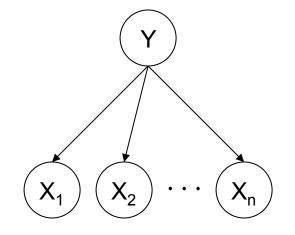
### Introduction to Bayesian methods (continued) - Lecture 17

David Sontag New York University

Slides adapted from Luke Zettlemoyer, Carlos Guestrin, Dan Klein, and Vibhav Gogate

# The Naïve Bayes Classifier

- Given:
  - Prior P(Y)
  - *n* conditionally independent features **X** given the class Y
  - For each X<sub>i</sub>, we have likelihood P(X<sub>i</sub>|Y)

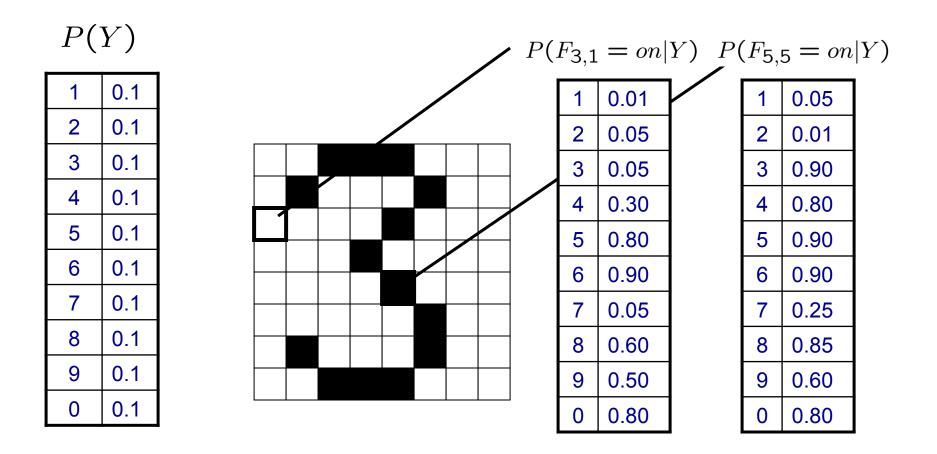


• Decision rule:

$$y^* = h_{NB}(\mathbf{x}) = \arg \max_{y} P(y) P(x_1, \dots, x_n \mid y)$$
$$= \arg \max_{y} P(y) \prod_{i} P(x_i \mid y)$$

If certain assumption holds, NB is optimal classifier! (they typically don't)

## What has to be learned?



## MLE for the parameters of NB

- Given dataset
  - − Count(A=a,B=b) ← number of examples where A=a and B=b
- MLE for discrete NB, simply:
  - Prior:

$$P(Y = y) = \frac{Count(Y = y)}{\sum_{y'} Count(Y = y')}$$

– Observation distribution:

$$P(X_i = x | Y = y) = \frac{Count(X_i = x, Y = y)}{\sum_{x'} Count(X_i = x', Y = y)}$$

## What about if there is missing data?

- One of the key strengths of Bayesian approaches is that they can naturally handle missing data
- Suppose don't have value for some attribute  $X_i$ 
  - applicant's credit history unknown
  - some medical test not performed on patient
  - how to compute  $P(X_1 = x_1 ... X_j = ? ... X_d = x_d | y)$
- Easy with Naïve Bayes
  - ignore attribute in instance where its value is missing

$$P(x_1...X_j...x_d|y) = \prod_{i \neq j}^d P(x_i|y)$$

- compute likelihood based on observed attributes
- no need to "fill in" or explicitly model missing values
- based on conditional independence between attributes

[Slide from Victor Lavrenko and Nigel Goddard]

## What about if there is missing data?

 $X_2 = H$ 

 $X_{3}=T$ 

 $X_1 = H$ 

- Ex: three coin tosses: Event = { $X_1$ =H,  $X_2$ =?,  $X_3$ =T}
  - event = head, unknown (either head or tail), tail
  - event =  $\{H,H,T\}$  +  $\{H,T,T\}$
  - P(event) = P(H,H,T) + P(H,T,T)
- $X_{p}=T$  General case: X<sub>i</sub> has missing value  $P(x_1...x_j...x_d|y) = P(x_1|y) \cdots P(x_j|y) \cdots P(x_d|y)$  $\sum_{\mathbf{x}_i} P(\mathbf{x}_1 \dots \mathbf{x}_j \dots \mathbf{x}_d | \mathbf{y}) = \sum_{\mathbf{x}_i} P(\mathbf{x}_1 | \mathbf{y}) \cdots P(\mathbf{x}_j | \mathbf{y}) \cdots P(\mathbf{x}_d | \mathbf{y})$  $= P(x_1|y) \cdots \left[ \sum_{x_i} P(x_j|y) \right] \cdots P(x_d|y)$  $= P(x_1|y)\cdots |1|\cdots P(x_d|y)$

[Slide from Victor Lavrenko and Nigel Goddard]

# Naive Bayes = Linear Classifier

Theorem: assume that  $x_i \in \{0, 1\}$  for all  $i \in [1, N]$ . Then, the Naive Bayes classifier is defined by

 $\mathbf{x} \mapsto \operatorname{sgn}(\mathbf{w} \cdot \mathbf{x} + b),$ 

[Slide from Mehyrar Mohri]

# **Outline of lectures**

- Review of probability
- Maximum likelihood estimation
- 2 examples of Bayesian classifiers:
- Naïve Bayes
- Logistic regression

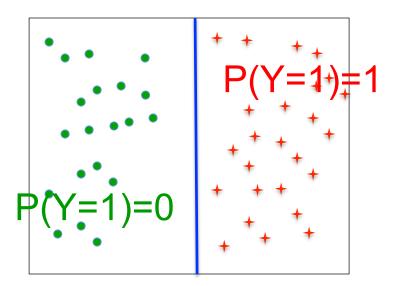
[Next several slides adapted from:

Vibhav Gogate, Luke Zettlemoyer, Carlos Guestrin, and Dan Weld]

# Logistic Regression

#### Learn P(Y|X) directly!

- □ Assume a particular functional form
- ★ Linear classifier? On one side we say P(Y=1|X)=1, and on the other P(Y=1|X)=0
- ★ But, this is not differentiable (hard to learn)... doesn't allow for label noise...

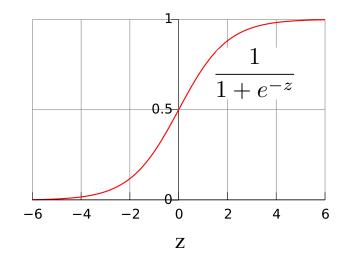


# Logistic Regression

#### Learn P(Y|X) directly!

- Assume a particular functional form
- Sigmoid applied to a linear function of the data:

#### Logistic function (Sigmoid):

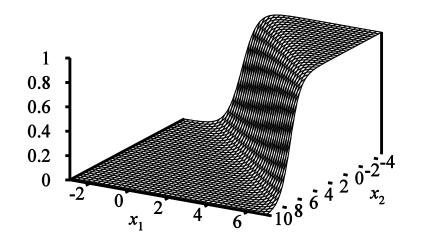


$$P(Y = 1|X) = \frac{1}{1 + \exp(w_0 + \sum_{i=1}^n w_i X_i)}$$
$$P(Y = 0|X) = \frac{\exp(w_0 + \sum_{i=1}^n w_i X_i)}{1 + \exp(w_0 + \sum_{i=1}^n w_i X_i)}$$

Features can be discrete or continuous!

# Logistic Function in n Dimensions $P(Y = 1|X) = \frac{1}{1 + \exp(w_0 + \sum_{i=1}^{n} w_i X_i)}$

Sigmoid applied to a linear function of the data:



#### Features can be discrete or continuous!

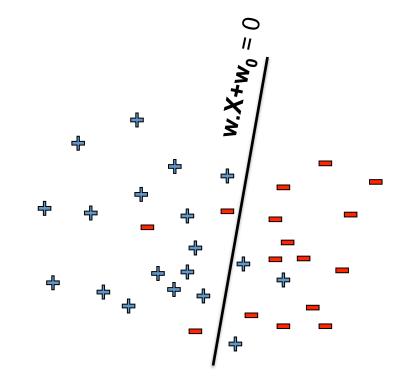
#### Logistic Regression: decision boundary

$$P(Y = 1|X) = \frac{1}{1 + \exp(w_0 + \sum_{i=1}^n w_i X_i)} \quad P(Y = 0|X) = \frac{\exp(w_0 + \sum_{i=1}^n w_i X_i)}{1 + \exp(w_0 + \sum_{i=1}^n w_i X_i)}$$

- Prediction: Output the Y with highest P(Y|X)
  - For binary Y, output Y=0 if

$$1 < \frac{P(Y = 0|X)}{P(Y = 1|X)}$$
$$1 < \exp(w_0 + \sum_{i=1}^{n} w_i X_i)$$
$$0 < w_0 + \sum_{i=1}^{n} w_i X_i$$

A Linear Classifier!



## Likelihood vs. Conditional Likelihood

Generative (Naïve Bayes) maximizes Data likelihood

$$n P(\mathcal{D} | \mathbf{w}) = \sum_{j=1}^{N} \ln P(\mathbf{x}^{j}, y^{j} | \mathbf{w})$$
$$= \sum_{j=1}^{N} \ln P(y^{j} | \mathbf{x}^{j}, \mathbf{w}) + \sum_{j=1}^{N} \ln P(\mathbf{x}^{j} | \mathbf{w})$$

Discriminative (Logistic Regr.) maximizes Conditional Data Likelihood

$$\ln P(\mathcal{D}_Y \mid \mathcal{D}_X, \mathbf{w}) = \sum_{j=1}^N \ln P(y^j \mid \mathbf{x}^j, \mathbf{w})$$

Focuses only on learning P(Y|X) - all that matters for classification

## Maximizing Conditional Log Likelihood

$$P(Y = 0|X, W) = \frac{1}{1 + exp(w_0 + \sum_i w_i X_i)}$$

$$P(Y = 1|X, W) = \frac{exp(w_0 + \sum_i w_i X_i)}{1 + exp(w_0 + \sum_i w_i X_i)}$$

$$= \sum_j y^j(w_0 + \sum_i^n w_i x_i^j) - \ln(1 + exp(w_0 + \sum_i^n w_i x_i^j))$$
**0 or 1!**

Bad news: no closed-form solution to maximize *l*(w)

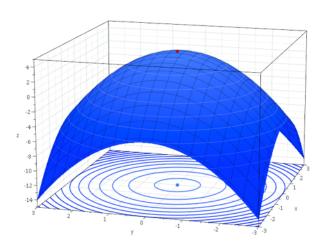
Good news:  $l(\mathbf{w})$  is concave function of  $\mathbf{w} \rightarrow$ 

No local maxima

Concave functions easy to optimize

# Optimizing concave function – Gradient ascent

- Conditional likelihood for Logistic Regression is concave ightarrow



Gradient: 
$$\nabla_{\mathbf{w}} l(\mathbf{w}) = \left[\frac{\partial l(\mathbf{w})}{\partial w_0}, \dots, \frac{\partial l(\mathbf{w})}{\partial w_n}\right]'$$
  
Learning rate,  $\eta > 0$   
Update rule:  $\Delta \mathbf{w} = \eta \nabla_{\mathbf{w}} l(\mathbf{w})$   
 $w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta \frac{\partial l(\mathbf{w})}{\partial w_i}$ 

#### Maximize Conditional Log Likelihood: Gradient ascent

$$P(Y = 1|X, W) = \frac{exp(w_0 + \sum_i w_i X_i)}{1 + exp(w_0 + \sum_i w_i X_i)}$$

$$P(Y = 1|X, W) = \frac{exp(w_0 + \sum_i w_i X_i)}{1 + exp(w_0 + \sum_i w_i X_i)}$$

$$\frac{\partial l(w)}{\partial w_i} = \sum_j \left[ \frac{\partial}{\partial w_i} y^j(w_0 + \sum_i w_i x_i^j) - \frac{\partial}{\partial w_i} \ln \left( 1 + \exp(w_0 + \sum_i w_i x_i^j) \right) \right]$$

$$= \sum_j \left[ y^j x_i^j - \frac{x_i^j \exp(w_0 + \sum_i w_i x_i^j)}{1 + \exp(w_0 + \sum_i w_i x_i^j)} \right]$$

$$= \sum_j x_i^j \left[ y^j - \frac{\exp(w_0 + \sum_i w_i x_i^j)}{1 + \exp(w_0 + \sum_i w_i x_i^j)} \right]$$

$$\frac{\partial l(w)}{\partial w_i} = \sum_j x_i^j \left( y^j - P(Y^j = 1|x^j, w) \right)$$

## **Gradient Ascent for LR**

Gradient ascent algorithm: (learning rate  $\eta > 0$ ) do:

$$w_0^{(t+1)} \leftarrow w_0^{(t)} + \eta \sum_j [y^j - \hat{P}(Y^j = 1 \mid \mathbf{x}^j, \mathbf{w})]$$

For i=1 to n: (iterate over features)

$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta \sum_j x_i^j [y^j - \hat{P}(Y^j = 1 \mid \mathbf{x}^j, \mathbf{w})]$$
  
until "change" <  $\varepsilon$   
Loop over training examples  
(could also do stochastic GD)

# That's all MLE. How about MAP? $p(\mathbf{w} | Y, \mathbf{X}) \propto P(Y | \mathbf{X}, \mathbf{w})p(\mathbf{w})$

- One common approach is to define priors on w
  - Normal distribution, zero mean, identity covariance
  - "Pushes" parameters towards zero

 $p(\mathbf{w}) = \prod_{i} \frac{1}{\kappa \sqrt{2\pi}} e^{\frac{-w_i^2}{2\kappa^2}}$ 

- Regularization
  - Helps avoid very large weights and overfitting
- MAP estimate:

$$\mathbf{w}^* = \arg \max_{\mathbf{w}} \ln \left[ p(\mathbf{w}) \prod_{j=1}^N P(y^j | \mathbf{x}^j, \mathbf{w}) \right]$$

## MAP as Regularization

$$\mathbf{w}^* = \arg\max_{\mathbf{w}} \ln \left[ p(\mathbf{w}) \prod_{j=1}^N P(y^j \mid \mathbf{x}^j, \mathbf{w}) \right] \quad p(\mathbf{w}) = \prod_i \frac{1}{\kappa \sqrt{2\pi}} e^{\frac{-w_i^2}{2\kappa^2}}$$

 $\mathbf{c}$ 

• Adds log p(w) to objective:

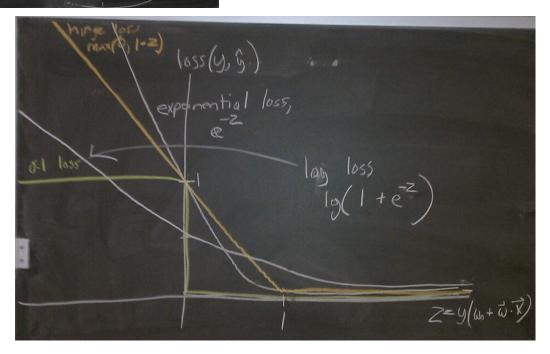
$$\ln p(w) \propto -\frac{\lambda}{2} \sum_{i} w_i^2 \qquad \frac{\partial \ln p(w)}{\partial w_i} = -\lambda w_i$$

- Quadratic penalty: drives weights towards zero
- Adds a negative linear term to the gradients

#### Quadratic penalty on weights, just like with SVMs!

MAP estimation of LR: yie {+1,-12  $\max_{i=1}^{N} \frac{1}{9} \left( \frac{1}{1+e^{-\frac{1}{9}(\omega \cdot x_{i})}} - \frac{1}{9} \| \overline{w} \|^{2} \right)$  $\begin{array}{c} n_{in} \\ \overrightarrow{c_{i}} \\ \overrightarrow{c_{i}}$ 

 $l(D; \vec{\omega}) = \underset{i=1}{\overset{\text{log}}{=}} \log \left( \frac{1 + e^{-y_i(w_0 + \vec{\omega} \cdot \vec{x}_i)}}{1 + e^{-y_i(w_0 + \vec{\omega} \cdot \vec{x}_i)}} + \frac{svm}{\vec{\omega}} \frac{svm}{i=1} \right) + \frac{svm}{\vec{\omega}} \frac{svm}{i=1}$ hinge loss  $\min_{\omega} \frac{1}{2} \sum_{i=1}^{N} L(y_i, \hat{y}(\vec{x}_i, \vec{\omega})) + \mathcal{R}(\vec{\omega})$ Learning:



## Naïve Bayes vs. Logistic Regression

**Learning**:  $h: X \mapsto Y$ 

X – features

Y – target classes

#### Generative

- Assume functional form for
  - P(X|Y) assume cond indepP(Y)
  - Est. params from train data
- Gaussian NB for cont. features
- Bayes rule to calc. P(Y | X = x):
   P(Y | X) ∝ P(X | Y) P(Y)
- Indirect computation
  - Can generate a sample of the data
  - Can easily handle missing data

#### Discriminative

- Assume functional form for
   P(Y|X) no assumptions
  - Est params from training data
- Handles discrete & cont features

Directly calculate P(Y|X=x)
 — Can't generate data sample

#### Naïve Bayes vs. Logistic Regression

[Ng & Jordan, 2002]

- Generative vs. Discriminative classifiers
- Asymptotic comparison
   (# training examples → infinity)
  - when model correct
    - NB, Linear Discriminant Analysis (with class independent variances), and Logistic Regression produce identical classifiers
  - when model incorrect
    - LR is less biased does not assume conditional independence

- therefore LR expected to outperform NB

#### Naïve Bayes vs. Logistic Regression

[Ng & Jordan, 2002]

- Generative vs. Discriminative classifiers
- Non-asymptotic analysis
  - convergence rate of parameter estimates,
     (n = # of attributes in X)
    - Size of training data to get close to infinite data solution
    - Naïve Bayes needs O(log n) samples
    - Logistic Regression needs O(n) samples
  - Naïve Bayes converges more quickly to its (perhaps less helpful) asymptotic estimates

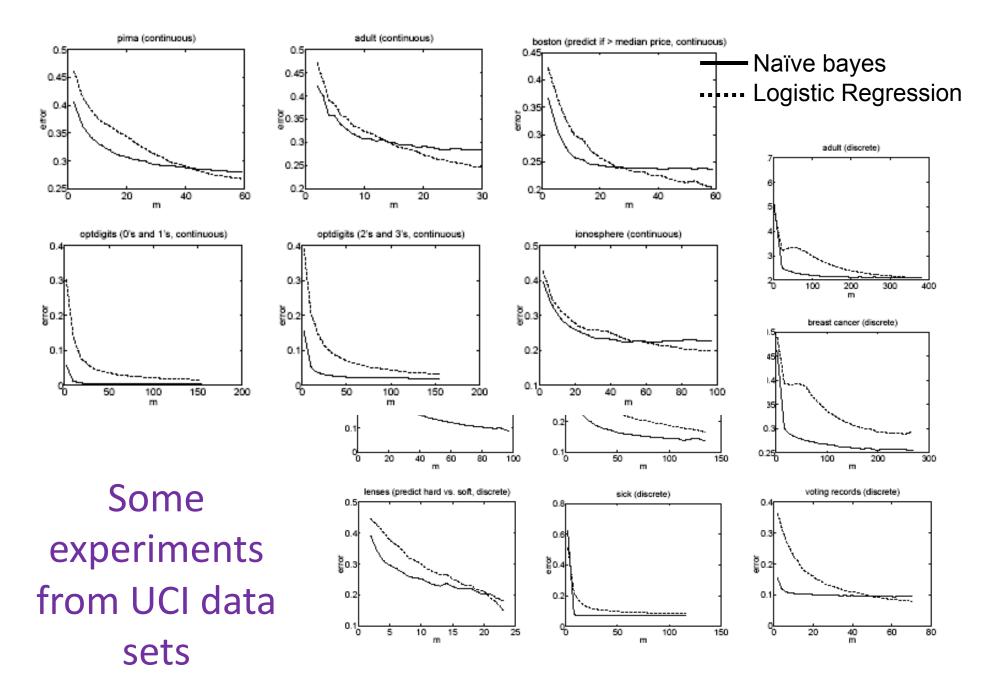


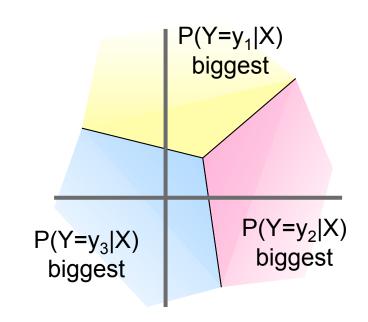
Figure 1: Results of 15 experiments on datasets from the UCI Machine Learning repository. Plots are of generalization error vs. m (averaged over 1000 random train/test splits). Dashed line is logistic regression; solid line is naive Bayes.

# Logistic regression for discrete classification

Logistic regression in more general case, where set of possible Y is  $\{y_1, ..., y_R\}$ 

• Define a weight vector  $w_i$  for each  $y_i$ , i=1,...,R

$$P(Y = 1|X) \propto \exp(w_{10} + \sum_{i} w_{1i}X_i)$$
$$P(Y = 2|X) \propto \exp(w_{20} + \sum_{i} w_{2i}X_i)$$



Also called "soft-max" loss