Machine Learning 10-601

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Today:
- Logistic regression
- Generative/Discriminative classifiers

Readings: (see class website)

Required:
- Mitchell: "Naïve Bayes and Logistic Regression"

Optional
- Ng & Jordan

Announcements

- HW3 due Wednesday Feb 4
- HW4 will be handed out next Monday Feb 9

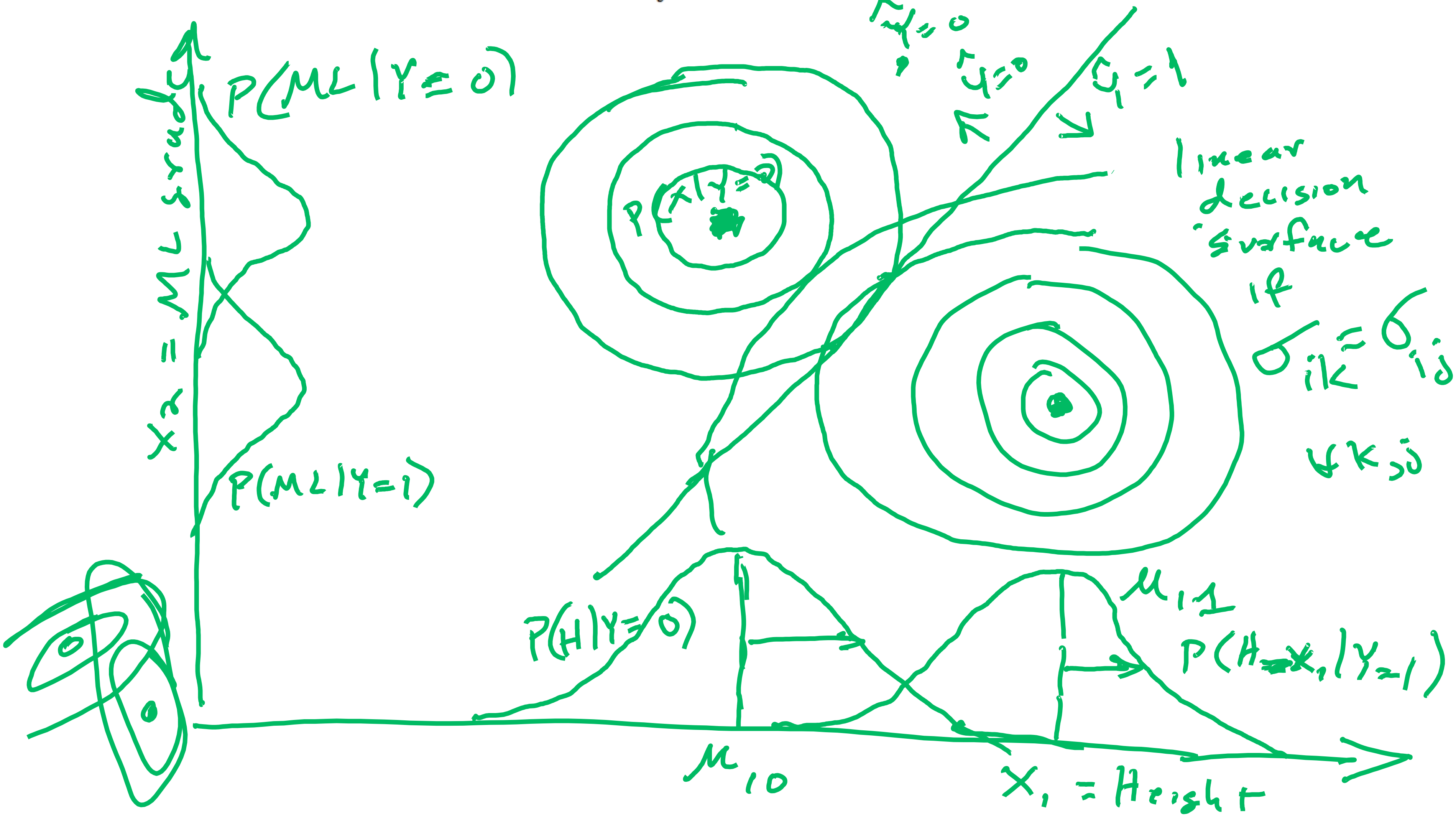
- new reading available:
  - Estimating Probabilities: MLE and MAP (Mitchell)
  - see Lecture tab of class website

- required reading for today:
  - Naïve Bayes and Logistic Regression (Mitchell)

Gaussian Naïve Bayes – Big Picture

Example: Y= PlayBasketball (boolean), X1=Height, X2=MLgrade

$$Y^{new} \leftarrow \arg\max_{y\in\{0,1\}} P(Y=y)\prod_i P(X_i^{new}|Y=y)$$ assume P(Y=1) = 0.5



Logistic Regression

Idea:

- Naïve Bayes allows computing P(Y|X) by learning P(Y) and P(X|Y)

- Why not learn P(Y|X) directly?

- Consider learning f: X → Y, where
  - X is a vector of real-valued features, < X_1 … X_n >
  - Y is boolean
  - assume all X_i are conditionally independent given Y
  - model $P(X_i \mid Y = y_k)$ as Gaussian $N(\mu_{ik}, \sigma_i)$ not σ_{ik}
  - model P(Y) as Bernoulli (π)

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

$$P(Y = 1|X = < X_1, ...X_n >) = \frac{1}{1 + exp(w_0 + \sum_i w_i X_i)}$$

Derive form for P(Y|X) for Gaussian $P(X_i|Y=y_k)$ assuming $\sigma_{ik} = \sigma_i$

$$P(Y=1|X) = \frac{P(Y=1)P(X|Y=1)}{P(Y=1)P(X|Y=1) + P(Y=0)P(X|Y=0)}$$

$$= \frac{1}{1 + \frac{P(Y=0)P(X|Y=0)}{P(Y=1)P(X|Y=1)}}$$

$x = \exp(\ln x)$

$$= \frac{1}{1 + \exp(\ln \frac{P(Y=0)P(X|Y=0)}{P(Y=1)P(X|Y=1)})}$$

$\pi \equiv P(Y=1)$

$$= \frac{1}{1 + \exp(\ (\ln \frac{1-\pi}{\pi}) + \boxed{\sum_i \ln \frac{P(X_i|Y=0)}{P(X_i|Y=1)}})}$$

e

$$P(x \mid y_k) = \frac{1}{\sigma_{ik}\sqrt{2\pi}} e^{\frac{-(x-\mu_{ik})^2}{2\sigma_{ik}^2}}$$

$$\boxed{\sum_i \left(\frac{\mu_{i0} - \mu_{i1}}{\sigma_i^2} X_i + \frac{\mu_{i1}^2 - \mu_{i0}^2)}{2\sigma_i^2} \right)}$$

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

Very convenient!

$$P(Y=1|X=<X_1,...X_n>) = \frac{1}{1+exp(w_0+\sum_i w_i X_i)}$$

implies

$$P(Y=0|X=<X_1,...X_n>) = \frac{exp(w_0+\sum_i w_i X_i)}{1+exp(w_0+\sum_i w_i X_i)}$$

implies

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

implies

$$0 \lessgtr \ln\frac{P(Y=0|X)}{P(Y=1|X)} = w_0+\sum_i w_i X_i$$

Very convenient!

$$P(Y=1|X=<X_1,...X_n>) = \frac{1}{1+exp(w_0+\sum_i w_i X_i)}$$

implies

$$P(Y=0|X=<X_1,...X_n>) = \frac{exp(w_0+\sum_i w_i X_i)}{1+exp(w_0+\sum_i w_i X_i)}$$

implies

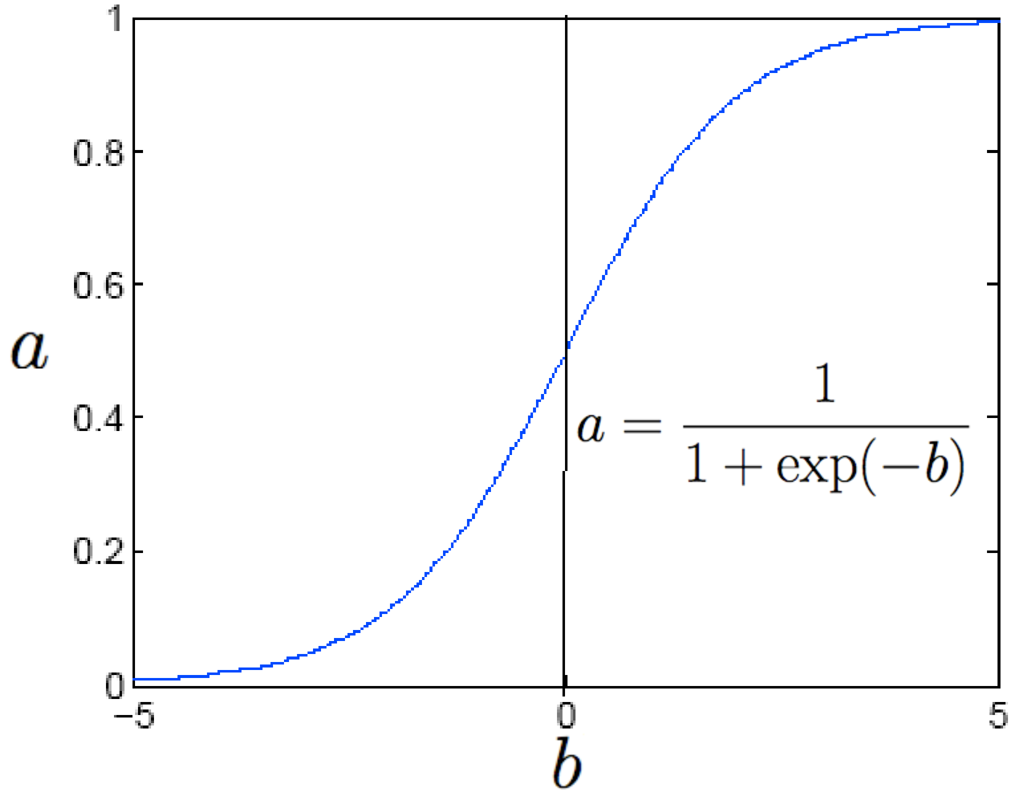
$$\frac{P(Y=0|X)}{P(Y=1|X)} = exp(w_0+\sum_i w_i X_i)$$

linear classification rule!

implies

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

Logistic function



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

Logistic regression more generally

- Logistic regression when Y not boolean (but still discrete-valued).
- Now $y \in \{y_1 \ldots y_R\}$: learn R-1 sets of weights

for *k<R* $$P(Y = y_k|X) = \frac{\exp(w_{k0} + \sum_{i=1}^n w_{ki} X_i)}{1 + \sum_{j=1}^{R-1} \exp(w_{j0} + \sum_{i=1}^n w_{ji} X_i)}$$

for *k=R* $$P(Y = y_R|X) = \frac{1}{1 + \sum_{j=1}^{R-1} \exp(w_{j0} + \sum_{i=1}^n w_{ji} X_i)}$$

Training Logistic Regression: MCLE

- we have L training examples: $\{\langle X^1, Y^1\rangle, \dots \langle X^L, Y^L\rangle\}$

- maximum likelihood estimate for parameters W

$$W_{MLE} = \arg\max_{\boxed{W}} P(< X^1, Y^1 > \dots < X^L, Y^L > |W)$$
$$= \arg\max_{W} \prod_l P(< X^l, Y^l > |W)$$

- maximum conditional likelihood estimate

$$W_{MCLE} = \arg\max_{W} \prod_l P(Y^l | X^l, W)$$

Training Logistic Regression: MCLE

- Choose parameters W=<w_0, ... w_n> to <u>maximize conditional likelihood</u> of training data

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

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

- Training data D = $\{\langle X^1, Y^1\rangle, \dots \langle X^L, Y^L\rangle\}$
- Data likelihood = $\prod_l P(X^l, Y^l|W)$
- Data <u>conditional</u> likelihood = $\prod_l P(Y^l|X^l, W)$

$$W_{MCLE} = \arg\max_W \prod_l P(Y^l|W, X^l)$$

Expressing Conditional Log Likelihood

$$l(W) \equiv \ln \underbrace{\prod_l P(Y^l|X^l, W)} = \sum_l \ln P(Y^l|X^l, W)$$

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

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

$$\begin{aligned} l(W) &= \sum_l Y^l \ln P(Y^l = 1|X^l, W) + (1 \underbrace{- Y^l) \ln P(Y^l = 0|X^l, W)} \\ &= \sum_l Y^l \ln \frac{P(Y^l = 1|X^l, W)}{P(Y^l = 0|X^l, W)} + \ln P(Y^l = 0|X^l, W) \\ &= \sum_l Y^l (w_0 + \sum_i^n w_i X_i^l) - \ln(1 + exp(w_0 + \sum_i^n w_i X_i^l)) \end{aligned}$$

Maximizing Conditional Log Likelihood

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

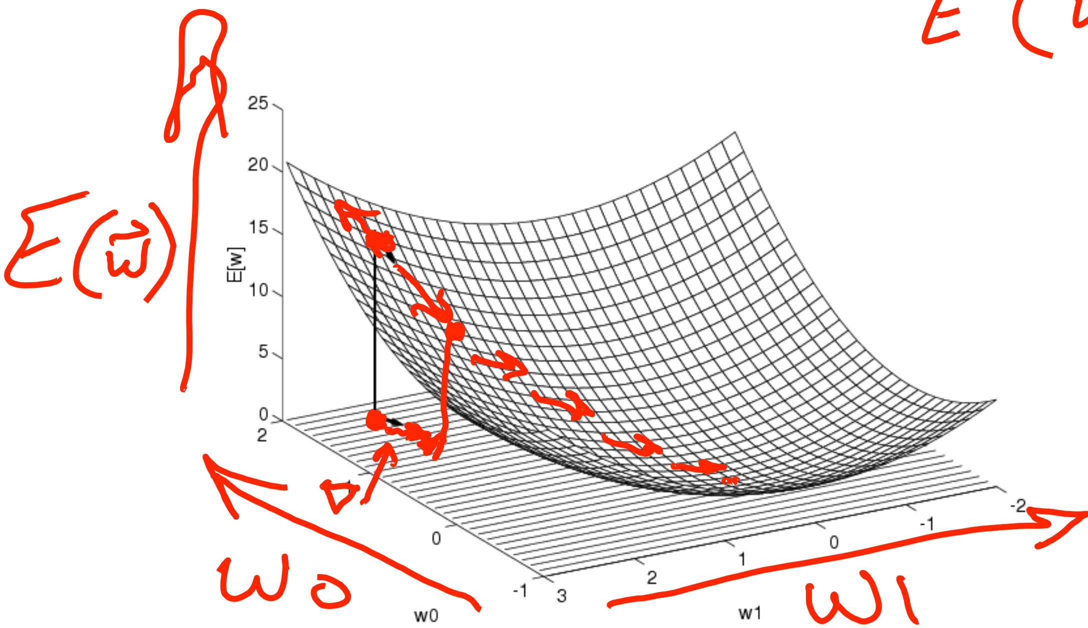
$$P(Y=1|X,W) = \frac{exp(w_0 + \sum_i w_i X_i)}{1+exp(w_0 + \sum_i w_i X_i)}$$

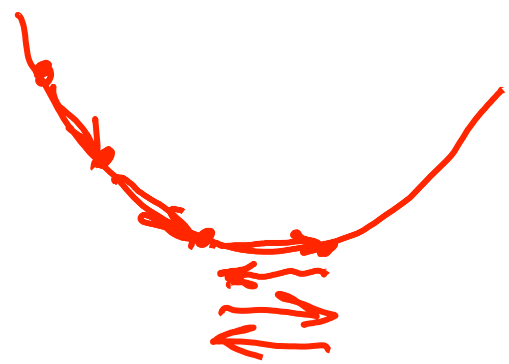
$$\begin{aligned} l(W) &\equiv \ln \prod_l P(Y^l|X^l,W) \\ &= \sum_l Y^l(w_0 + \sum_i^n w_i X_i^l) - \ln(1 + exp(w_0 + \sum_i^n w_i X_i^l)) \end{aligned}$$

Good news: *l(W)* is concave function of *W*
Bad news: no closed-form solution to maximize *l(W)*

Gradient Descent

$E(\vec{w})$





$\vec{w}^{(i+1)} = \vec{w}^{(i)} - \nabla E[\vec{w}]$

Gradient

$$\nabla E[\vec{w}] \equiv \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \cdots \frac{\partial E}{\partial w_n} \right]$$

Training rule:

$$\Delta \vec{w} = -\eta \nabla E[\vec{w}]$$

i.e.,

$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

Gradient Descent:

Batch gradient: use error $E_D(\mathbf{w})$ over entire training set D

Do until satisfied:

1. Compute the gradient $\nabla E_D(\mathbf{w}) = \left[\frac{\partial E_D(\mathbf{w})}{\partial w_0} \ldots \frac{\partial E_D(\mathbf{w})}{\partial w_n}\right]$
2. Update the vector of parameters: $\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla E_D(\mathbf{w})$

Stochastic gradient: use error $E_d(\mathbf{w})$ over single examples $d \in D$

Do until satisfied:

1. Choose (with replacement) a random training example $d \in D$
2. Compute the gradient just for d : $\nabla E_d(\mathbf{w}) = \left[\frac{\partial E_d(\mathbf{w})}{\partial w_0} \ldots \frac{\partial E_d(\mathbf{w})}{\partial w_n}\right]$
3. Update the vector of parameters: $\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla E_d(\mathbf{w})$

Stochastic approximates Batch arbitrarily closely as $\eta \rightarrow 0$

Stochastic can be much faster when D is very large

Intermediate approach: use error over subsets of D

Maximize Conditional Log Likelihood: Gradient Ascent

$$
\begin{aligned}
l(W) &\equiv \ln \prod_l P(Y^l | X^l, W) \\
&= \sum_l Y^l (w_0 + \sum_i^n w_i X_i^l) - \ln(1 + exp(w_0 + \sum_i^n w_i X_i^l))
\end{aligned}
$$

$$
\frac{\partial l(W)}{\partial w_i} = \sum_l X_i^l (Y^l - \hat{P}(Y^l = 1 | X^l, W))
$$

Maximize Conditional Log Likelihood: Gradient Ascent

$$
\begin{aligned}
l(W) &\equiv \ln \prod_l P(Y^l | X^l, W) \\
&= \sum_l Y^l (w_0 + \sum_i^n w_i X_i^l) - \ln(1 + exp(w_0 + \sum_i^n w_i X_i^l))
\end{aligned}
$$

$$
\frac{\partial l(W)}{\partial w_i} = \sum_l X_i^l (Y^l - \hat{P}(Y^l = 1 | X^l, W))
$$

Gradient ascent algorithm: iterate until change < ε

For all i, repeat

$$
w_i \leftarrow w_i + \eta \sum_l X_i^l (Y^l - \hat{P}(Y^l = 1 | X^l, W))
$$

That's all for M(C)LE. How about MAP?

- One common approach is to define priors on W
  - Normal distribution, zero mean, identity covariance
- Helps avoid very large weights and overfitting
- MAP estimate

$$W \leftarrow \arg\max_W \ \ln \ P(W) \prod_l P(Y^l | X^l, W)$$

- let's assume Gaussian prior: W ~ N(0, σ)

MLE vs MAP

#param GNB − $4n+1$ / $\sigma_{ik} = \sigma_i$ $3n+1$

$Y \in \{0,1\}$ $X_1, \ldots X_n$ $X_i \in \mathbb{R}$

- Maximum conditional likelihood estimate

$$W \leftarrow \arg\max_W \ \ln \prod_l P(Y^l | X^l, W)$$

LR: $n+1$

$$\boxed{w_i \leftarrow w_i + \eta \sum_l X_i^l (Y^l - \hat{P}(Y^l = 1 | X^l, W))}$$

- Maximum a posteriori estimate with prior W~N(0,σI)

$$W \leftarrow \arg\max_W \ \ln [P(W) \ \prod_l P(Y^l | X^l, W)]$$

$$\boxed{w_i \leftarrow w_i - \eta \lambda w_i + \eta \sum_l X_i^l (Y^l - \hat{P}(Y^l = 1 | X^l, W))}$$

MAP estimates and Regularization

- Maximum a posteriori estimate with prior W~N(0,σI)

$$W \leftarrow \arg\max_W \ \ln[P(W) \prod_l P(Y^l|X^l,W)]$$

$$\boxed{w_i \leftarrow w_i - \eta\lambda w_i + \eta \sum_l X_i^l (Y^l - \hat{P}(Y^l = 1|X^l, W))}$$

called a "<u>regularization</u>" term
- helps reduce overfitting
- keep weights nearer to zero (if P(W) is zero mean Gaussian prior), or whatever the prior suggests
- used very frequently in Logistic Regression

The Bottom Line

- Consider learning f: X → Y, where
  - X is a vector of real-valued features, < X_1 … X_n >
  - Y is boolean
  - assume all X_i are conditionally independent given Y
  - model $P(X_i \mid Y = y_k)$ as Gaussian $N(\mu_{ik},\sigma_i)$
  - model P(Y) as Bernoulli (π)

- Then P(Y|X) is of this form, and we can directly estimate W

$$P(Y = 1|X =< X_1, ...X_n >) = \frac{1}{1 + exp(w_0 + \sum_i w_i X_i)}$$

- Furthermore, same holds if the X_i are boolean
  - trying proving that to yourself

Generative vs. Discriminative Classifiers

Training classifiers involves estimating f: X → Y, or P(Y|X)

Generative classifiers (e.g., Naïve Bayes)
- 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 (e.g., Logistic regression)

- Assume some functional form for P(Y|X)
- Estimate parameters of P(Y|X) directly from training data

Use Naïve Bayes or Logisitic Regression?

Consider

- Restrictiveness of modeling assumptions

- Rate of convergence (in amount of training data) toward asymptotic hypothesis

Naïve Bayes vs Logistic Regression

Consider Y boolean, X_i continuous, $X = \langle X_1 \ldots X_n \rangle$

Number of parameters:

- NB: 4n +1
- LR: n+1

Estimation method:

- NB parameter estimates are uncoupled
- LR parameter estimates are coupled

G.Naïve Bayes vs. Logistic Regression

Recall two assumptions deriving form of LR from GNBayes:

1. X_i conditionally independent of X_k given Y
2. $P(X_i \mid Y = y_k) = N(\mu_{ik},\sigma_i)$, $\leftarrow$ not $N(\mu_{ik},\sigma_{ik})$

Consider three learning methods:

- GNB (assumption 1 only)
- GNB2 (assumption 1 and 2)
- LR

Which method works better if we have *infinite* training data, and…

- Both (1) and (2) are satisfied
- Neither (1) nor (2) is satisfied
- (1) is satisfied, but not (2)

G.Naïve Bayes vs. Logistic Regression

[Ng & Jordan, 2002]

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1. X_i conditionally independent of X_k given Y
2. $P(X_i \mid Y = y_k) = N(\mu_{ik},\sigma_i)$, $\leftarrow$ not $N(\mu_{ik},\sigma_{ik})$

Consider three learning methods:

•GNB (assumption 1 only) -- decision surface can be non-linear

•GNB2 (assumption 1 and 2) – decision surface linear

•LR -- decision surface linear, trained without assumption 1.

Which method works better if we have *infinite* training data, and...

•Both (1) and (2) are satisfied: LR = GNB2 = GNB

•(1) is satisfied, but not (2) : GNB > GNB2, GNB > LR, LR > GNB2

•Neither (1) nor (2) is satisfied: GNB>GNB2, LR > GNB2, LR><GNB

G.Naïve Bayes vs. Logistic Regression

[Ng & Jordan, 2002]

What if we have only finite training data?

They converge at different rates to their asymptotic (∞ data) error

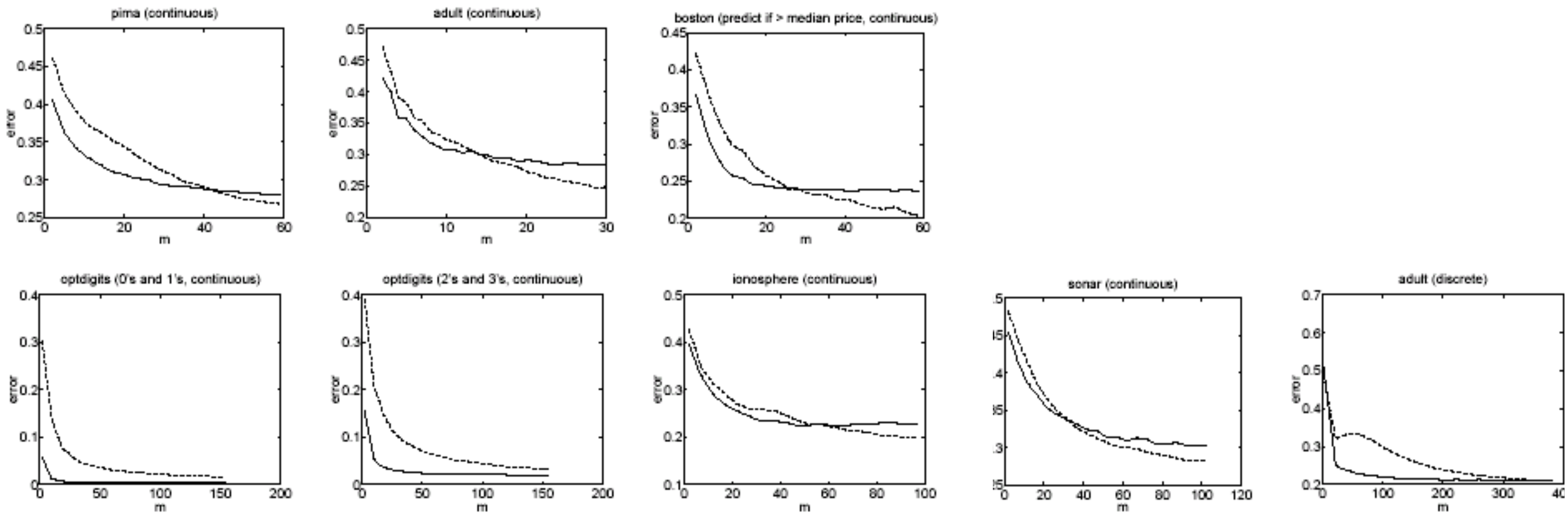
Let $\epsilon_{A,n}$ refer to expected error of learning algorithm A after *n* training examples

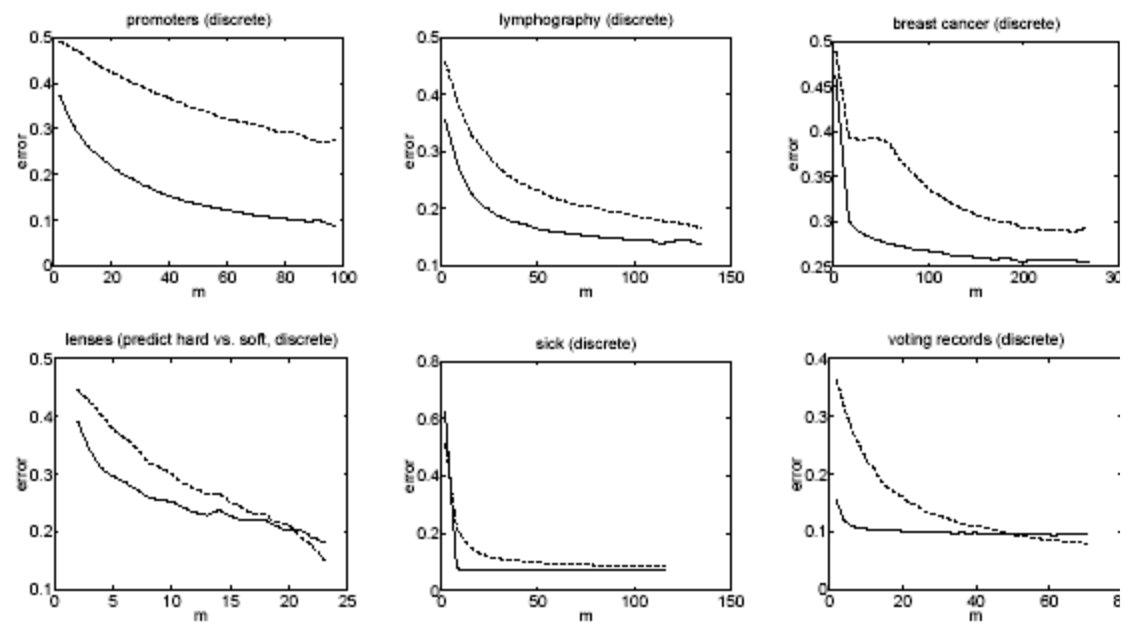
Let *d* be the number of features: <X_1 … X_d>

$$\epsilon_{LR,n} \leq \epsilon_{LR,\infty} + O\left(\sqrt{\frac{d}{n}}\right)$$

$$\epsilon_{GNB,n} \leq \epsilon_{GNB,\infty} + O\left(\sqrt{\frac{\log d}{n}}\right)$$

So, GNB requires *n = O(log d)* to converge, but LR requires *n = O(d)*





Some experiments from UCI data sets

[Ng & Jordan, 2002]

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

Naïve Bayes vs. Logistic Regression

The bottom line:

GNB2 and LR both use linear decision surfaces, GNB need not

Given infinite data, LR is better or equal to GNB2 because *training procedure* does not make assumptions 1 or 2 (though our derivation of the form of $P(Y|X)$ did).

But GNB2 converges more quickly to its perhaps-less-accurate asymptotic error

And GNB is both more biased (assumption1) and less (no assumption 2) than LR, so either might outperform the other

What you should know:

- Logistic regression
  - Functional form follows from Naïve Bayes assumptions
    - For Gaussian Naïve Bayes assuming variance $\sigma_{i,k} = \sigma_i$
    - For discrete-valued Naïve Bayes too
  - But training procedure picks parameters without making conditional independence assumption
  - MLE training: pick W to maximize P(Y | X, W)
  - MAP training: pick W to maximize P(W | X,Y)
    - 'regularization'
    - helps reduce overfitting

- Gradient ascent/descent
  - General approach when closed-form solutions unavailable

- Generative vs. Discriminative classifiers
  - Bias vs. variance tradeoff

extra slides

What is the minimum possible error?

Best case:

- conditional independence assumption is satistied
- we know P(Y), P(X|Y) perfectly (e.g., infinite training data)

Questions to think about:

- Can you use Naïve Bayes for a combination of discrete and real-valued X_i?
- How can we easily model the assumption that just 2 of the n attributes as dependent?
- What does the decision surface of a Naïve Bayes classifier look like?
- How would you select a subset of X_i's?