

Logistic Regression, Generative and Discriminative Classifiers

Recommended reading:

- Ng and Jordan paper “On Discriminative vs. Generative classifiers: A comparison of logistic regression and naïve Bayes,” A. Ng and M. Jordan, NIPS 2002.

Machine Learning 10-701

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Thanks to Ziv Bar-Joseph, Andrew Moore for some slides

Overview

Last lecture:

- Naïve Bayes classifier
- Number of parameters to estimate
- Conditional independence

This lecture:

- Logistic regression
- Generative and discriminative classifiers
- (if time) Bias and variance in learning

Naive Bayes Algorithm

Naive_Bayes_Learn(*examples*)

For each target value v_j

$$\hat{P}(v_j) \leftarrow \text{estimate } P(v_j)$$

For each attribute value a_i of each attribute a

$$\hat{P}(a_i|v_j) \leftarrow \text{estimate } P(a_i|v_j)$$

Classify_New_Instance(x)

$$v_{NB} = \operatorname{argmax}_{v_j \in V} \hat{P}(v_j) \prod_{a_i \in x} \hat{P}(a_i|v_j)$$

Generative vs. Discriminative Classifiers

Training classifiers involves estimating $f: X \rightarrow Y$, or $P(Y|X)$

Generative classifiers:

- Assume some functional form for $P(X|Y)$, $P(X)$
- Estimate parameters of $P(X|Y)$, $P(X)$ directly from training data
- Use Bayes rule to calculate $P(Y|X= x_i)$

Discriminative classifiers:

1. Assume some functional form for $P(Y|X)$
2. Estimate parameters of $P(Y|X)$ directly from training data

- Consider learning $f: X \rightarrow Y$, where
 - X is a vector of real-valued features, $\langle X_1 \dots X_n \rangle$
 - Y is boolean
- So we use a Gaussian Naïve Bayes classifier
 - assume all X_i are conditionally independent given Y
 - model $P(X_i | Y = y_k)$ as Gaussian $N(\mu_{ik}, \sigma)$
 - model $P(Y)$ as binomial (p)
- What does that imply about the form of $P(Y|X)$?

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- What does that imply about the form of $P(Y|X)$?

$$P(Y = 1 | X = \langle x_1, \dots, x_n \rangle) = \frac{1}{1 + \exp(w_0 + \sum_i w_i x_i)}$$

Logistic regression

- Logistic regression represents the probability of category i using a linear function of the input variables:

$$P(Y=i | X=x) = g(w_{i0} + w_{i1}x_1 + \dots + w_{id}x_d)$$

where for $i < k$

$$g(z_i) = \frac{e^{z_i}}{1 + \sum_{j=1}^{K-1} e^{z_j}}$$

and for k

$$g(z_k) = \frac{1}{1 + \sum_{j=1}^{K-1} e^{z_j}}$$

Logistic regression

- The name comes from the **logit** transformation:

$$\log \frac{p(Y = i | X = x)}{p(Y = K | X = x)} = \log \frac{g(z_i)}{g(z_k)} = w_0 + w_{i1}x_1 + \dots + w_{id}x_d$$

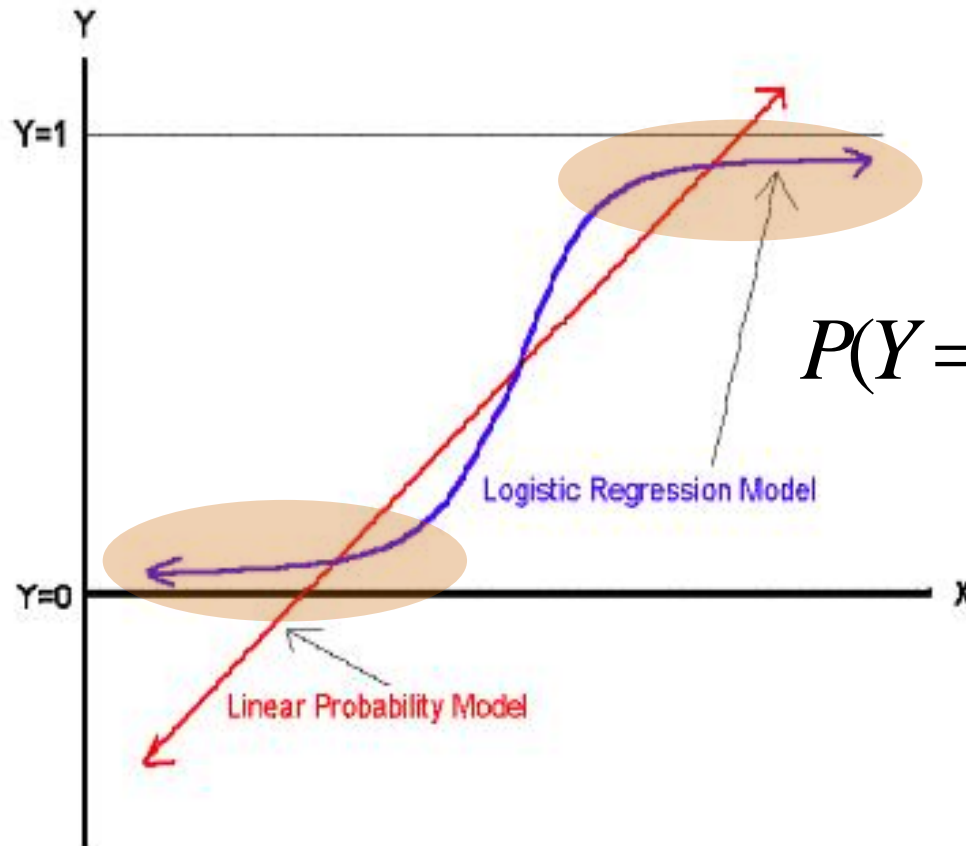
Binary logistic regression

- We only need one set of parameters

$$\begin{aligned} p(Y=1|X=x) &= \frac{e^{w_0+w_1x_1+\dots+w_dx_d}}{1+e^{w_0+w_1x_1+\dots+w_dx_d}} \\ &= \frac{1}{1+e^{-(w_0+w_1x_1+\dots+w_dx_d)}} \\ &= \frac{1}{1+e^{-z}} \end{aligned}$$

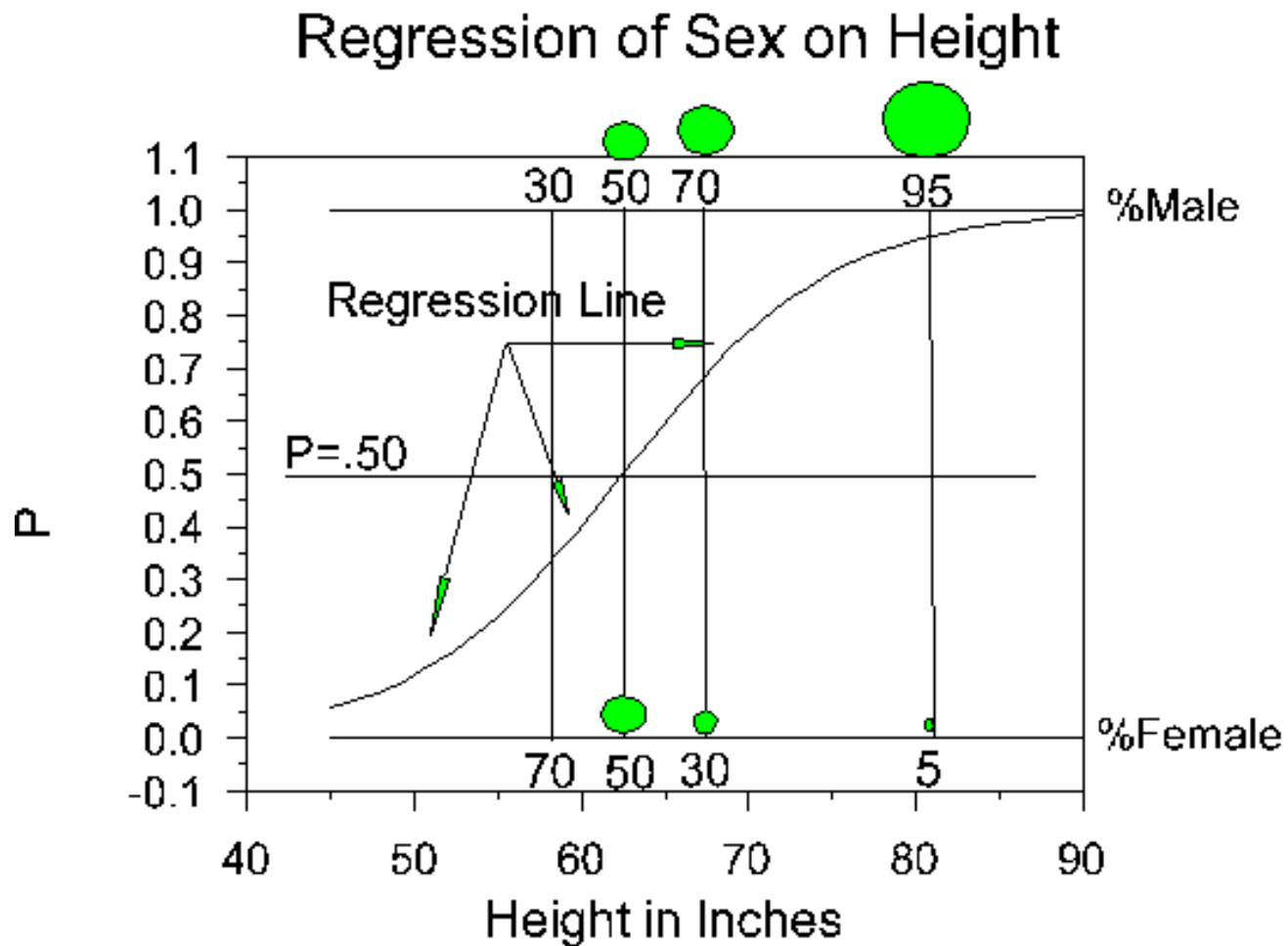
- This results in a “squashing function” which turns linear predictions into probabilities

Logistic regression vs. Linear regression



$$P(Y=1 | X=x) = \frac{1}{1+e^{-z}}$$

Example



Log likelihood

$$l(w) = \sum_{i=1}^N y_i \log p(x_i; w) + (1 - y_i) \log(1 - p(x_i; w))$$

Log likelihood

$$\begin{aligned}l(w) &= \sum_{i=1}^N y_i \log p(x_i; w) + (1 - y_i) \log(1 - p(x_i; w)) \\&= \sum_{i=1}^N y_i \log \frac{p(x_i; w)}{(1 - p(x_i; w))} + \log\left(\frac{1}{1 + e^{x_i w}}\right) \\&= \sum_{i=1}^N y_i x_i w - \log(1 + e^{x_i w})\end{aligned}$$

- Note: this likelihood is a concave in w

Maximum likelihood estimation

$$\frac{\partial}{\partial w_j} l(w) = \frac{\partial}{\partial w_j} \sum_{i=1}^N \{y_i x_{ij} w - \log(1 + e^{x_i w})\}$$

= ...

$$= \sum_{i=1}^N x_{ij} (y_i - p(x_i, w))$$


prediction error

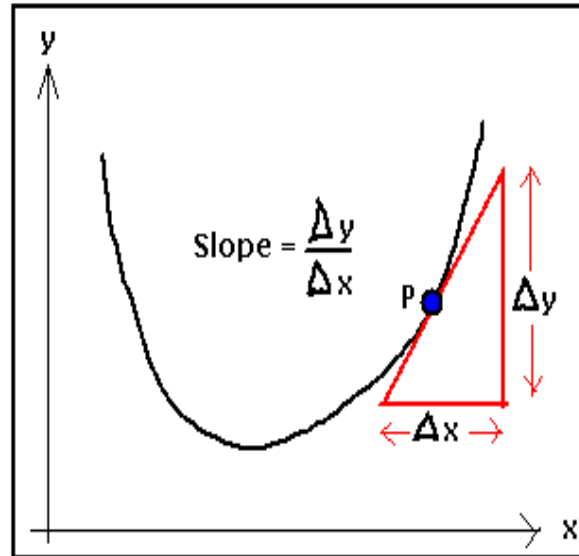
No close form solution!

Common (but not only) approaches:

Numerical Solutions:

- Line Search
- Simulated Annealing
- Gradient Descent
- Newton's Method
- Matlab glmfit function

Gradient descent



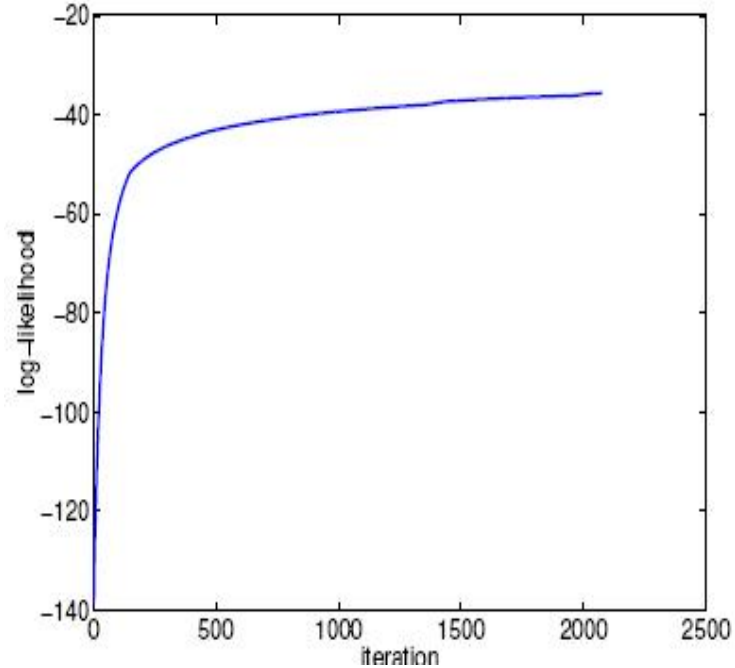
Gradient ascent

$$w_j^{t+1} \leftarrow w_j^t + \varepsilon \sum_i (x_{ij} (y_i - p(x_i, w)))$$

- Iteratively updating the weights in this fashion increases likelihood each round.
- We eventually reach the maximum
- We are near the maximum when changes in the weights are small.
- Thus, we can stop when the sum of the absolute values of the weight differences is less than some small number.

Example

- We get a monotonically increasing log likelihood of the training labels as a function of the iterations

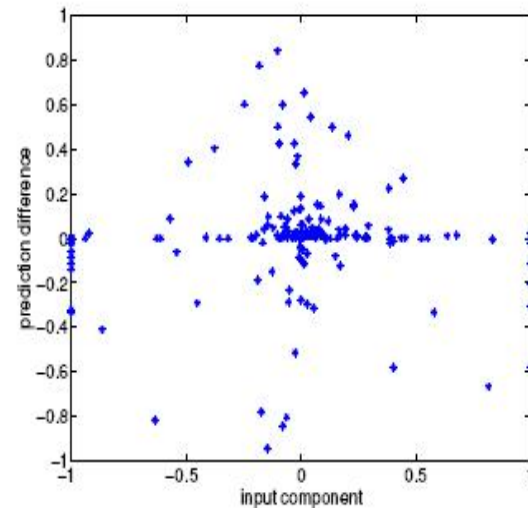


Convergence

- The gradient ascent learning method converges when there is no incentive to move the parameters in any particular direction:

$$\sum_i (x_{ij}(y_i - p(x_i, w))) = 0 \quad \forall k$$

- This condition means that the prediction error is uncorrelated with the components of the input vector



Naïve Bayes vs. Logistic Regression

[Ng & Jordan, 2002]

- Generative and Discriminative classifiers
- Asymptotic comparison (# training examples \rightarrow infinity)
 - when model correct
 - when model incorrect
- Non-asymptotic analysis
 - convergence rate of parameter estimates
 - convergence rate of expected error
- Experimental results

Generative-Discriminative Pairs

Example: assume Y boolean, $X = \langle X_1, X_2, \dots, X_n \rangle$, where x_i are boolean, perhaps dependent on Y , conditionally independent given Y

Generative model: naïve Bayes:

$$\hat{p}(x_i = 1 | y = b) = \frac{s\{x_i = 1, y = b\} + l}{s\{y = b\} + 2l}$$

$$\hat{p}(y = b) = \frac{s\{y = b\}}{\sum_j s\{y = j\}}$$

s indicates size of set.

l is smoothing parameter

Classify new example x based on ratio

$$\frac{\hat{p}(y = T | x)}{\hat{p}(y = F | x)} = \frac{\hat{p}(y = T) \prod_{i=1}^n \hat{p}(x_i | y = T)}{\hat{p}(y = F) \prod_{i=1}^n \hat{p}(x_i | y = F)}$$

Equivalently, based on sign of log of this ratio

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Discriminative model: logistic regression

$$\hat{p}(y = T | x; \beta, \theta) = 1 / (1 + \exp(-\sum_{i=1}^n \beta_i x_i - \theta))$$

Note both learn linear decision surface over X in this case

What is the difference asymptotically?

Notation: let $\epsilon(h_{A,m})$ denote error of hypothesis learned via algorithm A, from m examples

- If assumed model correct (e.g., naïve Bayes model), and finite number of parameters, then

$$\epsilon(h_{Dis,\infty}) = \epsilon(h_{Gen,\infty})$$

- If assumed model incorrect

$$\epsilon(h_{Dis,\infty}) \leq \epsilon(h_{Gen,\infty})$$

Note assumed discriminative model can be correct even when generative model incorrect, but not vice versa

Rate of convergence: logistic regression

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

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

Implication: if we want $\epsilon(h_{Dis,m}) \leq \epsilon(h_{Dis,\infty}) + \epsilon_0$ for some constant ϵ_0 , it suffices to pick $m = \Omega(n)$

→ Converges to its classifier, in order of n examples

(result follows from Vapnik's structural risk bound, plus fact that VCDim of n dimensional linear separators is n)

Rate of convergence: naïve Bayes

Consider first how quickly parameter estimates converge toward their asymptotic values.

Then we'll ask how this influences rate of convergence toward asymptotic classification error.

Rate of convergence: naïve Bayes parameters

Let any $\epsilon_1, \delta > 0$ and any $l \geq 0$ be fixed. Assume that for some fixed $\rho_0 > 0$, we have that $\rho_0 \leq p(y = T) \leq 1 - \rho_0$. Let $m = O((1/\epsilon_1^2) \log(n/\delta))$. Then with probability at least $1 - \delta$, after m examples:

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

Some experiments from UCI data sets

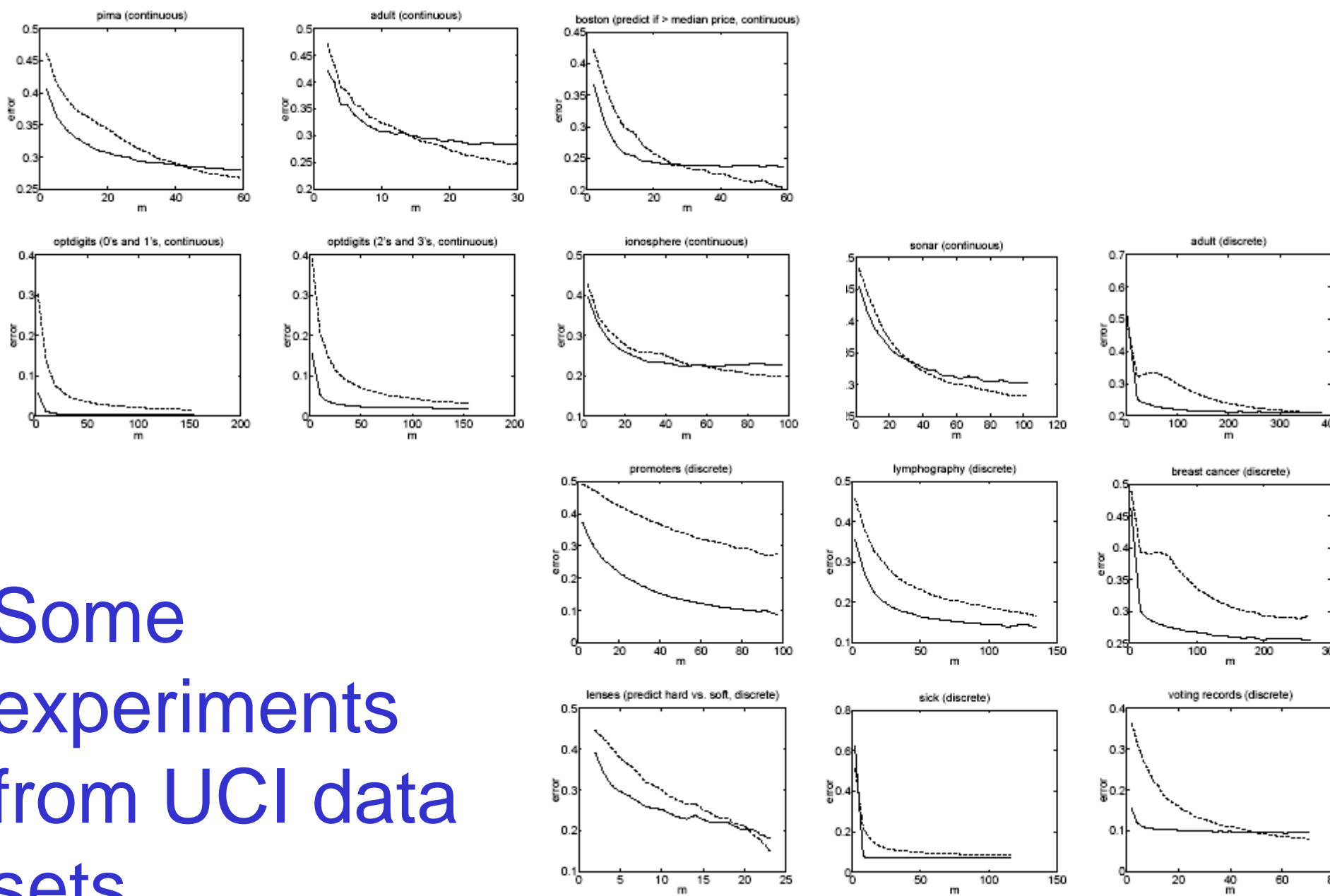


Figure 1: Results of 15 experiments on datasets from the UCI Machine Learning repository. Plots are of generalization error vs. m (averaged over 1000 random train/test splits). Dashed line is logistic regression; solid line is naive Bayes.

What you should know:

- Logistic regression
 - What it is
 - How to solve it
 - Log linear models
- Generative and Discriminative classifiers
 - Relation between Naïve Bayes and logistic regression
 - Which do we prefer, when?
- Bias and variance in learning algorithms

Acknowledgment

Some of these slides are based in part on slides from previous machine learning classes taught by Ziv Bar-Joseph, Andrew Moore at CMU, and by Tommi Jaakkola at MIT.

I thank them for providing use of their slides.