



10-601 Introduction to Machine Learning

Machine Learning Department School of Computer Science Carnegie Mellon University

Naïve Bayes

+

Generative vs. Discriminative

Matt Gormley Lecture 18 Mar. 25, 2019

Reminders

- Homework 6: Learning Theory / Generative Models
 - Out: Fri, Mar 22
 - Due: Fri, Mar 29 at 11:59pm (1 week)
- Midterm Exam 2
 - Thu, Apr 4 evening exam, details announced on Piazza
- Homework 7: HMMs
 - Out: Fri, Mar 29
 - Due: Wed, Apr 10 at 11:59pm
- Today's In-Class Poll
 - http://p18.mlcourse.org

Q&A

Q: Why would we use Naïve Bayes? Isn't it too Naïve?

A: Naïve Bayes has one **key advantage** over methods like Perceptron, Logistic Regression, Neural Nets:

Training is lightning fast!

While other methods require slow iterative training procedures that might require hundreds of epochs, Naïve Bayes computes its parameters in closed form by counting.

NAÏVE BAYES

Naïve Bayes Outline

Real-world Dataset

- Economist vs. Onion articles
- Document → bag-of-words → binary feature vector

Naive Bayes: Model

- Generating synthetic "labeled documents"
- Definition of model
- Naive Bayes assumption
- Counting # of parameters with / without
 NB assumption

Naïve Bayes: Learning from Data

- Data likelihood
- MLE for Naive Bayes
- MAP for Naive Bayes
- Visualizing Gaussian Naive Bayes

Naïve Bayes

- Why are we talking about Naïve Bayes?
 - It's just another decision function that fits into our "big picture" recipe from last time
 - But it's our first example of a Bayesian Network and provides a clearer picture of probabilistic learning
 - Just like the other Bayes Nets we'll see, it admits
 a closed form solution for MLE and MAP
 - So learning is extremely efficient (just counting)

Fake News Detector

Today's Goal: To define a generative model of emails of two different classes (e.g. real vs. fake news)

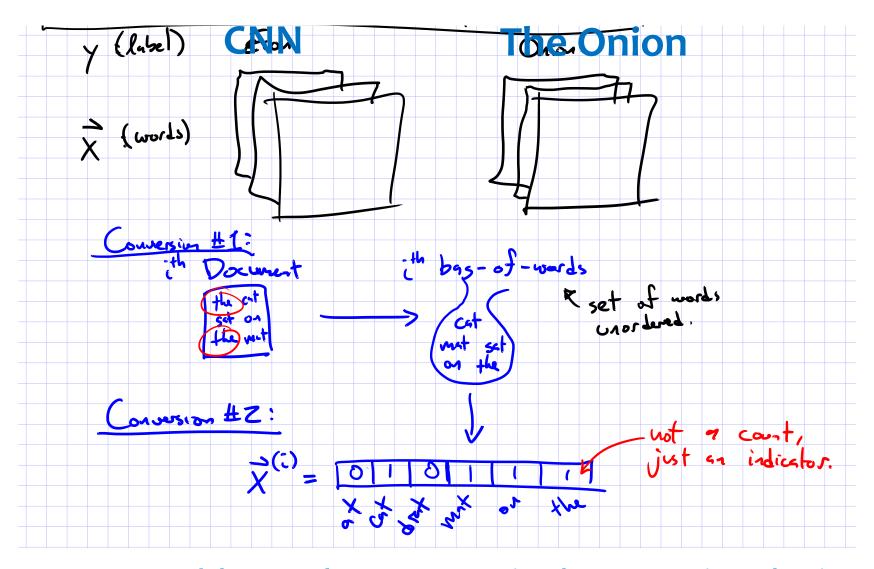
CNN



The Onion



Fake News Detector



We can pretend the natural process generating these vectors is stochastic...

Naive Bayes: Model

Whiteboard

- Document → bag-of-words → binary feature vector
- Generating synthetic "labeled documents"
- Definition of model
- Naive Bayes assumption
- Counting # of parameters with / without NB assumption

Flip weighted coin



If HEADS, flip each red coin



 x_2

 x_3

 x_M

y

 x_1

If TAILS, flip each blue coin



We can **generate** data in this fashion. Though in practice we never would since our data is **given**.

Instead, this provides an explanation of **how** the data was generated (albeit a terrible one).

Each red coin corresponds to $an x_m$

What's wrong with the Naïve Bayes Assumption?

The features might not be independent!!

Example 1:

- If a document contains the word "Donald", it's extremely likely to contain the word "Trump"
- These are not independent!

* ELECTION 2016 * MORE ELECTION COVERAGE

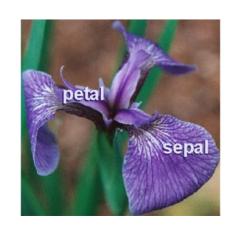
Trump Spends Entire Classified National
Security Briefing Asking About Egyptian
Mummies



NEWS IN BRIEF August 18, 2016 VOL 52 ISSUE 32 · Politics · Politicians · Election 2016 · Donald Trump

Example 2:

If the petal width is very high,
 the petal length is also likely to
 be very high



Naïve Bayes: Learning from Data

Whiteboard

- Data likelihood
- MLE for Naive Bayes
- Example: MLE for Naïve Bayes with Two Features
- MAP for Naive Bayes

Recipe for Closed-form MLE

- 1. Assume data was generated i.i.d. from some model (i.e. write the generative story) $x^{(i)} \sim p(x|\theta)$
- 2. Write log-likelihood

$$\ell(\boldsymbol{\theta}) = \log p(\mathbf{x}^{(1)}|\boldsymbol{\theta}) + \dots + \log p(\mathbf{x}^{(N)}|\boldsymbol{\theta})$$

3. Compute partial derivatives (i.e. gradient)

$$\frac{\partial \ell(\boldsymbol{\theta})}{\partial \theta_1} = \dots$$
$$\frac{\partial \ell(\boldsymbol{\theta})}{\partial \theta_2} = \dots$$
$$\frac{\partial \ell(\boldsymbol{\theta})}{\partial \theta_M} = \dots$$

4. Set derivatives to zero and solve for θ

$$\partial \ell(\theta)/\partial \theta_{\rm m} = \text{o for all } m \in \{1, ..., M\}$$

 $\theta^{\rm MLE} = \text{solution to system of } M \text{ equations and } M \text{ variables}$

5. Compute the second derivative and check that $\ell(\theta)$ is concave down at θ^{MLE}

NAÏVE BAYES: MODEL DETAILS

Data: Binary feature vectors, Binary labels

$$\mathbf{x} \in \{0, 1\}^M$$

$$y \in \{0, 1\}$$

Generative Story:

$$y \sim \mathsf{Bernoulli}(\phi)$$

$$x_1 \sim \mathsf{Bernoulli}(\theta_{y,1})$$

$$x_2 \sim \mathsf{Bernoulli}(\theta_{y,2})$$

:

 $x_M \sim \mathsf{Bernoulli}(\theta_{y,M})$

Model:

$$p_{\phi,\theta}(\boldsymbol{x},y) = p_{\phi,\theta}(x_1,\dots,x_M,y)$$

$$= p_{\phi}(y) \prod_{m=1}^{M} p_{\theta}(x_m|y)$$

$$= \left[(\phi)^y (1-\phi)^{(1-y)} \right]$$

$$\prod_{m=1}^{M} (\theta_{y,m})^{x_m} (1-\theta_{y,m})^{(1-x_m)}$$

Maximum Likelihood Estimation

Training: Find the class-conditional MLE parameters

Count
$$N_{y=1} = \sum_{i=1}^{N} \mathbb{I}(y^{(i)} = 1)$$

$$N_{y=0} = \sum_{i=1}^{N} \mathbb{I}(y^{(i)} = 0)$$

$$N_{y=0,x_m=1} = \sum_{i=1}^{N} \mathbb{I}(y^{(i)} = 0 \land x_m^{(i)} = 1)$$

Maximum Likelihood **Estimators:**

$$\phi = \frac{N_{y=1}}{N}$$

$$\theta_{0,m} = \frac{N_{y=0,x_m=1}}{N_{y=0}}$$

$$\theta_{1,m} = \frac{N_{y=1,x_m=1}}{N_{y=1}}$$

$$\forall m \in \{1, \dots, M\}$$

Maximum Likelihood Estimation

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$$\forall m \in \{1, \dots, M\}$$

Data: χ_2 χ_3 χ_{M}

Question 1:

What is the MLE of ϕ ? (A) 0/6 (B) 1/6 (C) 2/6 (D) 3/6 (E) 4/6 (F) 5/6 (G) 6/6 (H) None of the above

Maximum Likelihood Estimation

Training: Find the class-conditional MLE parameters

Count
$$N_{y=1} = \sum_{i=1}^{N} \mathbb{I}(y^{(i)} = 1)$$

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Maximum Likelihood **Estimators:**

$$\phi = \frac{N_{y=1}}{N}$$

$$\theta_{0,m} = \frac{N_{y=0,x_m=1}}{N_{y=0}}$$

$$\theta_{1,m} = \frac{N_{y=1,x_m=1}}{N_{y=1}}$$

$$\forall m \in \{1, \dots, M\}$$

Data: χ_2 χ_3 χ_{M}

Question 2:

What is the MLE of $\theta_{0.1}$? (A) 0/6 (B) 1/6 (C) 2/6 (D) 3/6 (E) 4/6 (F) 5/6 (G) 6/6 (H) None of the above

MLE

What does maximizing likelihood accomplish?

- There is only a finite amount of probability mass (i.e. sum-to-one constraint)
- MLE tries to allocate as much probability mass as possible to the things we have observed...

... at the expense of the things we have not observed

A Shortcoming of MLE

For Naïve Bayes, suppose we never observe the word "serious" in an Onion article.

In this case, what is the MLE of $p(x_k | y)$?

$$\theta_{k,0} = \frac{\sum_{i=1}^{N} \mathbb{I}(y^{(i)} = 0 \land x_k^{(i)} = 1)}{\sum_{i=1}^{N} \mathbb{I}(y^{(i)} = 0)}$$

Now suppose we observe the word "serious" at test time. What is the posterior probability that the article was an Onion article?

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

MAP Estimation (Beta Prior)

1. Generative Story:

The parameters are drawn once for the entire dataset.

$$\begin{aligned} &\text{for } m \in \{1, \dots, M\}\text{:} \\ &\text{for } y \in \{0, 1\}\text{:} \\ &\theta_{m,y} \sim \text{Beta}(\alpha, \beta) \\ &\text{for } i \in \{1, \dots, N\}\text{:} \\ &y^{(i)} \sim \text{Bernoulli}(\phi) \\ &\text{for } m \in \{1, \dots, M\}\text{:} \\ &x_m^{(i)} \sim \text{Bernoulli}(\theta_{y^{(i)}, m}) \end{aligned}$$

$$N_{y=1} = \sum_{i=1}^{N} \mathbb{I}(y^{(i)} = 1)$$

$$N_{y=0} = \sum_{i=1}^{N} \mathbb{I}(y^{(i)} = 0)$$

$$N_{y=0,x_m=1} = \sum_{i=1}^{N} \mathbb{I}(y^{(i)} = 0 \land x_m^{(i)} = 1)$$

2. Likelihood:

$$\ell_{MAP}(\phi, \boldsymbol{\theta})$$

$$= \log \left[p(\phi, \boldsymbol{\theta} | \alpha, \beta) p(\mathcal{D} | \phi, \boldsymbol{\theta}) \right]$$

$$= \log \left[\left(p(\phi | \alpha, \beta) \prod_{m=1}^{M} p(\theta_{0,m} | \alpha, \beta) \right) \left(\prod_{i=1}^{N} p(\mathbf{x}^{(i)}, y^{(i)} | \phi, \boldsymbol{\theta}) \right) \right]$$

3. MAP Estimates:
$$(\phi^{MAP}, \boldsymbol{\theta}^{MAP}) = \operatorname*{argmax}_{\phi, \boldsymbol{\theta}} \ell_{MAP}(\phi, \boldsymbol{\theta})$$

Take derivatives, set to zero and solve...

$$\phi = \frac{N_{y=1}}{N}$$

$$\theta_{0,m} = \frac{(\alpha - 1) + N_{y=0,x_m=1}}{(\alpha - 1) + (\beta - 1) + N_{y=0}}$$

$$\theta_{1,m} = \frac{(\alpha - 1) + N_{y=1,x_m=1}}{(\alpha - 1) + (\beta - 1) + N_{y=1}}$$

$$\forall m \in \{1, \dots, M\}$$

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Other NB Models

- Bernoulli Naïve Bayes:
 - for binary features
- 2. Multinomial Naïve Bayes:
 - for integer features
- 3. Gaussian Naïve Bayes:
 - for continuous features
- 4. Multi-class Naïve Bayes:
 - for classification problems with > 2 classes
 - event model could be any of Bernoulli, Gaussian,
 Multinomial, depending on features

Model 2: Multinomial Naïve Bayes

Support:

Option 1: Integer vector (word IDs)

 ${\bf x} = [x_1, x_2, \dots, x_M]$ where $x_m \in \{1, \dots, K\}$ a word id.

Generative Story:

$$\begin{aligned} &\textbf{for } i \in \{1,\dots,N\} \textbf{:} \\ &y^{(i)} \sim \text{Bernoulli}(\phi) \\ &\textbf{for } j \in \{1,\dots,M_i\} \textbf{:} \\ &x_j^{(i)} \sim \text{Multinomial}(\boldsymbol{\theta}_{y^{(i)}},1) \end{aligned}$$

Model:

$$p_{\phi,\boldsymbol{\theta}}(\boldsymbol{x},y) = p_{\phi}(y) \prod_{k=1}^{K} p_{\boldsymbol{\theta}_k}(x_k|y)$$
$$= (\phi)^y (1-\phi)^{(1-y)} \prod_{j=1}^{M_i} \theta_{y,x_j}$$

Model 3: Gaussian Naïve Bayes

Support:

$$\mathbf{x} \in \mathbb{R}^K$$

Model: Product of prior and the event model

$$p(\mathbf{x}, y) = p(x_1, \dots, x_K, y)$$
$$= p(y) \prod_{k=1}^K p(x_k | y)$$

Gaussian Naive Bayes assumes that $p(x_k|y)$ is given by a Normal distribution.

Model 4: Multiclass Naïve Bayes

Model:

The only change is that we permit y to range over C classes.

$$p(\mathbf{x}, y) = p(x_1, \dots, x_K, y)$$
$$= p(y) \prod_{k=1}^K p(x_k | y)$$

Now, $y \sim \text{Multinomial}(\phi, 1)$ and we have a separate conditional distribution $p(x_k|y)$ for each of the C classes.

Generic Naïve Bayes Model

Support: Depends on the choice of **event model**, $P(X_k|Y)$

Model: Product of prior and the event model

$$P(\mathbf{X}, Y) = P(Y) \prod_{k=1}^{K} P(X_k | Y)$$

Training: Find the class-conditional MLE parameters

For P(Y), we find the MLE using all the data. For each $P(X_k|Y)$ we condition on the data with the corresponding

Classification: Find the class that maximizes the posterior

$$\hat{y} = \operatorname*{argmax}_{y} p(y|\mathbf{x})$$

Generic Naïve Bayes Model

Classification:

$$\hat{y} = \operatorname*{argmax} p(y|\mathbf{x})$$
 (posterior)
$$= \operatorname*{argmax} \frac{p(\mathbf{x}|y)p(y)}{p(x)}$$
 (by Bayes' rule)
$$= \operatorname*{argmax} p(\mathbf{x}|y)p(y)$$

$$= \operatorname*{argmax} p(\mathbf{x}|y)p(y)$$

VISUALIZING GAUSSIAN NAÏVE BAYES

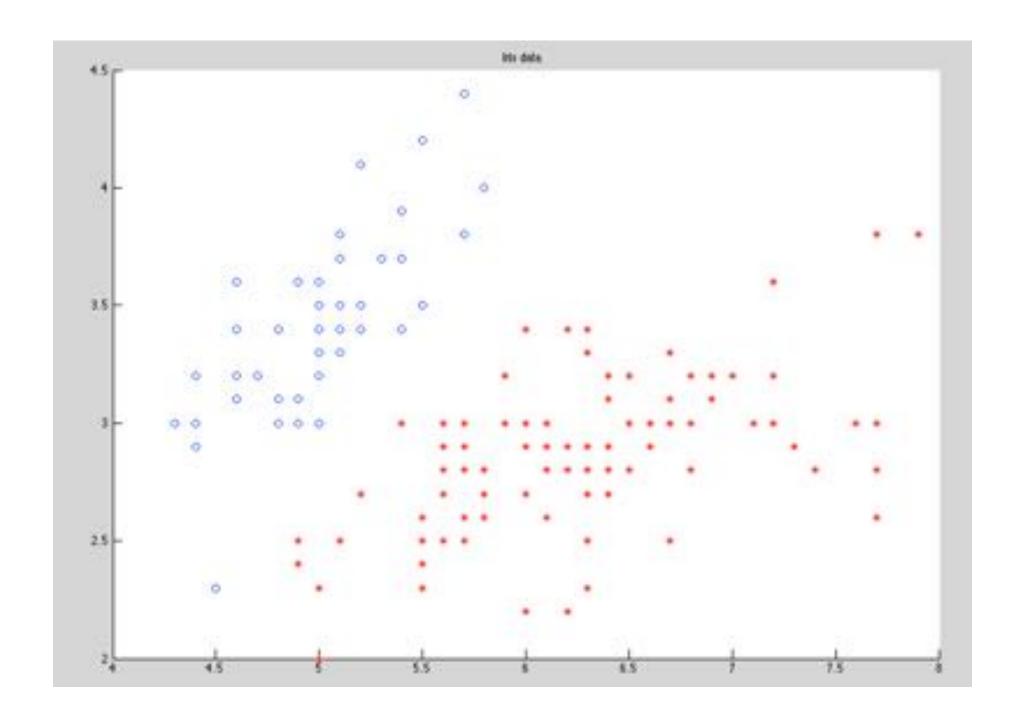


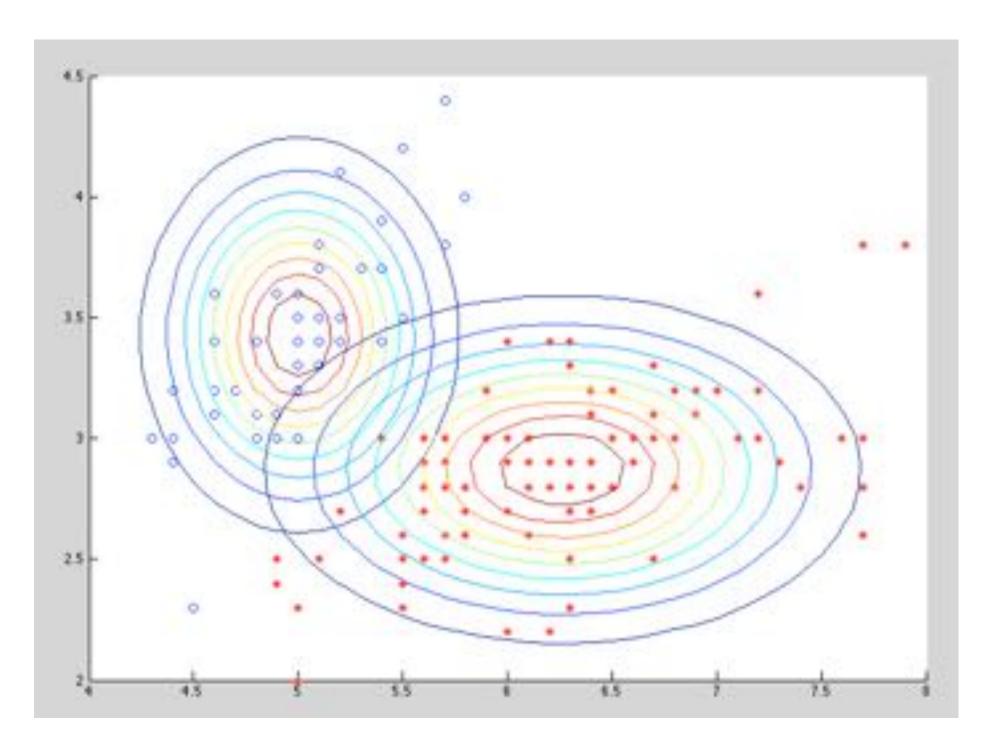


Fisher Iris Dataset

Fisher (1936) used 150 measurements of flowers from 3 different species: Iris setosa (0), Iris virginica (1), Iris versicolor (2) collected by Anderson (1936)

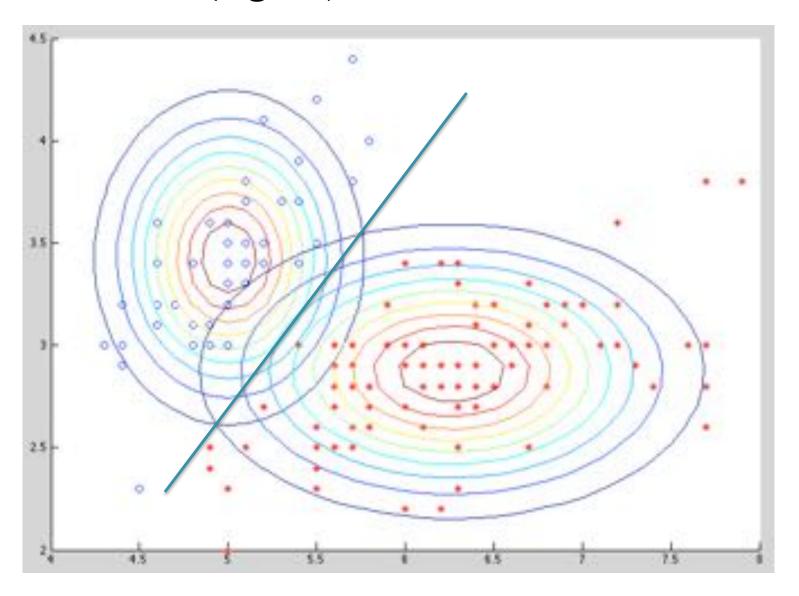
Species	Sepal Length	Sepal Width	Petal Length	Petal Width
0	4.3	3.0	1.1	0.1
0	4.9	3.6	1.4	0.1
0	5.3	3.7	1.5	0.2
1	4.9	2.4	3.3	1.0
1	5.7	2.8	4.1	1.3
1	6.3	3.3	4.7	1.6
1	6.7	3.0	5.0	1.7



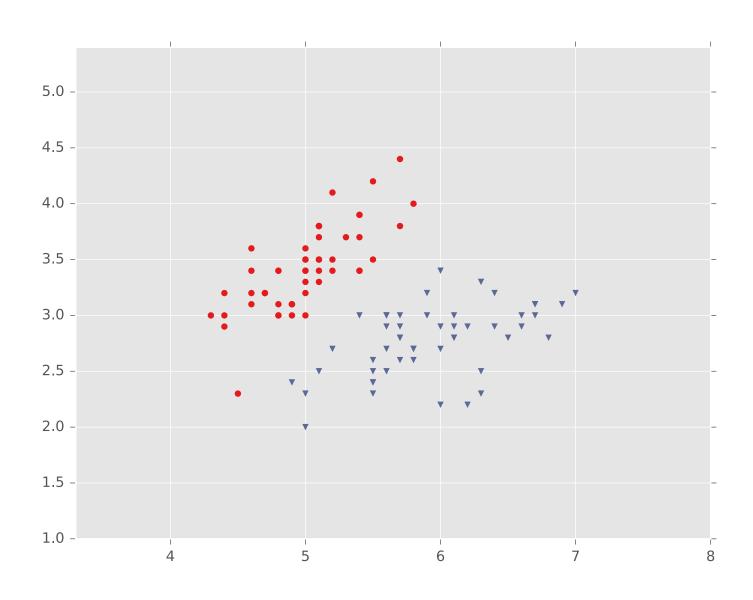


Slide from William Cohen

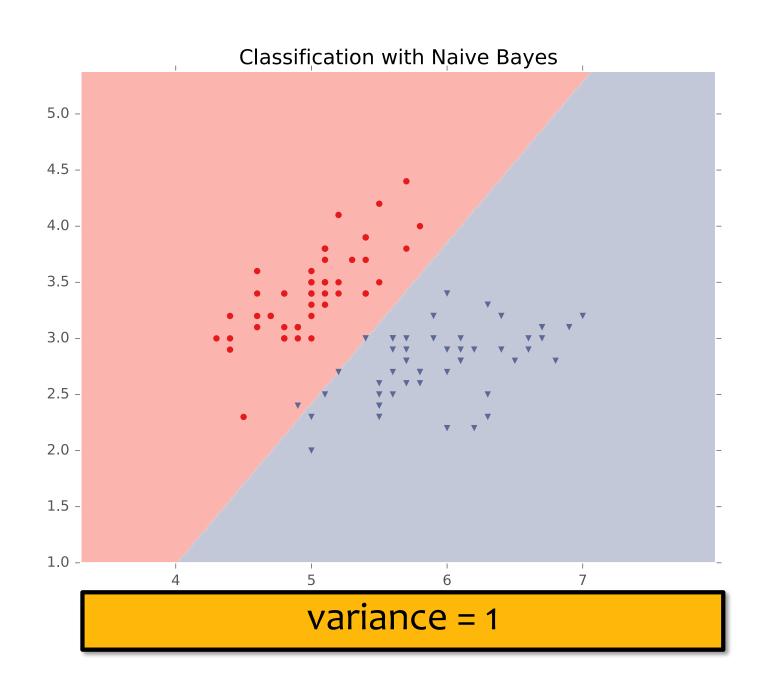
Naïve Bayes has a **linear** decision boundary if variance (sigma) is constant across classes



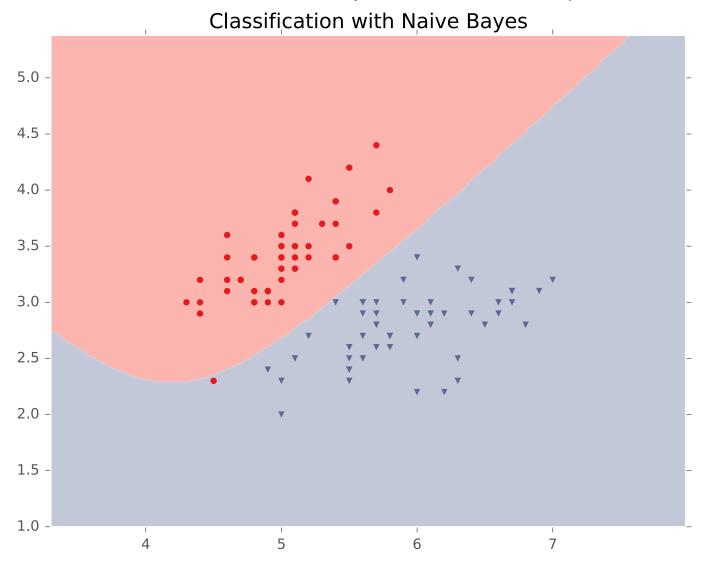
Iris Data (2 classes)



Iris Data (2 classes)

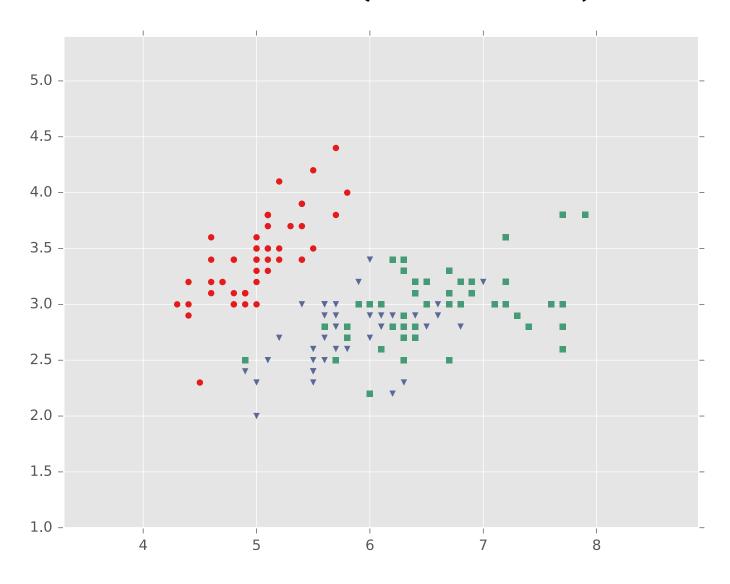


Iris Data (2 classes)

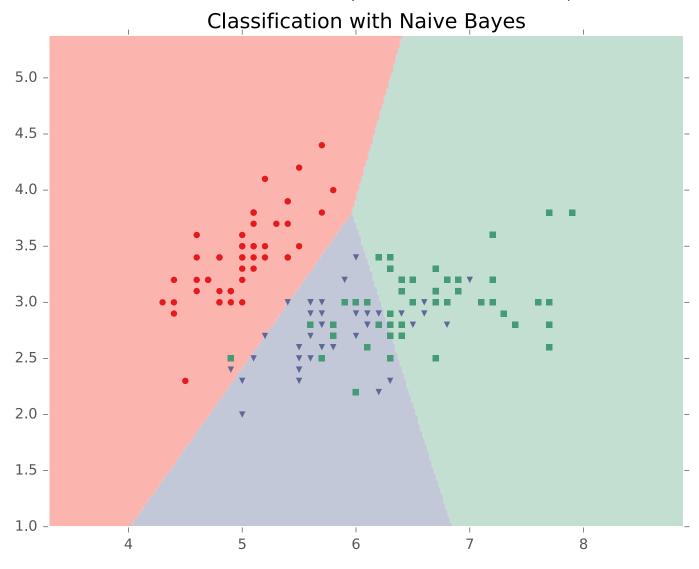


variance learned for each class

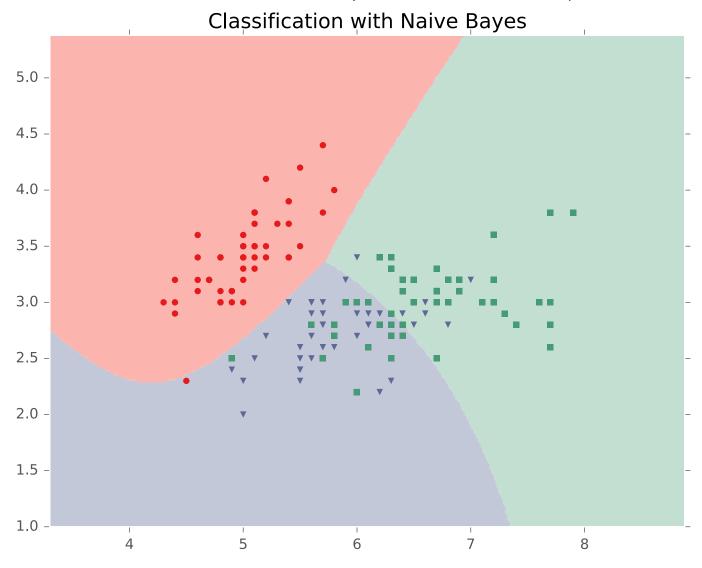
Iris Data (3 classes)



Iris Data (3 classes)

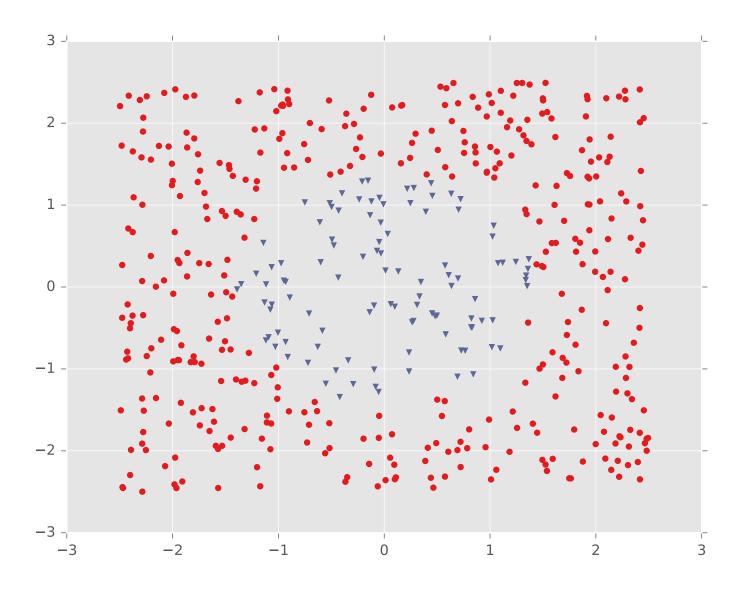


Iris Data (3 classes)

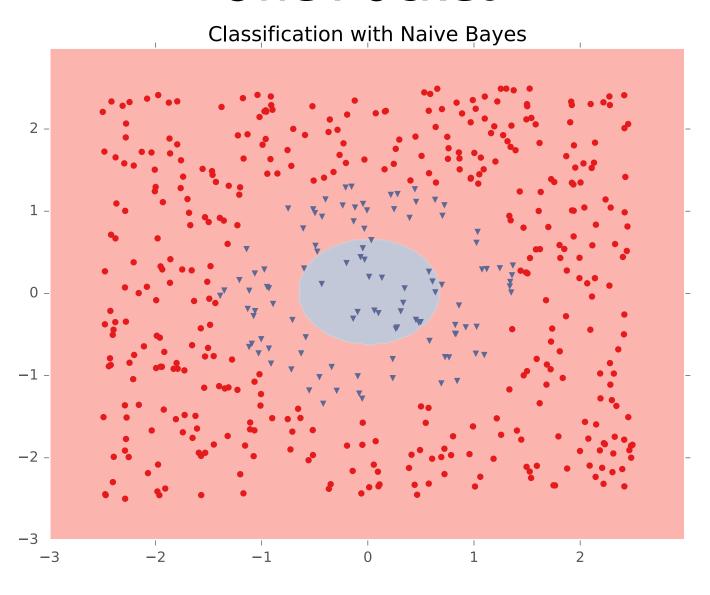


variance learned for each class

One Pocket

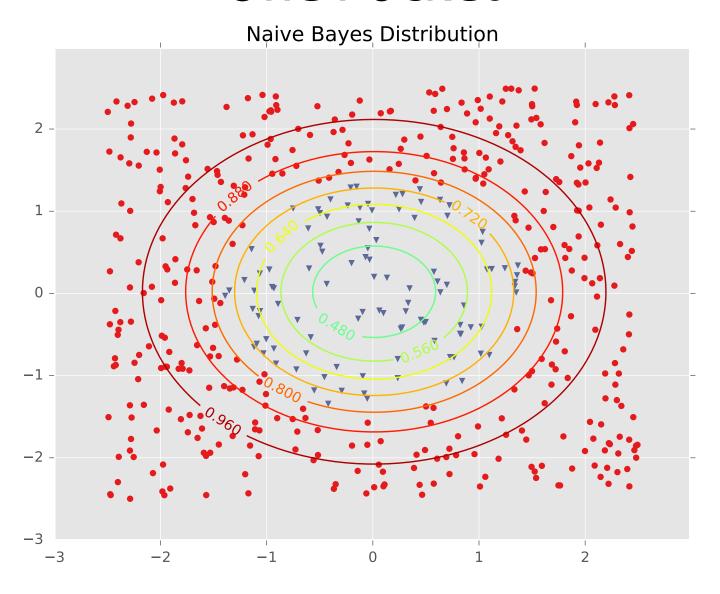


One Pocket



variance learned for each class

One Pocket



Summary

- Naïve Bayes provides a framework for generative modeling
- Choose p(x_m | y) appropriate to the data (e.g. Bernoulli for binary features, Gaussian for continuous features)
- 3. Train by MLE or MAP
- 4. Classify by maximizing the posterior

Learning Objectives

Naïve Bayes

You should be able to...

- 1. Write the generative story for Naive Bayes
- 2. Create a new Naive Bayes classifier using your favorite probability distribution as the event model
- 3. Apply the principle of maximum likelihood estimation (MLE) to learn the parameters of Bernoulli Naive Bayes
- 4. Motivate the need for MAP estimation through the deficiencies of MLE
- 5. Apply the principle of maximum a posteriori (MAP) estimation to learn the parameters of Bernoulli Naive Bayes
- 6. Select a suitable prior for a model parameter
- 7. Describe the tradeoffs of generative vs. discriminative models
- 8. Implement Bernoulli Naives Bayes
- 9. Employ the method of Lagrange multipliers to find the MLE parameters of Multinomial Naive Bayes
- 10. Describe how the variance affects whether a Gaussian Naive Bayes model will have a linear or nonlinear decision boundary

DISCRIMINATIVE AND GENERATIVE CLASSIFIERS

Generative Classifiers:

- Example: Naïve Bayes
- Define a joint model of the observations ${\bf x}$ and the labels y: $p({\bf x},y)$
- Learning maximizes (joint) likelihood
- Use Bayes' Rule to classify based on the posterior:

$$p(y|\mathbf{x}) = p(\mathbf{x}|y)p(y)/p(\mathbf{x})$$

Discriminative Classifiers:

- Example: Logistic Regression
- Directly model the conditional: $p(y|\mathbf{x})$
- Learning maximizes conditional likelihood

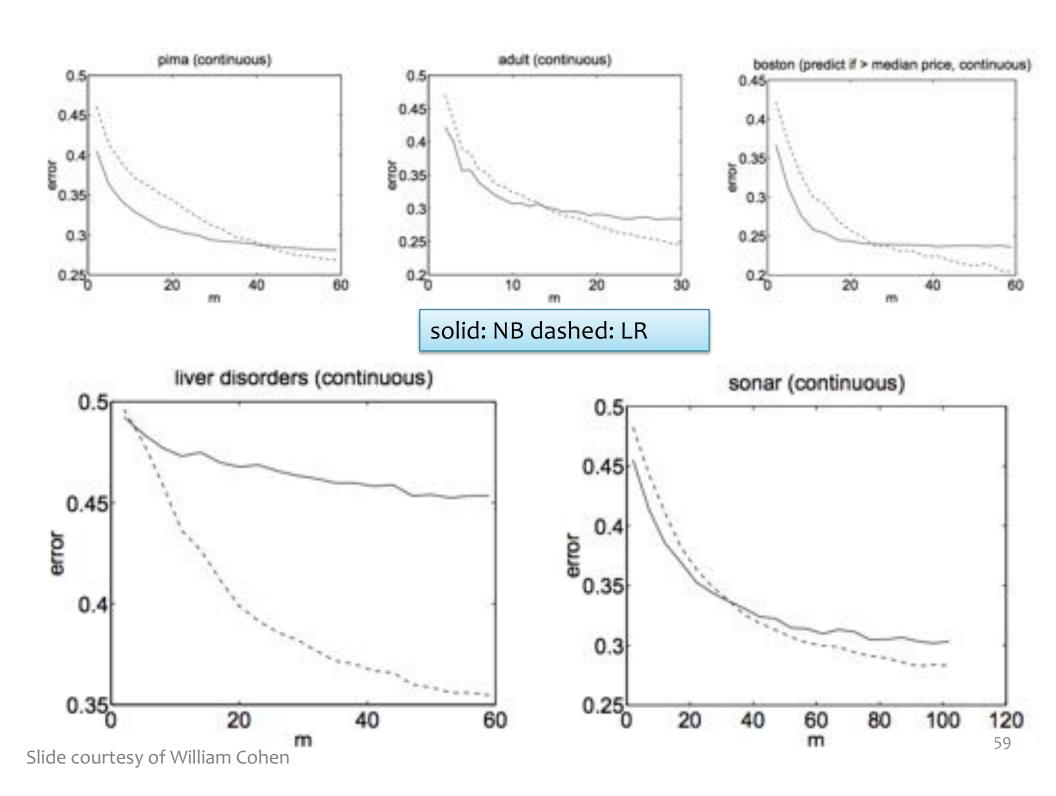
	Gen.	Disc.
MLE	$\prod_{i} p(\mathbf{x}^{(i)}, y^{(i)} \boldsymbol{\theta})$	$\prod_{i} p(y^{(i)} \mathbf{x}^{(i)},\boldsymbol{\theta})$
MAP	$p(\boldsymbol{\theta}) \prod_{i} p(\mathbf{x}^{(i)}, y^{(i)} \boldsymbol{\theta})$	$\frac{\prod_{i} p(y^{(i)} \mathbf{x}^{(i)}, \boldsymbol{\theta})}{p(\boldsymbol{\theta}) \prod_{i} p(y^{(i)} \mathbf{x}^{(i)}, \boldsymbol{\theta})}$

Finite Sample Analysis (Ng & Jordan, 2002)

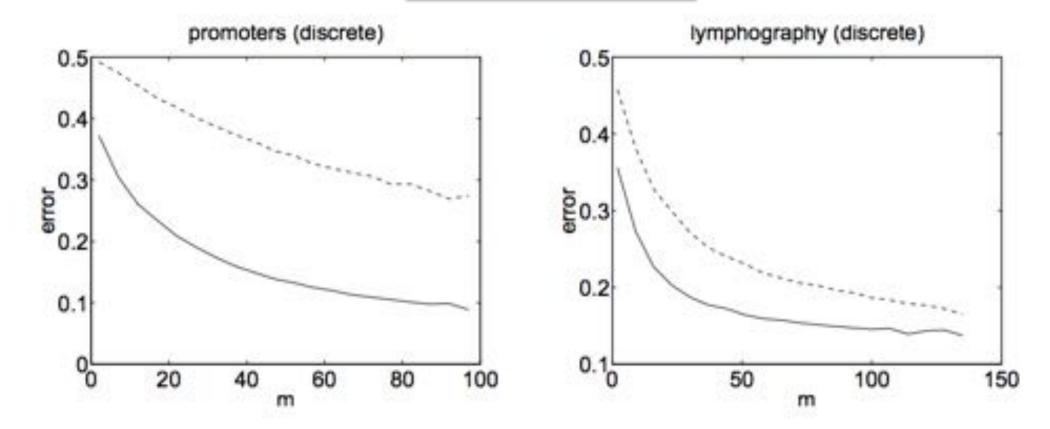
[Assume that we are learning from a finite training dataset]

If model assumptions are correct: Naive Bayes is a more efficient learner (requires fewer samples) than Logistic Regression

If model assumptions are incorrect: Logistic Regression has lower asymtotic error, and does better than Naïve Bayes



solid: NB dashed: LR



Naïve Bayes makes stronger assumptions about the data but needs fewer examples to estimate the parameters

"On Discriminative vs Generative Classifiers:" Andrew Ng and Michael Jordan, NIPS 2001.

Learning (Parameter Estimation)

Naïve Bayes:

Parameters are decoupled -> Closed form solution for MLE

Logistic Regression:

Parameters are coupled \rightarrow No closed form solution – must use iterative optimization techniques instead

Naïve Bayes vs. Logistic Reg.

Learning (MAP Estimation of Parameters)

Bernoulli Naïve Bayes:

Parameters are probabilities → Beta prior (usually) pushes probabilities away from zero / one extremes

Logistic Regression:

Parameters are not probabilities -> Gaussian prior encourages parameters to be close to zero

(effectively pushes the probabilities away from zero / one extremes)

Naïve Bayes vs. Logistic Reg.

Features

Naïve Bayes:

Features x are assumed to be conditionally independent given y. (i.e. Naïve Bayes Assumption)

Logistic Regression:

No assumptions are made about the form of the features x. They can be dependent and correlated in any fashion.

MOTIVATION: STRUCTURED PREDICTION

Structured Prediction

 Most of the models we've seen so far were for classification

- Given observations: $\mathbf{x} = (x_1, x_2, ..., x_K)$
- Predict a (binary) label: y
- Many real-world problems require structured prediction
 - Given observations: $\mathbf{x} = (x_1, x_2, ..., x_K)$
 - Predict a structure: $y = (y_1, y_2, ..., y_J)$
- Some classification problems benefit from latent structure

Structured Prediction Examples

Examples of structured prediction

- Part-of-speech (POS) tagging
- Handwriting recognition
- Speech recognition
- Word alignment
- Congressional voting

Examples of latent structure

Object recognition

Dataset for Supervised Part-of-Speech (POS) Tagging

Data: $\mathcal{D} = \{oldsymbol{x}^{(n)}, oldsymbol{y}^{(n)}\}_{n=1}^N$

Sample 1:	n	v flies	p like	an	$y^{(1)}$ $x^{(1)}$
Sample 2:	n	n	like	an	$y^{(2)}$ $x^{(2)}$
Sample 3:	n	fly	with	heir	$y^{(3)}$ $x^{(3)}$
Sample 4:	with	n	you	will	$y^{(4)}$ $x^{(4)}$

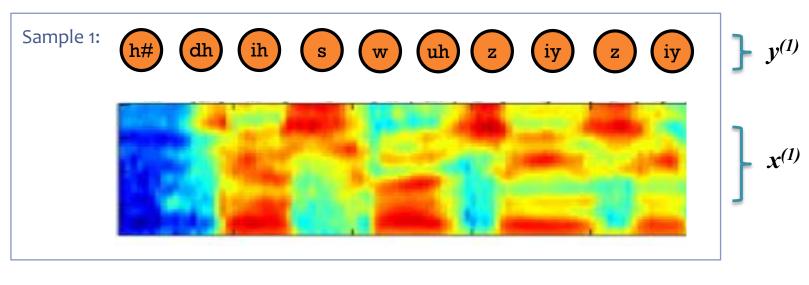
Dataset for Supervised Handwriting Recognition

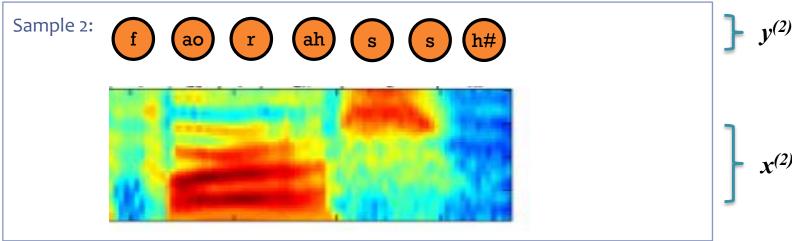
Data: $\mathcal{D} = \{oldsymbol{x}^{(n)}, oldsymbol{y}^{(n)}\}_{n=1}^N$



Dataset for Supervised Phoneme (Speech) Recognition

Data: $\mathcal{D} = \{ oldsymbol{x}^{(n)}, oldsymbol{y}^{(n)} \}_{n=1}^N$



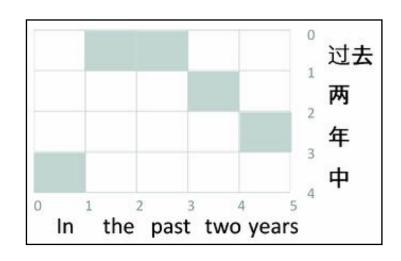


Application:

Word Alignment / Phrase Extraction

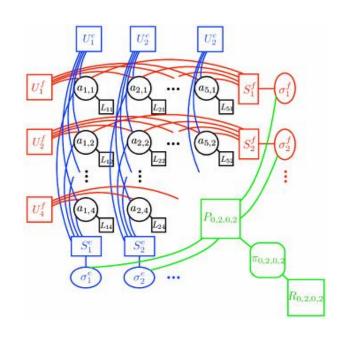
Variables (boolean):

For each (Chinese phrase, English phrase) pair, are they linked?



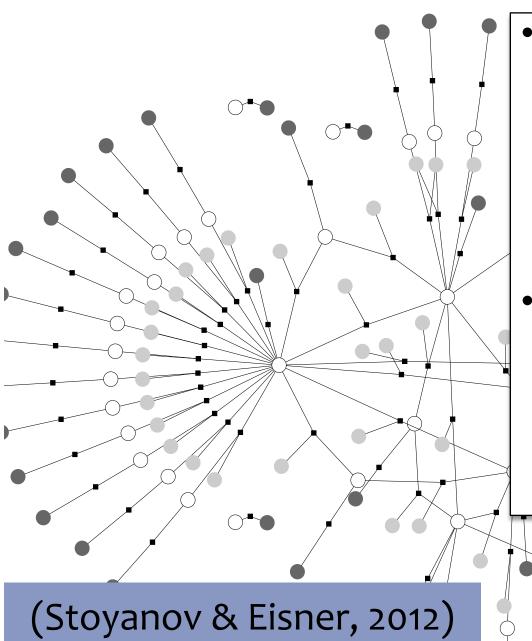
Interactions:

- Word fertilities
- Few "jumps" (discontinuities)
- Syntactic reorderings
- "ITG contraint" on alignment
- Phrases are disjoint (?)



Application:

Congressional Voting



Variables:

- Representative's vote
- Text of all speeches of a representative
- Local contexts of references between two representatives

• Interactions:

- Words used by representative and their vote
- Pairs of representatives and their local context

Structured Prediction Examples

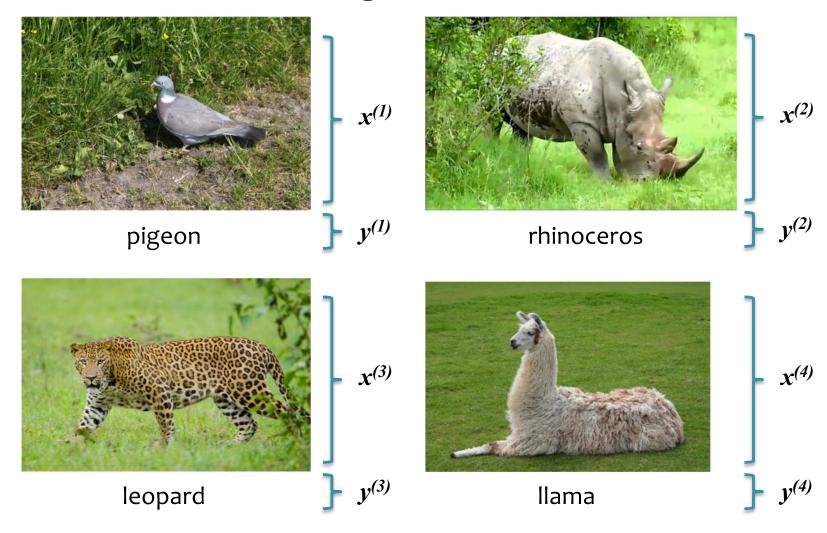
Examples of structured prediction

- Part-of-speech (POS) tagging
- Handwriting recognition
- Speech recognition
- Word alignment
- Congressional voting

Examples of latent structure

Object recognition

Data consists of images x and labels y.



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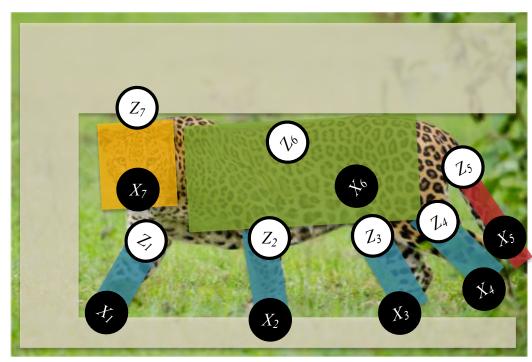
- Preprocess data into "patches"
- Posit a latent labeling z describing the object's parts (e.g. head, leg, tail, torso, grass)
- Define graphical model with these latent variables in mind
- z is not observed at train or test time



leopard

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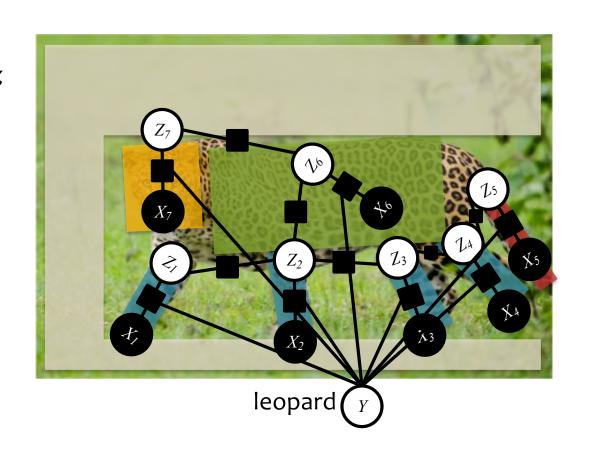
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leopard (y)

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Structured Prediction

Preview of challenges to come...

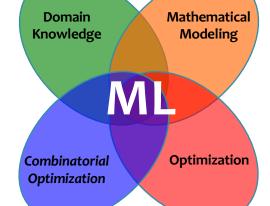
 Consider the task of finding the most probable assignment to the output

Classification
$$\hat{y} = \operatorname*{argmax}_{y} p(y|\mathbf{x})$$
 where $y \in \{+1, -1\}$

Structured Prediction
$$\hat{\mathbf{y}} = \operatorname*{argmax}_{\mathbf{y}} p(\mathbf{y}|\mathbf{x})$$
 where $\mathbf{y} \in \mathcal{Y}$ and $|\mathcal{Y}|$ is very large

Machine Learning

The data inspires
the structures
we want to
predict



Our **model**defines a score
for each structure

It also tells us what to optimize

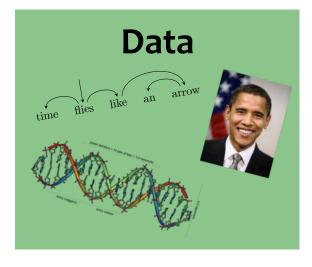
Inference finds

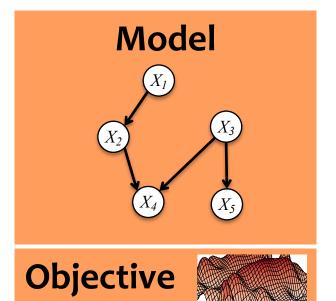
{best structure, marginals, partition function} for a new observation

(Inference is usually called as a subroutine in learning)

Learning tunes the parameters of the model

Machine Learning

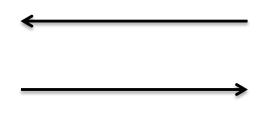




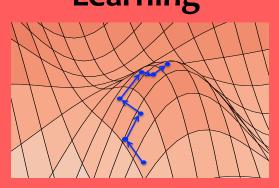




(Inference is usually called as a subroutine in learning)







BACKGROUND

Background: Chain Rule of Probability

For random variables A and B:

$$P(A,B) = P(A|B)P(B)$$

For random variables X_1, X_2, X_3, X_4 :

$$P(X_1, X_2, X_3, X_4) = P(X_1 | X_2, X_3, X_4)$$

$$P(X_2 | X_3, X_4)$$

$$P(X_3 | X_4)$$

$$P(X_4)$$

Background: Conditional Independence

Random variables A and B are conditionally independent given C if:

$$P(A,B|C) = P(A|C)P(B|C)$$
 (1)

or equivalently:

$$P(A|B,C) = P(A|C) \tag{2}$$

We write this as:

$$A \perp \!\!\! \perp B | C$$

Later we will also write: $I \le A$, $\{C\}$, $B \ge$