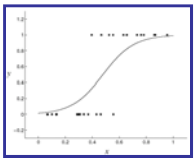
# Machine Learning

**10-701/15-781, Fall 2011**

## Generative verses discriminative classifier

**Eric Xing**



**Lecture 3, September 19, 2011**

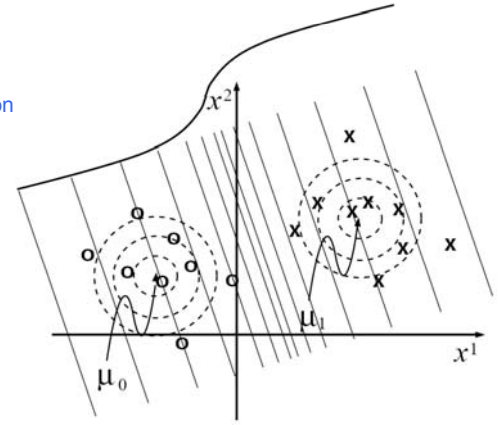
**Reading:**




- Homework 1 out today! Save at least 10 hours for it.
- About project
- Midterm and final

# Generative vs. Discriminative classifiers

- Goal: Wish to learn f: X → Y, e.g., P(Y|X)
- Generative:
  - Modeling the joint distribution of all data
- Discriminative:
  - Modeling only points at the boundary

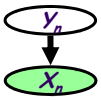




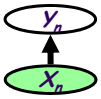


# Learning Generative and Discriminative Classifiers

- Goal: Wish to learn f: X → Y, e.g., P(Y|X)
- Generative classifiers (e.g., Naïve Bayes):
  - Assume some functional form for P(X|Y), P(Y)
    This is a '***generative***' model of the data!
  - Estimate parameters of P(X|Y), P(Y) directly from training data
  - Use Bayes rule to calculate P(Y|X= x)

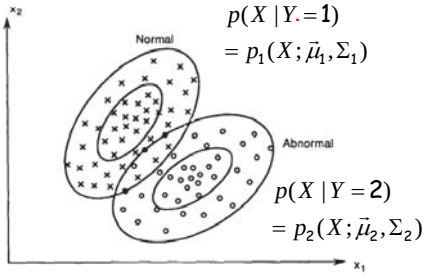



- Discriminative classifiers (e.g., logistic regression)
  - Directly assume some functional form for P(Y|X)
    This is a '***discriminative***' model of the data!
  - Estimate parameters of P(Y|X) directly from training data



# Suppose you know the following …

- Class-specific Dist.: P(X|Y)




**Bayes classifier:**

$$P(Y|X) = \frac{P(X|Y)P(Y)}{P(X)}$$

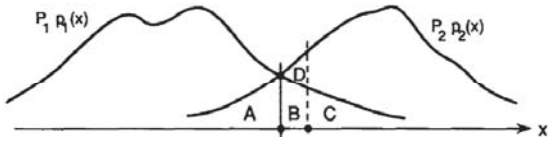
- Class prior (i.e., "weight"): P(Y)
- This is a generative model of the data!



# Optimal classification

- **Theorem:** Bayes classifier is optimal!
  - That is

$$error_{true}(h_{Bayes})) \leq error_{true}(h), \ \forall h(\mathbf{x})$$




- How to learn a Bayes classifier?
  - Recall density estimation. We need to estimate P(X|y=k), and P(y=k) for all k

# Learning Bayes Classifier

- Training data (discrete case):


| Sky | Temp | Humid | Wind | Water | Forecst | EnjoySpt |
|---|---|---|---|---|---|---|
| Sunny | Warm | Normal | Strong | Warm | Same | Yes |
| Sunny | Warm | High | Strong | Warm | Same | Yes |
| Rainy | Cold | High | Strong | Warm | Change | No |
| Sunny | Warm | High | Strong | Cool | Change | Yes |

- Learning = estimating P(X|Y), and P(Y)
- Classification = using Bayes rule to calculate $P(Y \mid X_{new})$




# Parameter learning from *iid* data: The Maximum Likelihood Est.

- Goal: estimate distribution parameters $\theta$ from a dataset of $N$ independent, identically distributed (*iid*), fully observed, training cases

$$D = \{x_1, \ldots, x_N\}$$

- Maximum likelihood estimation (MLE)
  1. One of the most common estimators
  2. With iid and full-observability assumption, write $L(\theta)$ as the likelihood of the data:

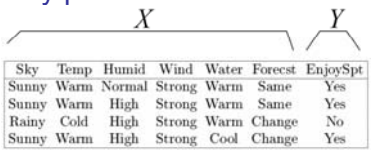
$$\begin{aligned} L(\theta) &= P(x_1, x_2, \ldots, x_N; \theta) \\ &= P(x;\theta)P(x_2;\theta),\ldots,P(x_N;\theta) \\ &= \prod_{n=1}^{N} P(x_n;\theta) \end{aligned}$$

  3. pick the setting of parameters most likely to have generated the data we saw:

$$\theta^* = \arg\max_{\theta} L(\theta) \quad = \arg\max_{\theta} \log L(\theta)$$

# How hard is it to learn the optimal classifier?

- How do we represent these? How many parameters?
  - Prior, P(Y):
    - Suppose Y is composed of *k* classes




| Sky | Temp | Humid | Wind | Water | Forecst | EnjoySpt |
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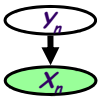
  - Likelihood, P(**X**|Y):
    - Suppose **X** is composed of *n* binary features

- Complex model → High variance with limited data!!!



# Gaussian Discriminative Analysis

- learning f: X → Y, where
  - X is a vector of real-valued features, $\mathbf{X}_n = < X_n^1, \ldots X_n^m >$
  - Y is an indicator vector
- What does that imply about the form of P(Y|X)?




  - The joint probability of a datum and its label is:

$$p(\mathbf{x}_n, y_n^k = 1 \mid \mu, \sigma) = p(y_n^k = 1) \times p(\mathbf{x}_n \mid y_n^k = 1, \mu, \Sigma)$$
$$= \pi_k \frac{1}{(2\pi|\Sigma|)^{1/2}} \exp\left\{-\tfrac{1}{2}(\mathbf{x}_n - \vec{\mu}_k)^T \Sigma^{-1}(\mathbf{x}_n - \vec{\mu}_k)\right\}$$

  - Given a datum $\mathbf{x}_n$, we predict its label using the conditional probability of the label given the datum:

$$p(y_n^k = 1 \mid \mathbf{x}_n, \mu, \Sigma) = \frac{\pi_k \frac{1}{(2\pi|\Sigma|)^{1/2}} \exp\left\{-\tfrac{1}{2}(\mathbf{x}_n - \vec{\mu}_k)^T \Sigma^{-1}(\mathbf{x}_n - \vec{\mu}_k)\right\}}{\sum_{k'} \pi_{k'} \frac{1}{(2\pi|\Sigma|)^{1/2}} \exp\left\{-\tfrac{1}{2}(\mathbf{x}_n - \vec{\mu}_k)^T \Sigma^{-1}(\mathbf{x}_n - \vec{\mu}_{k'})\right\}}$$

## Conditional Independence

- X is **conditionally independent** of Y given Z, if the probability distribution governing X is independent of the value of Y, given the value of Z

$$(\forall i,j,k) P(X=i|Y=j,Z=k) = P(X=i|Z=k)$$

Which we often write

$$P(X \mid Y,Z) = P(X \mid Z)$$

- e.g.,

$$P(Thunder|Rain,Lightning) = P(Thunder|Lightning)$$

- Equivalent to:

$$P(X,Y \mid Z) = P(X \mid Z)P(Y \mid Z)$$



## The Naïve Bayes assumption

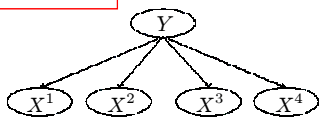
- Naïve Bayes assumption:
  - Features are conditionally independent given class:

$$\begin{aligned} P(X_1,X_2|Y) &= P(X_1|X_2,Y)P(X_2|Y) \\ &= P(X_1|Y)P(X_2|Y) \end{aligned}$$

  - More generally:

$$P(X^1 \ldots X^n|Y) = \prod_i P(X^i|Y)$$

- How many parameters now?
  - Suppose **X** is composed of *m* binary features



# The Naïve Bayes Classifier

- Given:
  - Prior P(Y)
  - *m* conditionally independent features **X** given the class Y
  - For each $X_n$, we have likelihood $P(X_n|Y)$
- Decision rule:

$$y^* = h_{NB}(\mathbf{x}) = \arg\max_y P(y)P(x^1,\ldots,x^m \mid y)$$
$$= \arg\max_y P(y)\prod_i P(x^i|y)$$

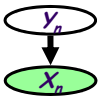
- If assumption holds, NB is optimal classifier!




# The A Gaussian Discriminative Naïve Bayes Classifier

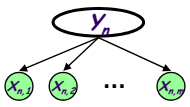
- When X is multivariate-Gaussian vector:
  - The joint probability of a datum and it label is:

$$p(\mathbf{x}_n, y_n^k = 1 \mid \vec{\mu}, \Sigma) = p(y_n^k = 1) \times p(\mathbf{x}_n \mid y_n^k = 1, \vec{\mu}, \Sigma)$$
$$= \pi_k \frac{1}{(2\pi|\Sigma|)^{1/2}} \exp\left\{-\tfrac{1}{2}(\mathbf{x}_n - \vec{\mu}_k)^T \Sigma^{-1}(\mathbf{x}_n - \vec{\mu}_k)\right\}$$




  - The naïve Bayes simplification

$$p(\mathbf{x}_n, y_n^k = 1 \mid \mu, \sigma) = p(y_n^k = 1) \times \prod_j p(x_n^j \mid y_n^k = 1, \mu_k^j, \sigma_k^j)$$
$$= \pi_k \prod_j \frac{1}{\sqrt{2\pi}\sigma_k^j} \exp\left\{-\tfrac{1}{2}\left(\frac{x_n^j - \mu_k^j}{\sigma_k^j}\right)^2\right\}$$




  - More generally: $p(\mathbf{x}_n, y_n \mid \eta, \pi) = p(y_n \mid \pi) \times \prod_{j=1}^{m} p(x_n^j \mid y_n, \eta)$
    - Where $p(. \mid .)$ is an arbitrary conditional (discrete or continuous) 1-D density

# The predictive distribution

- Understanding the predictive distribution

$$p(y_n^k = 1 \mid x_n, \vec{\mu}, \Sigma, \pi) = \frac{p(y_n^k = 1, x_n \mid \vec{\mu}, \Sigma, \pi)}{p(x_n \mid \vec{\mu}, \Sigma)} = \frac{\pi_k N(x_n, \mid \mu_k, \Sigma_k)}{\sum_{k'} \pi_{k'} N(x_n, \mid \mu_{k'}, \Sigma_{k'})} \quad *$$

- Under naïve Bayes assumption:

$$p(y_n^k = 1 \mid x_n, \vec{\mu}, \Sigma, \pi) = \frac{\pi_k \exp\left\{-\sum_j \left(\frac{1}{2}\left(\frac{x_n^j - \mu_k^j}{\sigma_k^j}\right)^2 - \log \sigma_k^j - C\right)\right\}}{\sum_{k'} \pi_{k'} \exp\left\{-\sum_j \left(\frac{1}{2}\left(\frac{x_n^j - \mu_{k'}^j}{\sigma_{k'}^j}\right)^2 - \log \sigma_{k'}^j - C\right)\right\}} \quad **$$

- For two class (i.e., *K*=2), and when the two classes haves the same variance, ** turns out to be a logistic function

$$p(y_n^1 = 1 \mid x_n) = \frac{1}{1 + \frac{\pi_2 \exp\left\{-\sum_j \left(\frac{1}{2\sigma_j^2}(x_n^j - \mu_2^j)^2 - \log \sigma_j - C\right)\right\}}{\pi_1 \exp\left\{-\sum_j \left(\frac{1}{2\sigma_j^2}(x_n^j - \mu_1^j)^2 - \log \sigma_j - C\right)\right\}}} = \frac{1}{1 + \exp\left\{-\sum_j \left(x_n^j \frac{1}{\sigma_j^2}(\mu_1^j - \mu_2^j) + \frac{1}{\sigma_j^2}([\mu_1^j]^2 - [\mu_2^j]^2)\right) + \log \frac{(1-\pi_1)}{\pi_1}\right\}}$$

$$= \frac{1}{1 + e^{-\theta^T x_n}}$$



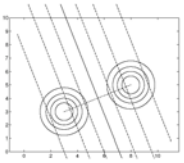
# The decision boundary

- The predictive distribution

$$p(y_n^1 = 1 \mid x_n) = \frac{1}{1 + \exp\left\{-\sum_{j=1}^{M} \theta_j x_n^j - \theta_0\right\}} = \frac{1}{1 + e^{-\theta^T x_n}}$$

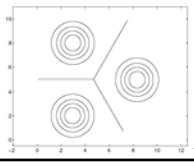
- The Bayes decision rule:

$$\ln \frac{p(y_n^1 = 1 \mid x_n)}{p(y_n^2 = 1 \mid x_n)} = \ln \left( \frac{\frac{1}{1 + e^{-\theta^T x_n}}}{\frac{e^{-\theta^T x_n}}{1 + e^{-\theta^T x_n}}} \right) = \theta^T x_n$$

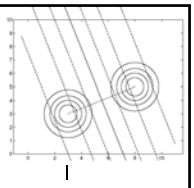


- For multiple class (i.e., *K*>2), * correspond to a softmax function

$$p(y_n^k = 1 \mid x_n) = \frac{e^{-\theta_k^T x_n}}{\sum_j e^{-\theta_j^T x_n}}$$



# Summary: The Naïve Bayes Algorithm



- Train Naïve Bayes (examples)
  - for each* value $y_k$
  - estimate $\pi_k \equiv P(Y = y_k)$
  - for each* value $x_{ij}$ of each attribute $X_i$
  - estimate $\theta_{ijk} \equiv P(X^i = x_{ij}|Y = y_k)$

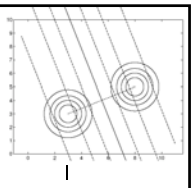
- Classify ($X_{new}$)

$$Y^{new} \leftarrow \arg\max_{y_k} P(Y = y_k) \prod_i P(X^i = x_{ij}|Y = y_k)$$

$$Y^{new} \leftarrow \arg\max_{y_k} \pi_k \prod_i \theta_{ijk}$$

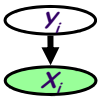


# Generative vs. Discriminative Classifiers

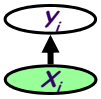


- Goal: Wish to learn f: X → Y, e.g., P(Y|X)

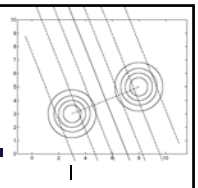
- Generative classifiers (e.g., Naïve Bayes):
  - Assume some functional form for P(X|Y), P(Y)
    This is a '***generative***' model of the data!
  - Estimate parameters of P(X|Y), P(Y) directly from training data
  - Use Bayes rule to calculate P(Y|X= x)




- Discriminative classifiers:
  - Directly assume some functional form for P(Y|X)
    This is a '***discriminative***' model of the data!
  - Estimate parameters of P(Y|X) directly from training data



# Logistic regression (sigmoid classifier)

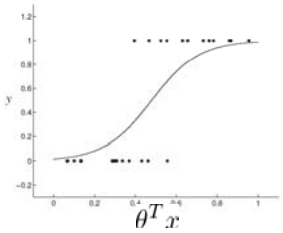


- The condition distribution: a Bernoulli

$$p(y \mid x) = \mu(x)^y (1-\mu(x))^{1-y}$$

where $\mu$ is a logistic function

$$\mu(x) = \frac{1}{1+e^{-\theta^T x}}$$




- We can used the brute-force gradient method as in LR

- But we can also apply generic laws by observing the $p(y|x)$ is an exponential family function, more specifically, a generalized linear model (see future lectures …)




# Training Logistic Regression: MCLE

- Estimate parameters $\theta$=<$\theta_0$, $\theta_1$, ... $\theta_m$> to maximize the **conditional likelihood** of training data

- Training data $\mathcal{D} = \{(x_1, y_1), \ldots, (x_N, y_N)\}$

- Data likelihood = $\prod_{i=1}^{N} P(x_i, y_i; \theta)$

- Data conditional likelihood = $\prod_{i=1}^{N} P(x_i|y_i; \theta)$

$$\theta = \arg\max_{\theta} \ln \prod_i P(y_i|x_i; \theta)$$

# Expressing Conditional Log Likelihood

$$l(\theta) \equiv \ln \prod_i P(y_i|x_i;\theta) = \sum_i \ln P(y_i|x_i;\theta)$$

- Recall the logistic function: $\mu = \frac{1}{1+e^{-\theta^T x}}$

  and conditional likelihood: $P(y|x) = \mu(x)^y (1-\mu(x))^{1-y}$

$$\begin{aligned} l(\theta) = \sum_i \ln P(y_i|x_i;\theta) &= \sum_i y_i \ln u(x_i) + (1-y_i)\ln(1-\mu(x_i)) \\ &= \sum_i y_i \ln \frac{u(x_i)}{1-\mu(x_i)} + \ln(1-\mu(x_i)) \\ &= \sum_i y_i \theta^T x_i - \theta^T x_i + \ln(1+e^{-\theta^T x_i}) \\ &= \sum (y_i - 1)\theta^T x_i + \ln(1+e^{-\theta^T x_i}) \end{aligned}$$




# Maximizing Conditional Log Likelihood

- The objective:

$$\begin{aligned} l(\theta) &= \ln \prod_i P(y_i|x_i;\theta) \\ &= \sum_i (y_i - 1)\theta^t x_i + \ln(1+e^{-\theta^T x_i}) \end{aligned}$$

- Good news: $l(\theta)$ is concave function of $\theta$
- Bad news: no closed-form solution to maximize $l(\theta)$

## Gradient Ascent

$$l(\theta) = \ln \prod_i P(y_i|x_i;\theta)$$
$$= \sum_i (y_i - 1)\theta^T x_i + \ln(1 + e^{-\theta^T x_i}) = \sum_i (y_i - 1)\theta^T x_i - \ln \mu(\theta^T x_i)$$

- Property of sigmoid function:

$$\mu = \frac{1}{1+e^{-t}} \qquad \frac{d\mu}{dt} = \mu(1-\mu)$$

- The gradient:

$$\frac{\partial l(\theta)}{\partial \theta_j} =$$

The gradient ascent algorithm iterate until change < ε

For all *i*, $\theta_j \leftarrow \theta_j + \eta \sum_i (y_i - P(y_i = 0|x_i;\theta))x_i^j$

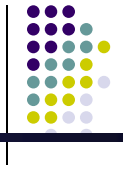
repeat

## The Newton's method

- Finding a zero of a function

$$\theta^{t+1} := \theta^t - \frac{f(\theta^t)}{f'(\theta^t)}$$

## The Newton's method (con'd)



- To maximize the conditional likelihood $l(\theta)$:

$$l(\theta) = \sum_i (y_i - 1)\theta^T x_i + \ln(1 + e^{-\theta^T x_i})$$

since $l$ is convex, we need to find $\theta^*$ where $l'(\theta^*)=0$ !

- So we can perform the following iteration:

$$\theta^{t+1} := \theta^t + \frac{l'(\theta^t)}{l''(\theta^t)}$$



## The Newton-Raphson method

- In LR the $\theta$ is vector-valued, thus we need the following generalization:

$$\theta^{t+1} := \theta^t + H^{-1}\nabla_{\theta^t} l(\theta^t)$$

- $\nabla$ is the gradient operator over the function

- H is known as the Hessian of the function

## The Newton-Raphson method

- In LR the $\theta$ is vector-valued, thus we need the following generalization:

$$\theta^{t+1} := \theta^t + H^{-1}\nabla_{\theta^t} l(\theta^t)$$

- $\nabla$ is the gradient operator over the function

$$\nabla_\theta l(\theta) = \sum_i (y_i - u_i)x_i = \mathbf{X}^T(\mathbf{y} - \mathbf{u})$$

- H is known as the Hessian of the function

$$H = \nabla_\theta \nabla_\theta l(\theta) = \sum_i u_i(1-u_i)x_i x_i^T = \mathbf{X}^T\mathbf{R}\mathbf{X}$$
$$\text{where} \quad R_{ii} = u_i(1-u_i)$$




## Iterative reweighed least squares (IRLS)

- Recall in the least square est. in linear regression, we have:

$$\theta = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

which can also derived from Newton-Raphson

- Now for logistic regression:

$$\begin{aligned}
\theta^{t+1} &= \theta^t + H^{-1}\nabla_{\theta^t} l(\theta^t) \\
&= \theta^t - (\mathbf{X}^T\mathbf{R}\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{u} - \mathbf{y}) \\
&= (\mathbf{X}^T\mathbf{R}\mathbf{X})^{-1}\{\mathbf{X}^T\mathbf{R}\mathbf{X}\theta^t - \mathbf{X}^T(\mathbf{u} - \mathbf{y})\} \\
&= (\mathbf{X}^T\mathbf{R}\mathbf{X})^{-1}\mathbf{X}^T\mathbf{R}\mathbf{z}
\end{aligned}$$

# IRLS

- Recall in the least square est. in linear regression, we have:

$$\theta = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

  which can also derived from Newton-Raphson

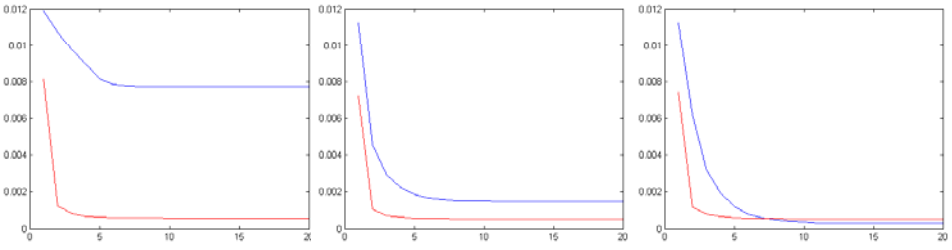
- Now for logistic regression:

$$\theta^{t+1} = (\mathbf{X}^T\mathbf{R}\mathbf{X})^{-1}\mathbf{X}^T\mathbf{R}\mathbf{z}$$

$$\text{where} \quad \mathbf{z} = \mathbf{X}\theta^t - \mathbf{R}^{-1}(\mathbf{u} - \mathbf{y})$$

$$\text{and} \quad R_{ii} = u_i(1 - u_i)$$

# Convergence curves



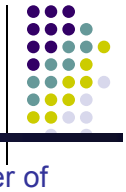
**alt.atheism** **vs.** **comp.graphics**

**rec.autos** **vs.** **rec.sport.baseball**

**comp.windows.x** **vs.** **rec.motorcycles**

**Legend:** **- X-axis: Iteration #; Y-axis: error**
**- In each figure, red for IRLS and blue for gradient descent**

# Logistic regression: practical issues

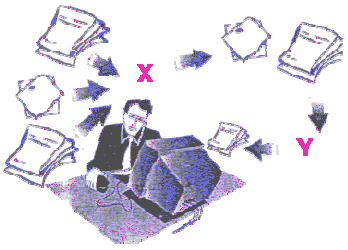


- NR (IRLS) takes $O(N+d^3)$ per iteration, where $N$ = number of training cases and $d$ = dimension of input $x$, but converge in fewer iterations
- Quasi-Newton methods, that approximate the Hessian, work faster.
- Conjugate gradient takes $O(Nd)$ per iteration, and usually works best in practice.
- Stochastic gradient descent can also be used if $N$ is large c.f. perceptron rule:




# Case Study: Text classification

- Classify e-mails
  - Y = {Spam,NotSpam}
- Classify news articles
  - Y = {what is the topic of the article?}
- Classify webpages
  - Y = {Student, professor, project, …}
- What about the features **X**?
  - The text!



## Features X are entire document – $X^i$ for $i^{th}$ word in article


| | |
|---|---|
| aardvark | 0 |
| about | 2 |
| all | 2 |
| Africa | 1 |
| apple | 0 |
| anxious | 0 |
| ... | |
| gas | 1 |
| ... | |
| oil | 1 |
| … | |
| Zaire | 0 |



## Bag of words model

- Typical additional assumption – **Position in document doesn't matter**: $P(X^i=x^i|Y=y) = P(X^k=x^i|Y=y)$
  - "Bag of words" model – order of words on the page ignored
  - Sounds really silly, but often works very well!

$$P(y)\prod_{i=1}^{LengthDoc} P(x^i|y) \quad \textbf{or} \quad P(y)\prod_{k=1}^{LengthVol} P(w^k|y)$$

**When the lecture is over, remember to wake up the person sitting next to you in the lecture room.**

# Bag of words model

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**in is lecture lecture next over person remember room sitting the the the to to up wake when you**



# NB with Bag of Words for text classification

- Learning phase:
  - Prior P(Y)
    - Count how many documents you have from each topic (+ prior)
  - $P(X^i|Y)$
    - For each topic, count how many times you saw word in documents of this topic (+ prior)
- Test phase:
  - For each document $\mathbf{x}_{new}$
    - Use naïve Bayes decision rule

$$h_{NB}(\mathbf{x}_{\text{new}}) = \arg\max_y P(y)\prod_{i=1}^{LengthDoc} P(x^i_{\text{new}}|y)$$

# Back to our 20 NG Case study

- Dataset
  - 20 News Groups (20 classes)
  - 61,118 words, 18,774 documents

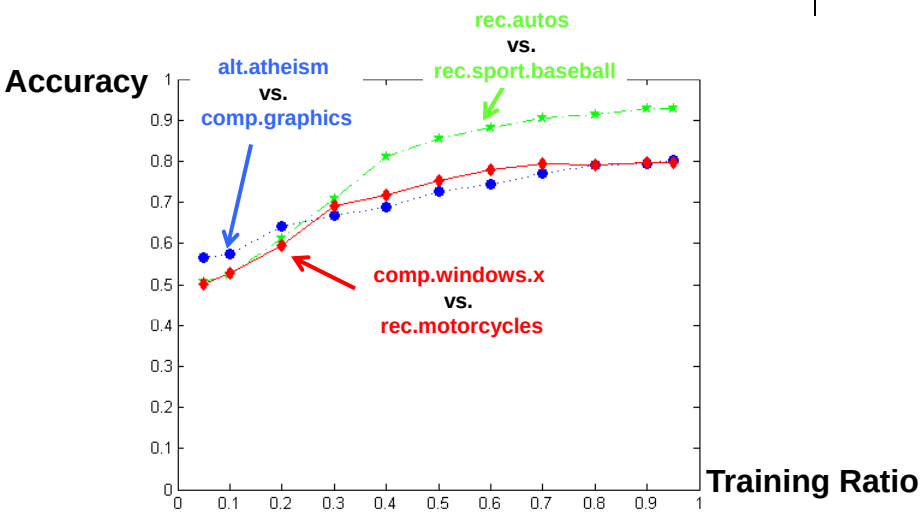
| | | |
|---|---|---|
| comp.graphics<br>comp.os.ms-windows.misc<br>comp.sys.ibm.pc.hardware<br>comp.sys.mac.hardware<br>comp.windows.x | rec.autos<br>rec.motorcycles<br>rec.sport.baseball<br>rec.sport.hockey | sci.crypt<br>sci.electronics<br>sci.med<br>sci.space |
| misc.forsale | talk.politics.misc<br>talk.politics.guns<br>talk.politics.mideast | talk.religion.misc<br>alt.atheism<br>soc.religion.christian |

- Experiment:
  - Solve only a two-class subset: 1 vs 2.
  - 1768 instances, 61188 features.
  - Use dimensionality reduction on the data (SVD).
  - Use 90% as training set, 10% as test set.
  - Test prediction error used as accuracy measure.

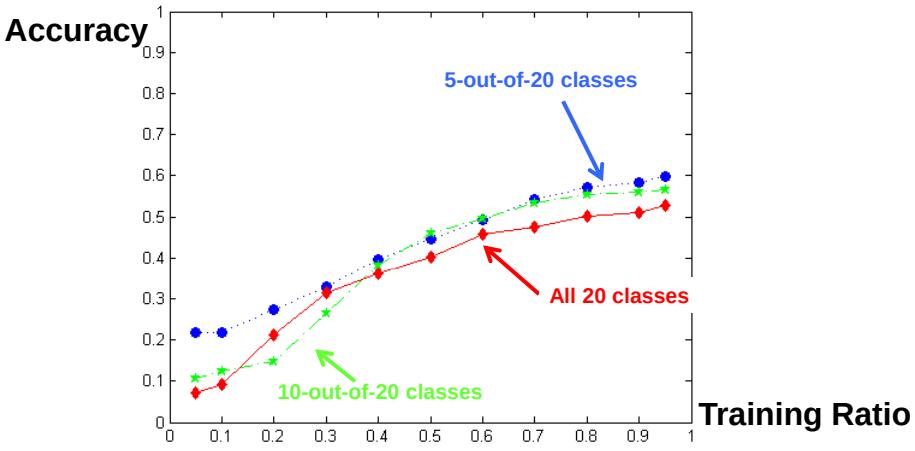
$$Accuracy = \frac{\sum_{\text{test set}} \mathrm{I}(predict_i = true\ label_i)}{\#\ of\ test\ samples}$$



# Results: Binary Classes



# Results: Multiple Classes

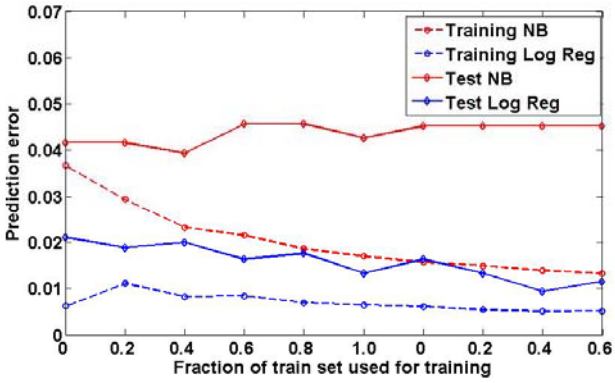






# NB vs. LR

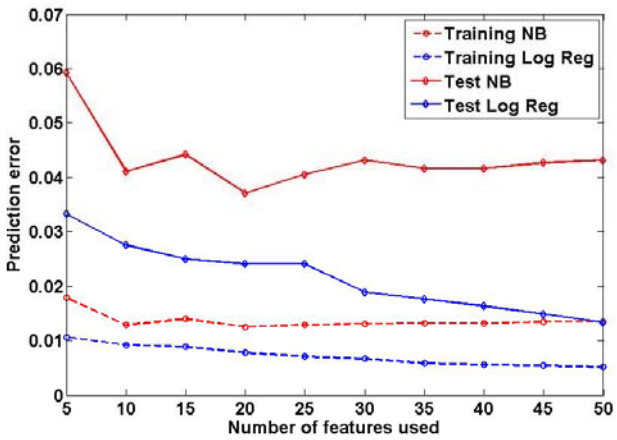
- Versus training size




- 30 features.
- A fixed test set
- Training set varied from 10% to 100% of the training set

# NB vs. LR

- Versus model size




**Number of dimensions of the data varied from 5 to 50 in steps of 5**

**The features were chosen in decreasing order of their singular values**

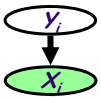
**90% versus 10% split on training and test**



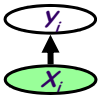

# Generative vs. Discriminative Classifiers

- Goal: Wish to learn f: X → Y, e.g., P(Y|X)

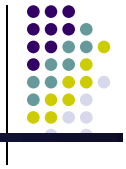
- Generative classifiers (e.g., Naïve Bayes):
  - Assume some functional form for P(X|Y), P(Y)
    This is a '***generative***' model of the data!
  - Estimate parameters of P(X|Y), P(Y) directly from training data
  - Use Bayes rule to calculate P(Y|X= x)




- Discriminative classifiers:
  - Directly assume some functional form for P(Y|X)
    This is a '***discriminative***' model of the data!
  - Estimate parameters of P(Y|X) directly from training data



# Naïve Bayes vs Logistic Regression



- Consider Y boolean, X continuous, X=<$X^1$ ... $X^m$>
- Number of parameters to estimate:

NB:

$$p(y \mid \mathbf{x}) = \frac{\pi_k \exp\left\{-\sum_j \left(\frac{1}{2\sigma_{k,j}^2}(x_j - \mu_{k,j})^2 - \log \sigma_{k,j} - C\right)\right\}}{\sum_{k'} \pi_{k'} \exp\left\{-\sum_j \left(\frac{1}{2\sigma_{k',j}^2}(x_j - \mu_{k',j})^2 - \log \sigma_{k',j} - C\right)\right\}} \quad **$$

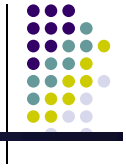
LR:

$$\mu(x) = \frac{1}{1 + e^{-\theta^T x}}$$

- Estimation method:
  - NB parameter estimates are uncoupled
  - LR parameter estimates are coupled




# Naïve Bayes vs Logistic Regression



- Asymptotic comparison (# training examples → infinity)
- when model assumptions correct
  - NB, LR produce identical classifiers
- when model assumptions incorrect
  - LR is less biased – does not assume conditional independence
  - therefore expected to outperform NB

# Naïve Bayes vs Logistic Regression

- Non-asymptotic analysis (see [Ng & Jordan, 2002] )
- convergence rate of parameter estimates – how many training examples needed to assure good estimates?

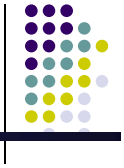
  NB order log m (where m = # of attributes in X)

  LR order m

- NB converges more quickly to its (perhaps less helpful) asymptotic estimates




# Rate of convergence: logistic regression



- Let $h_{Dis,m}$ be logistic regression trained on *n* examples in *m* dimensions. Then with high probability:

$$\epsilon(h_{Dis,n}) \leq \epsilon(h_{Dis,\infty}) + O\left(\sqrt{\frac{m}{n}\log\frac{n}{m}}\right)$$

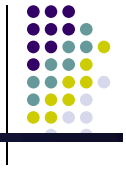
- Implication: if we want $\epsilon(h_{Dis,m}) \leq \epsilon(h_{Dis,\infty}) + \epsilon_0$

  for some small constant $\varepsilon_0$, it suffices to pick order *m* examples

  → Convergences to its asymptotic classifier, in order *m* examples

  - result follows from Vapnik's structural risk bound, plus fact that the "VC Dimension" of an *m*-dimensional linear separators is *m*

# Rate of convergence: naïve Bayes parameters



- Let any $\varepsilon_1$, $\delta$>0, and any $n \geq 0$ be fixed.
  Assume that for some fixed $\rho_0 > 0$,
  we have that $\rho_0 \leq p(y = T) \leq 1 - \rho_0$

- Let $n = O((1/\epsilon_1^2)\log(m/\delta))$

- Then with probability at least 1-$\delta$, after $n$ examples:

1. For discrete input, $|\hat{p}(x_i|y=b) - p(x_i|y=b)| \leq \epsilon_1$ and $|\hat{p}(y=b) - p(y=b)| \leq \epsilon_1$ for all $i$ and $b$
2. For continuous inputs, $|\hat{\mu}_{i|y=b} - \mu_{i|y=b}| \leq \epsilon_1$ and $|\hat{\sigma}^2_{i|y=b} - \sigma^2_{i|y=b}| \leq \epsilon_1$ for all $i$ and $b$



# Some experiments from UCI data sets

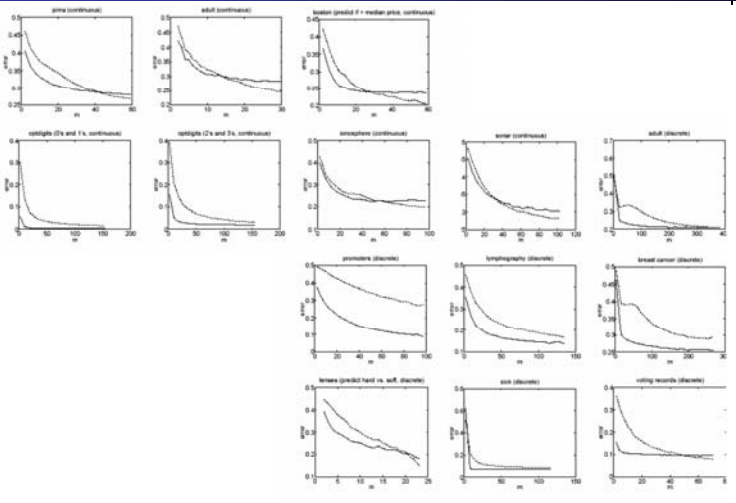
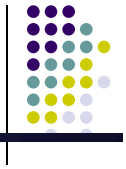


Figure 1: Results of 15 experiments on datasets from the UCI Machine Learning repository. Plots are of generalization error vs. $m$ (averaged over 1000 random train/test splits). Dashed line is logistic regression; solid line is naive Bayes.

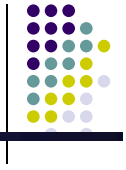
# Summary



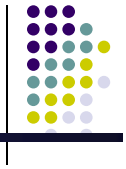
- Naïve Bayes classifier
  - What's the assumption
  - Why we use it
  - How do we learn it
- Logistic regression
  - Functional form follows from Naïve Bayes assumptions
  - For Gaussian Naïve Bayes assuming variance
  - For discrete-valued Naïve Bayes too
  - But training procedure picks parameters without the conditional independence assumption
- Gradient ascent/descent
  - – General approach when closed-form solutions unavailable
- Generative vs. Discriminative classifiers
  - – Bias vs. variance tradeoff




# Appendix



# Subtleties of NB classifier 1 – Violating the NB assumption



- Often the $X^i$ are not really conditionally independent

- We use Naïve Bayes in many cases anyway, and it often works pretty well
  - Often the right classification, even when not the right probability (see [Domingos&Pazzani, 1996])
  - But the resulting probabilities $P(Y|X_{new})$ are biased toward 1 or 0 (why?)

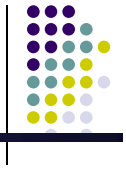



# Subtleties of NB classifier 2 – Insufficient training data

- What if you never see a training instance where $w^{1000}>0$ when Y=b?
  - e.g., Y={SpamEmail or not}, $w^{1:999} \equiv$ {'pill', 'enhancement', 'Rolex', 'enlarge' … }
  - P( enlargement>0 | Y=T) = 0
- Thus, no matter what the values $w_1,\ldots,w_n$/'enlargement' take:
  - $P(Y=T \mid w^1,w^2,\ldots,\text{enlargement}, \ldots, w^k) = 0$

- What now???

# Learning NB: parameter estimation



- Maximum Likelihood Estimate (MLE):
  choose $\theta$ that maximizes probability of observed data $\mathcal{D}$

$$\hat{\theta} = \arg\max_{\theta} P(\mathcal{D}|\theta)$$

- Maximum a Posteriori (MAP) estimate:
  choose $\theta$ that is most probable given prior probability and the data

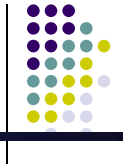
$$\begin{aligned}\hat{\theta} &= \arg\max_{\theta} p(\theta|\mathcal{D}) \\ &= \arg\max_{\theta} \frac{P(\mathcal{D}|\theta)p(\theta)}{P(\mathcal{D})}\end{aligned}$$

- Bayesian estimate:

$$\hat{\theta} = \int \theta p(\theta|\mathcal{D}) d\theta$$




# MAP for the parameters of NB



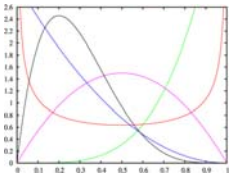
**Discrete features:**

- Maximum *a Posteriori* (MAP) estimate: (MAP's):

$$\hat{\theta} = \arg\max_{\theta} \frac{P(\mathcal{D}|\theta)\mathcal{P}(\theta)}{P(\mathcal{D})}$$

- Given prior:
  - Consider binary feature
  - $\theta$ is a *Bernoulli* rate

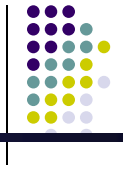
$$P(\theta;\alpha_T,\alpha_F) = \frac{\Gamma(\alpha_T+\alpha_F)}{\Gamma(\alpha_T)\Gamma(\alpha_F)}\theta^{\alpha_T-1}(1-\theta)^{\alpha_F-1} = \frac{\theta^{\alpha_T-1}(1-\theta)^{\alpha_F-1}}{B(\alpha_T,\alpha_F)}$$



  - Let $\beta_a$=Count(X=a) ← number of examples where X=a

$$P(\theta \mid \mathcal{D}) = \frac{\theta^{\beta_T+\alpha_T-1}(1-\theta)^{\beta_F+\alpha_F-1}}{B(\beta_T+\alpha_T,\beta_F+\alpha_F)} \sim Beta(\beta_H+\alpha_H,\beta_T+\alpha_T)$$

# Bayesian learning for NB parameters – a.k.a. smoothing



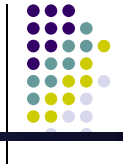
- **Posterior distribution of $\theta$**
  - Bernoulli: $P(\theta \mid \mathcal{D}) = \frac{\theta^{\beta_T+\alpha_T-1}(1-\theta)^{\beta_F+\alpha_F-1}}{B(\beta_T+\alpha_T,\beta_F+\alpha_F)} \sim Beta(\beta_H+\alpha_H,\beta_T+\alpha_T)$
  - Multinomial $P(\theta \mid \mathcal{D}) = \frac{\prod_{j=1}^{K}\theta_j^{\beta_j+\alpha_j-1}}{B(\beta_1+\alpha_1,\ldots,\beta_K+\alpha_K)} \sim Dirichlet(\beta_1+\alpha_1,\ldots,\beta_K+\alpha_K)$
- MAP estimate:

$$\hat{\theta} = \arg\max_{\theta} P(\theta|\mathcal{D}) =$$

  - Beta prior equivalent to extra thumbtack flips
  - As $N \rightarrow \infty$, prior is "forgotten"
  - **But, for small sample size, prior is important!**



# MAP for the parameters of NB



- Dataset of $N$ examples
  - Let $\beta_{iab}$=Count($X^i$=a,Y=b) ← number of examples where $X_i$=a and Y=b
  - Let $\gamma_b$=Count(Y=b)
- Prior

  Q($X^i$|Y) ∝ Multinomial($\alpha_{i1}$, …, $\alpha_{iK}$) or Multinomial($\alpha/K$)

  Q(Y) ∝ Multinomial($\tau_{i1}$, …, $\tau_{iM}$) or Multinomial($\tau/M$)

  $m$ "virtual" examples
- MAP estimate

$$\hat{\pi}_k = \arg\max_{\pi_k} \prod_k P(Y=y_k;\pi_k)P(\pi_k|\vec{\tau}) = ?$$

$$\hat{\theta}_{ijk} = \arg\max_{\theta_{ijk}} \prod_j P(X^i=x_{ij}|Y=y_k;\theta_{ijk})P(\theta_{ijk}|\vec{\alpha}_{ik}) = ?$$

  - Now, even if you never observe a feature/class, posterior probability never zero