthestocks - Licensed under CC0 via Wikimedia Commons

## 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

- $\mathfrak{X} = \left\{ \left( X_1, X_2, X_3, X_4 \right) \in \left\{ 0, 1 \right\}^4 \right) \right\}$   $\mathfrak{Y} = \left\{ 0, 1 \right\}$  be a class label.
- Consider the Bayesian network depicted below:



• BN structure implies joint distribution factors as:

$$p(x_1, x_2, x_3, x_4, y) = p(y)p(x_1 | y)p(x_2 | y)p(x_3 | y)p(x_4 | y)$$

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

KPM Figure 10.2(a).

## 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:

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

Joint distribution is

$$\begin{split} & p(x_1, \dots x_d, y) \\ &= p(y) \prod_{i=1}^n p(x_i \mid y) \\ &= (\theta_y)^y (1 - \theta_y)^{1-y} \\ &\times \prod_{i=1}^n (\theta_{i1})^{yx_i} (1 - \theta_{i1})^{y(1-x_i)} (\theta_{i0})^{(1-y)x_i} (1 - \theta_{i0})^{(1-y)(1-x_i)} \end{split}$$

#### 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

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

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

# Posterior Class Probability

• Let  $x = (x_1, ..., x_d)$ , 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?  $p(y \mid x)$  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.

## Naive Bayes and Logistic Regression

Recall the logistic regression prediction function is of the form

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

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

#### **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  $w \in \mathbb{R}^d$ .

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  $x = (x_1, ..., x_d)$ .
- 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  $X_1$  and  $X_2$  from the input vector.
- Just predict with

$$\mathbb{P}(y \mid x_3, \dots x_d) \propto p(y, x_3, \dots, x_d)$$

$$= \sum_{x_1, x_2 \in \{0,1\}} p(y, x)$$

• 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.

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

- Wasted effort to model all features if you only care about  $p(y \mid x)$ ?
- 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:

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

## 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

$$\begin{split} p(x,y) &= (\theta_y)^y (1 - \theta_y)^{1 - y} \\ &\times \prod_{i=1}^n (\theta_{i1})^{yx_i} (1 - \theta_{i1})^{y(1 - x_i)} \\ &\times \prod_{i=1}^n (\theta_{i0})^{(1 - y)x_i} (1 - \theta_{i0})^{(1 - y)(1 - x_i)} \end{split}$$

- Theorem: MLE is exactly the plug-in estimator.
- Proof: Optional Homework.

#### Class Prediction

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

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

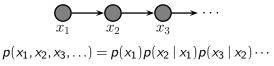
One approach to this is to write

$$\begin{split} \frac{\rho(Y=1 \mid x)}{\rho(Y=0 \mid x)} &= \frac{\rho(Y=1,x)/\rho(x)}{\rho(Y=0,x)/\rho(x)} = \frac{\rho(Y=1,x)}{\rho(Y=0,x)} \\ &= \frac{\rho(Y=1) \prod_{i=1}^{d} \rho(x_i \mid Y=1)}{\rho(Y=0) \prod_{i=1}^{d} \rho(x_i \mid Y=0)} \\ &= \frac{\rho(Y=1)}{\rho(Y=0)} \prod_{i=1}^{d} \frac{\rho(x_i \mid Y=1)}{\rho(x_i \mid Y=0)} \end{split}$$

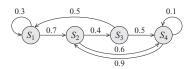
• Compare ratio to 1 to get prediction.

#### Markov Chain Model

• A Markov chain model has structure:



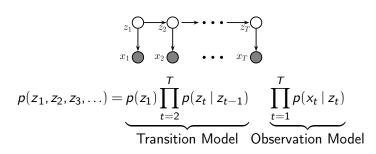
- Conditional distributions  $p(x_i | x_{i-1})$  is called the **transition model**.
- When conditional distribution independent of i, called time-homogeneous.
- 4-state transition model for  $X_i \in \{S_1, S_2, S_3, S_4\}$ :



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

#### Hidden Markov Model

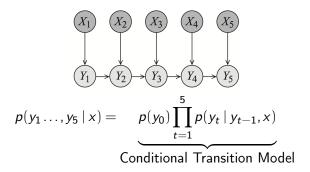
• A hidden Markov model (HMM) has structure:



- 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  $(Z_1, ..., Z_T)$  . (Use **Viterbi** algorithm.)

# 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).

# 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

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