Machine Learning 10-601

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Today:
- Gaussian Naïve Bayes
- Logistic regression
- Gradient ascent/descent

Readings: (see class website)

Required:
- Mitchell: “Naïve Bayes and Logistic Regression”

What if we have continuous X_i ?

Eg., image classification: X_i is real-valued i[th] pixel

Naïve Bayes requires $P(X_i \mid Y{=}y_k)$, but X_i is real (continuous)

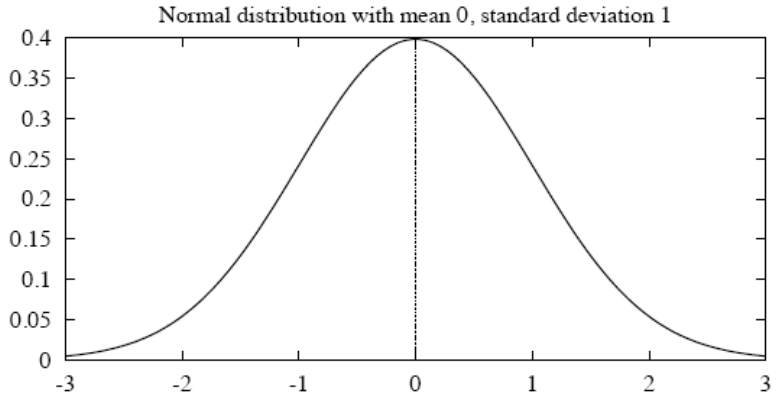
$$P(Y = y_k | X_1 \ldots X_n) = \frac{P(Y = y_k) \prod_i P(X_i | Y = y_k)}{\sum_j P(Y = y_j) \prod_i P(X_i | Y = y_j)}$$

Common approach: assume $P(X_i \mid Y{=}y_k)$ follows a Normal (Gaussian) distribution

Gaussian Distribution

(also called “Normal”)

p(x) is a *probability density function*, whose integral (not sum) is 1



$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})^2}$$

The probability that X will fall into the interval (a, b) is given by

$$\int_a^b p(x)dx$$

- Expected, or mean value of X, $E[X]$, is

$$E[X] = \mu$$

- Variance of X is

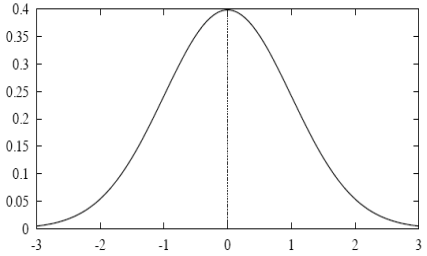
$$Var(X) = \sigma^2$$

- Standard deviation of X, σ_X, is

$$\sigma_X = \sigma$$

What if we have continuous X_i ?

Gaussian Naïve Bayes (GNB): assume



$$p(X_i = x | Y = y_k) = \frac{1}{\sqrt{2\pi\sigma_{ik}^2}} \; e^{-\frac{1}{2}\left(\frac{x-\mu_{ik}}{\sigma_{ik}}\right)^2}$$

Sometimes assume variance σ_{ik}

- is independent of Y (i.e., σ_i),
- or independent of X_i (i.e., σ_k)
- or both (i.e., σ)

Gaussian Naïve Bayes Algorithm – continuous X_i (but still discrete Y)

- Train Naïve Bayes (examples)

  for each value y_k

  estimate* $\pi_k \equiv P(Y = y_k)$

  for each attribute X_i estimate $P(X_i|Y = y_k)$

  - class conditional mean μ_{ik}, variance σ_{ik}

- Classify (X^{new})

$$Y^{new} \leftarrow \arg\max_{y_k} \; P(Y = y_k) \prod_i P(X_i^{new}|Y = y_k)$$

$$Y^{new} \leftarrow \arg\max_{y_k} \; \pi_k \prod_i \mathcal{N}(X_i^{new}; \mu_{ik}, \sigma_{ik})$$

* probabilities must sum to 1, so need estimate only n-1 parameters...

Estimating Parameters: Y discrete, X_i continuous

Maximum likelihood estimates:

$$\hat{\mu}_{ik} = \frac{1}{\sum_j \delta(Y^j = y_k)} \sum_j X_i^j \delta(Y^j = y_k)$$

jth training example

ith feature

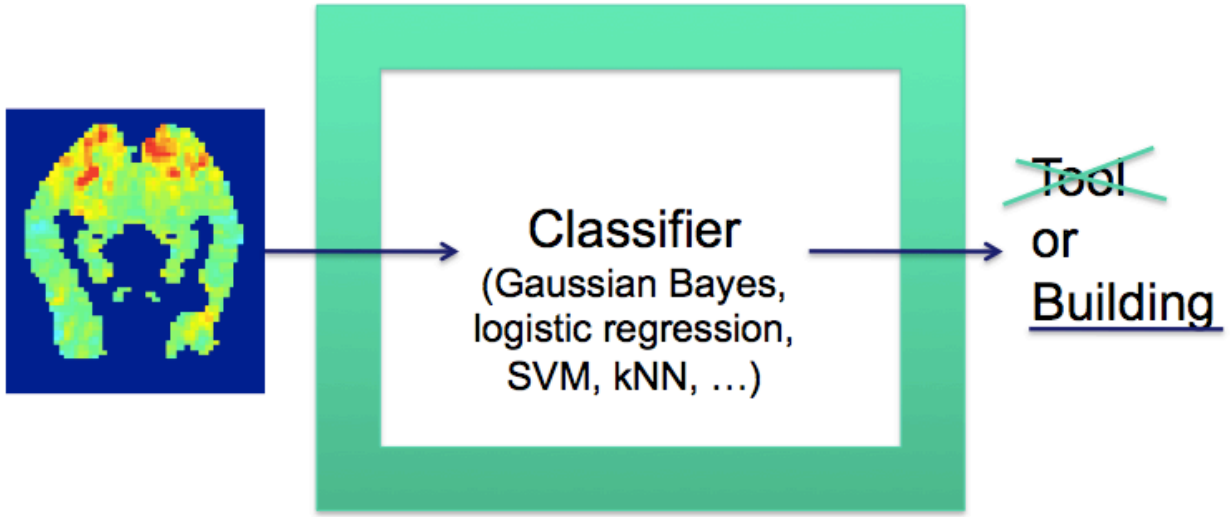
kth class

δ()=1 if (y^j=y_k) else 0

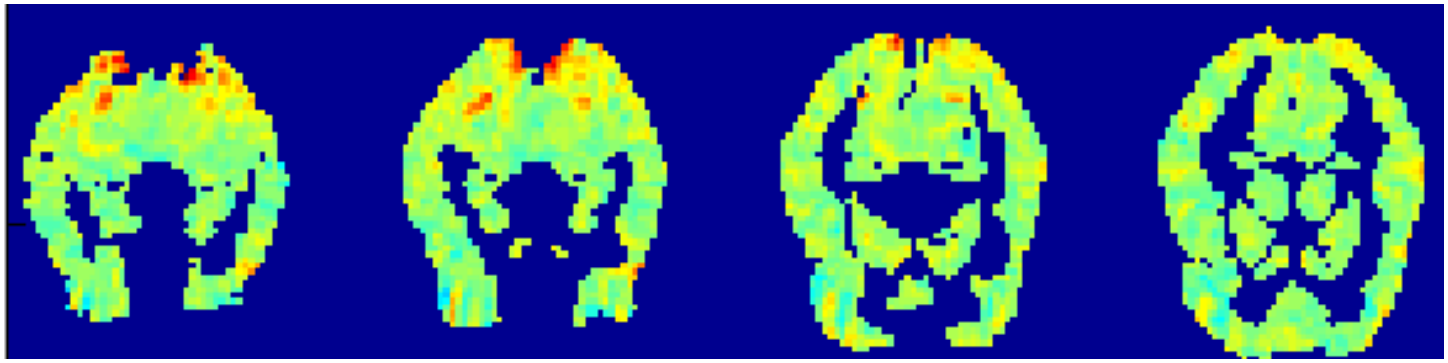
$$\hat{\sigma}_{ik}^2 = \frac{1}{\sum_j \delta(Y^j = y_k)} \sum_j (X_i^j - \hat{\mu}_{ik})^2 \delta(Y^j = y_k)$$

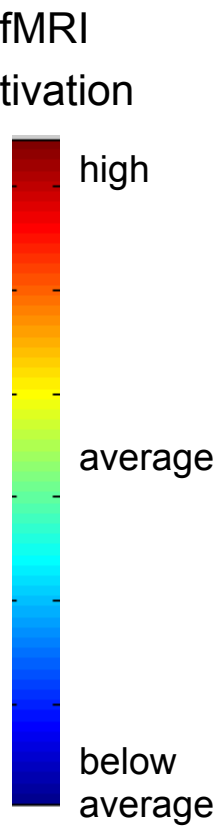
GNB Example: Classify a person's cognitive state, based on brain image

- reading a sentence or viewing a picture?
- reading the word describing a "Tool" or "Building"?
- answering the question, or getting confused?



Mean activations over all training examples for Y="bottle"

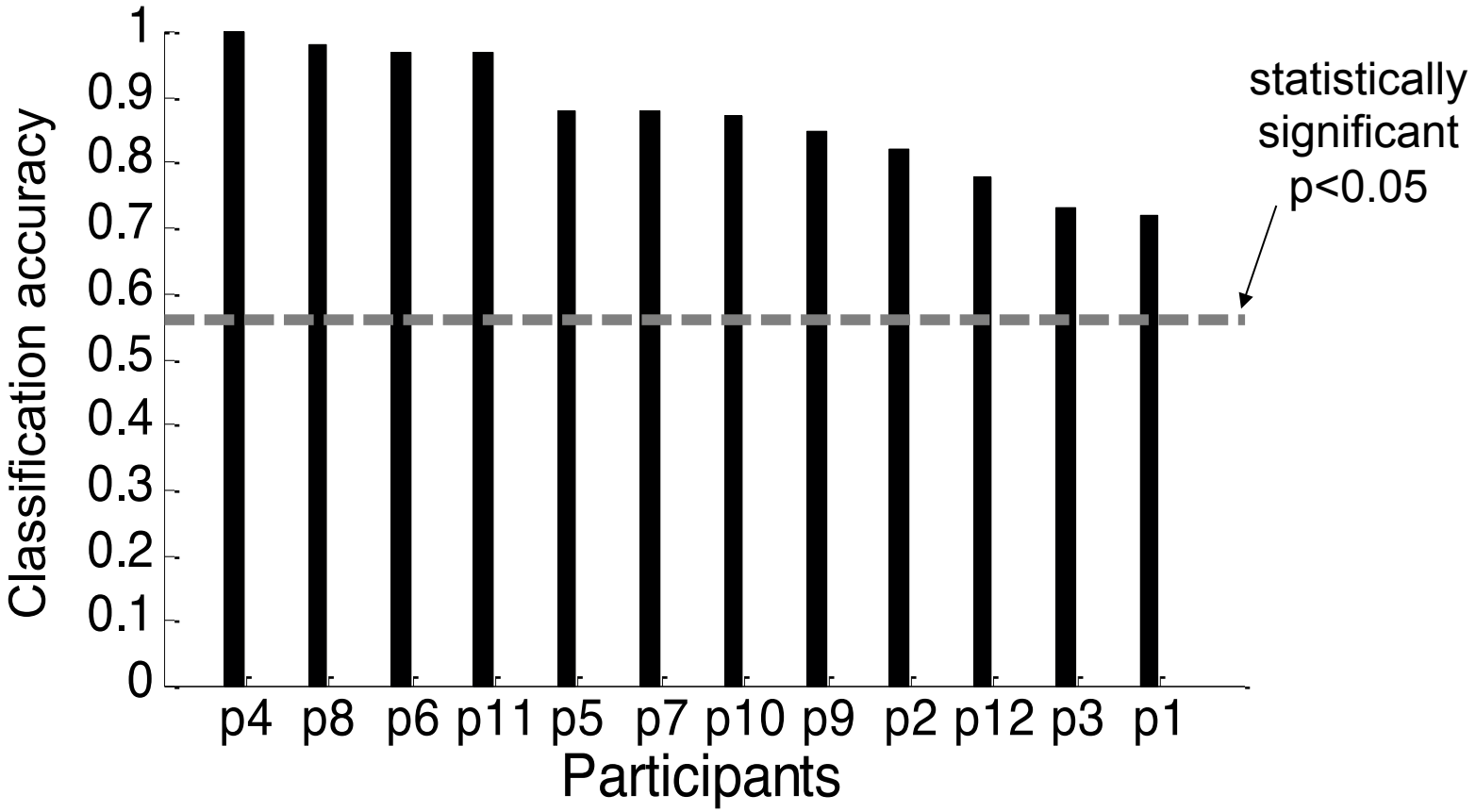




Y is the mental state (reading "house" or "bottle")
X_i are the voxel activities,

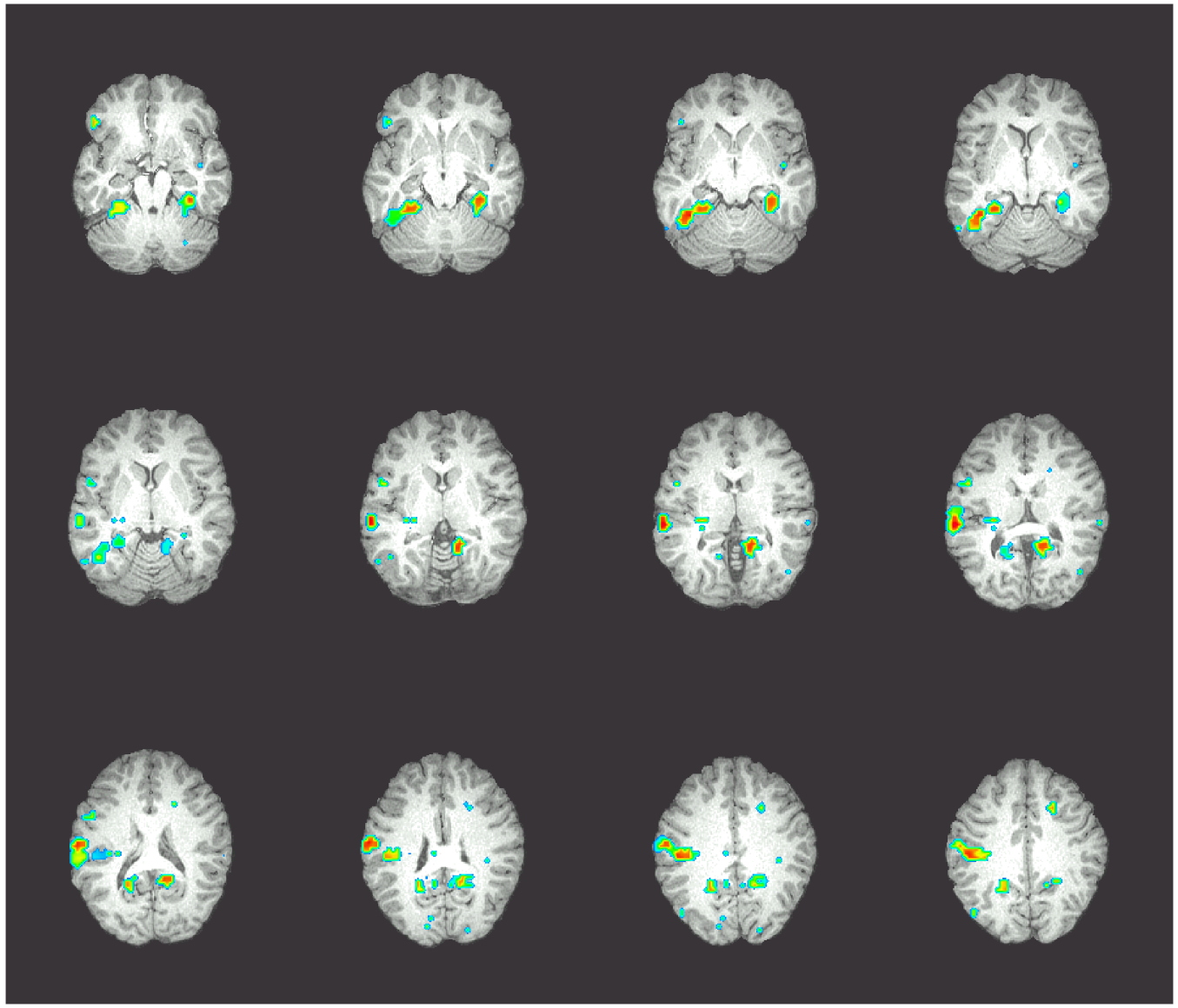
this is a plot of the μ's defining $P(X_i \mid Y=\text{"bottle"})$

Classification task: is person viewing a “tool” or “building”?



Where is information encoded in the brain?

Tools vs. Buildings
Accuracies of cubical 27-voxel classifiers centered at each significant voxel
[0.7-0.8]



Naïve Bayes: What you should know

- Designing classifiers based on Bayes rule
- Conditional independence
  - What it is
  - Why it's important
- Naïve Bayes assumption and its consequences
  - Which (and how many) parameters must be estimated under different generative models (different forms for P(X|Y))
    - and why this matters
- How to train Naïve Bayes classifiers
  - MLE and MAP estimates
  - with discrete and/or continuous inputs X_i

Questions to think about:

- Can you use Naïve Bayes for a combination of discrete and real-valued X_i?
- How can we extend Naïve Bayes to model that two of the X_i's are dependent?
- What does the decision surface of a Naïve Bayes classifier look like?
- What error will Naïve Bayes achive if cond. indep. is satisfied and we have infinite training data?

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 $N(\mu_{ik},\sigma_i)$
  - 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 $\sigma_{ik} = \sigma_i$

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

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

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

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

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

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

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

Very convenient!

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

implies

$$P(Y = 0|X =< X_1, ...X_n >) =$$

implies

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

implies

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

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

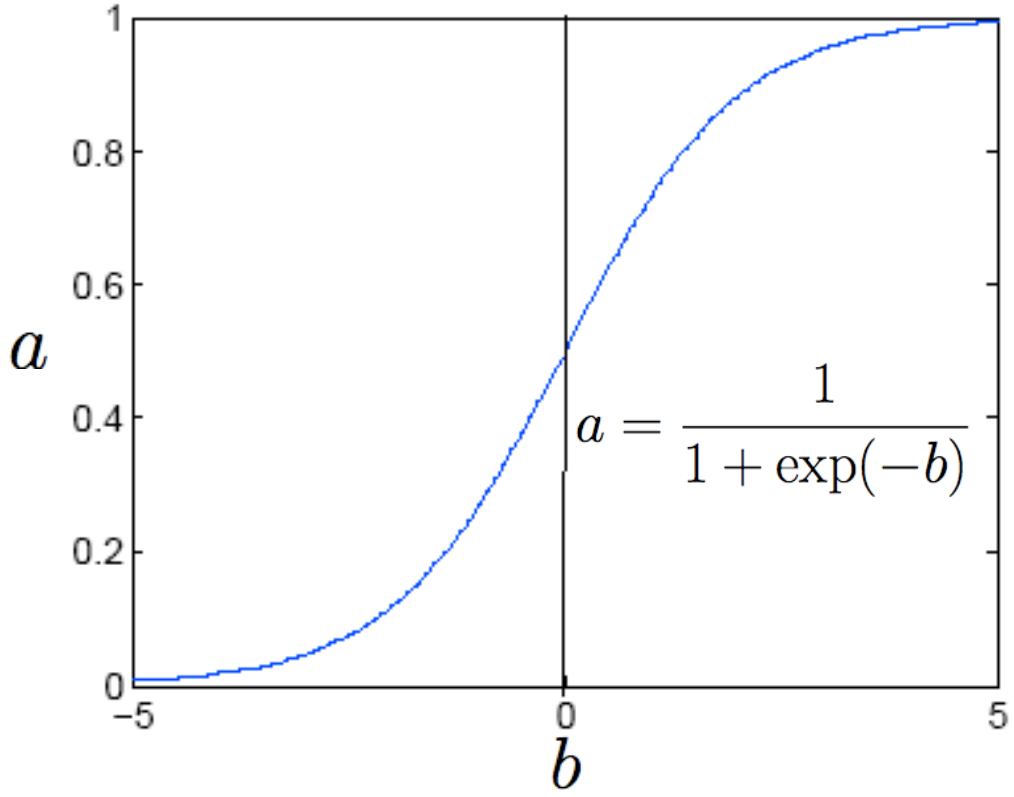
$$\frac{P(Y=0|X)}{P(Y=1|X)}=exp(w_0+\sum_i w_i X_i)$$

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: MLE, MCLE

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

- maximum likelihood estimate for parameters W

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

- maximum conditional likelihood estimate…

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 = $\{\langle X^1, Y^1\rangle, \ldots \langle X^L, Y^L\rangle\}$
- 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

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

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

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

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

Maximizing Conditional Log Likelihood

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

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

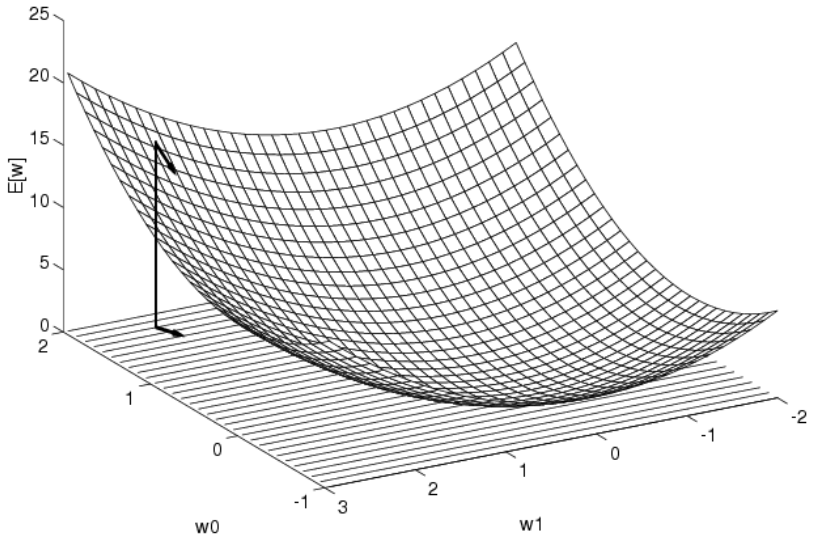
$$l(W) \equiv \ln \prod_l P(Y^l|X^l,W) = \sum_l \ln P(Y^l|X^l,W)$$

$$= \sum_l Y^l(w_0 + \sum_i^n w_i X_i^l) - \ln(1+exp(w_0+\sum_i^n w_i X_i^l))$$

Good news: $l(W)$ is concave function of W

Bad news: no closed-form solution to maximize $l(W)$

Gradient Descent



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

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

$$= \sum_l Y^l(w_0 + \sum_i^n w_i X_i^l) - \ln(1 + exp(w_0 + \sum_i^n w_i X_i^l))$$

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

Maximize Conditional Log Likelihood: Gradient Ascent

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

$$= \sum_l Y^l(w_0 + \sum_i^n w_i X_i^l) - \ln(1 + exp(w_0 + \sum_i^n w_i X_i^l))$$

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

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?

- For MAP, need to define prior on W
  - given $W = \langle w_1, \ldots w_n \rangle$
    let's assume prior $P(w_i) = N(0, \sigma)$
  - i.e., assume zero mean, Gaussian prior for each w_i

- A kind of Occam's razor (simplest is best) prior

- Helps avoid very large weights and overfitting

MAP Estimates for Logistic Regression

$$W^{MAP} = \arg\max_{W} P(W|Y,X) = \frac{P(Y|W,X)P(W,X)}{P(Y,X)}$$

MAP Estimates for Logistic Regression

$$W^{MAP} = \arg\max_W P(W|Y,X) = \frac{P(Y|W,X)P(W,X)}{P(Y,X)}$$

$$= \arg\max_W P(Y|W,X)P(W,X)$$

let's assume P(W,X)=P(W) P(X)

$$= \arg\max_W P(Y|W,X)P(W)P(X)$$

$$= \arg\max_W P(Y|W,X)P(W)$$

$$W^{MAP} = \arg\max_W [\ln P(Y|W,X) + \ln P(W)]$$

zero mean Gaussian P(W)

$$P(W) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}\sum_i w_i^2\right)$$

$$W^{MAP} = \arg\max_W [\ln P(Y|W,X) - \left(\frac{1}{2\sigma^2}\sum_i w_i^2\right)]$$

MLE vs MAP

- Maximum conditional likelihood estimate

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

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

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

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

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

MAP estimates and Regularization

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

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

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

called a "regularization" term

- helps reduce overfitting
- if P(W) is Gaussian, then encourages W to be near the mean of P(W) : zero here, but can easily use any mean
- 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

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

Extra slides

for more details, see Ng & Jordan paper

http://www.cs.cmu.edu/~awm/10701/readings/NgJordanNIPS2001.ps

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=<X_1 ... X_n>

Number of parameters to estimate:

- NB:

- LR:

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

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

Naïve Bayes vs Logistic Regression

Consider Y boolean, X_i continuous, $X=<X_1 \ldots X_n>$

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. $P(X_i \mid Y = y_k) = N(\mu_{ik},\sigma_i)$, ← 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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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]

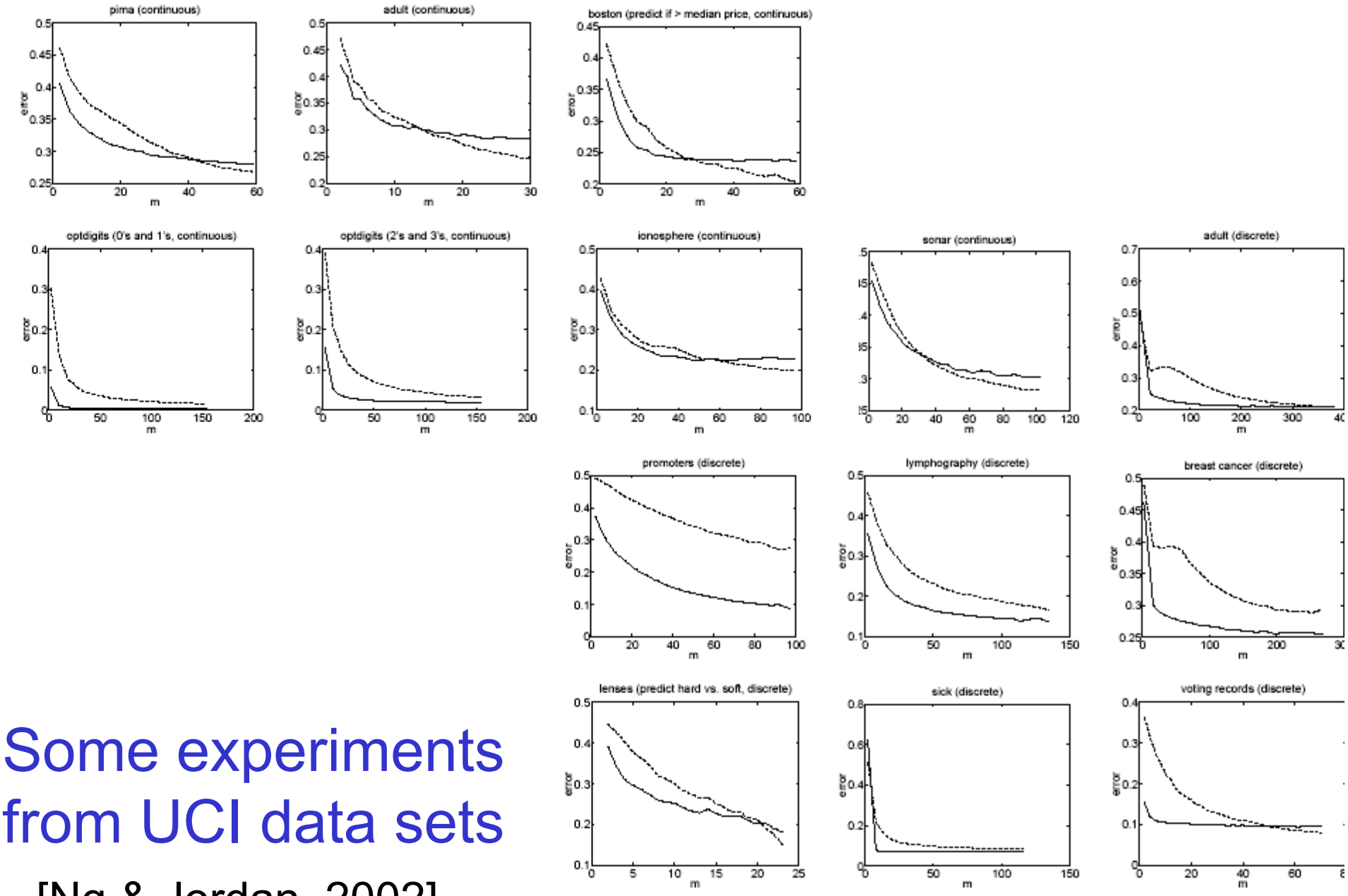

Figure 1: Results of 15 experiments on datasets from the UCI Machine Learnin repository. Plots are of generalization error vs. m (averaged over 1000 randor train/test splits). Dashed line is logistic regression; solid line is naive Bayes.

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