# Machine Learning 10-701

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Today:
- Naïve Bayes – Big Picture
- Logistic regression
- Gradient ascent
- Generative – discriminative classifiers

Readings:

Required:
- Mitchell: "Naïve Bayes and Logistic Regression"
  (see class website)

Optional
- Ng and Jordan paper (class website)

# Gaussian Naïve Bayes – Big Picture

## 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 ($\pi$)

- 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 continuous $X_i$

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

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

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

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

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

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

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

## Very convenient!

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

implies

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

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

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

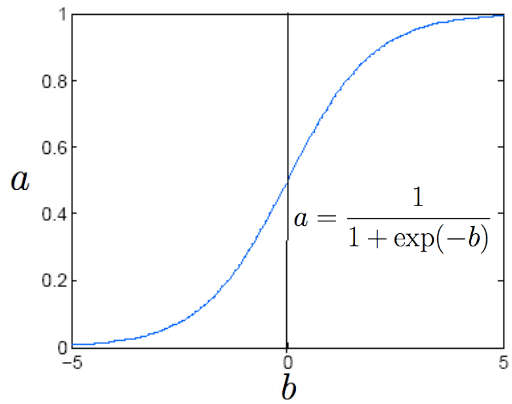
linear classification rule!

implies

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

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

# 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: $\{\langle X^1, Y^1\rangle, \ldots \langle X^L, Y^L\rangle\}$
- 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 maximize conditional likelihood 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 conditional 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

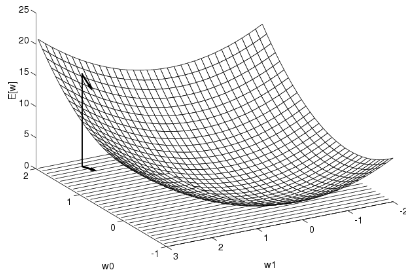
$$P(Y=0|X,W) = \frac{1}{1 + exp(w_0 + \sum_i w_i X_i)}$$

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

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

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

Gradient Descent



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.,

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

## 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

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

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

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

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

- Maximum conditional likelihood estimate

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

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

- 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 "regularization" term
• helps reduce overfitting, especially when training data is sparse
• 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 ($\pi$)

- 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
  - i.e., the learning curve

## 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, $X=<X_1 ... X_n>$

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

[Ng & Jordan, 2002]

- Generative and Discriminative classifiers

- *Asymptotic comparison* (# training examples → infinity)
  - when conditional independence assumptions correct
    - GNB, LR produce identical classifiers
  - when conditional independence assumptions incorrect
    - LR is less biased – does not assume cond indep.
    - therefore expected to outperform GNB when both given infinite training data

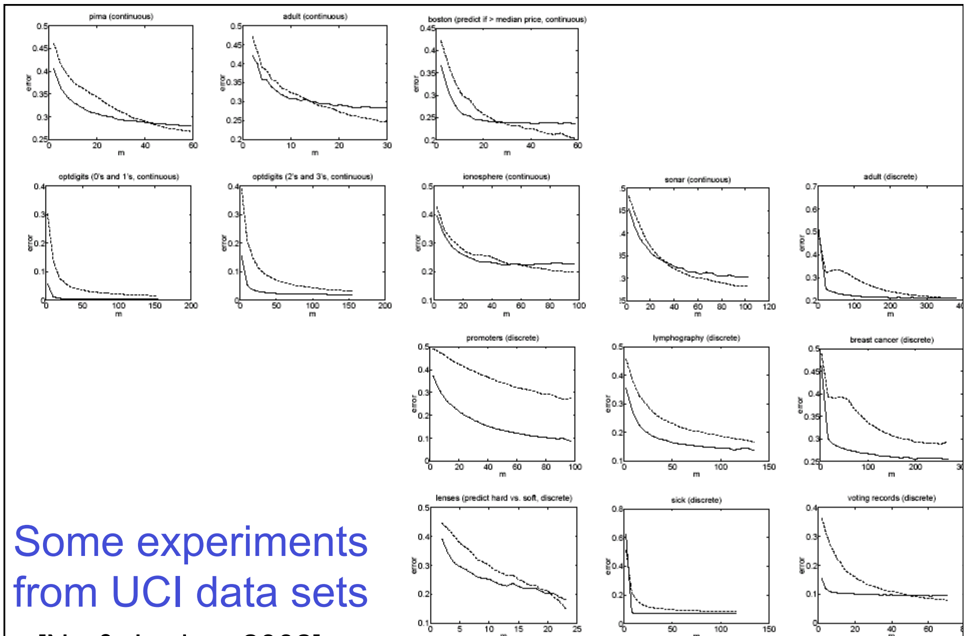
## Naïve Bayes vs. Logistic Regression

- Generative and Discriminative classifiers

- *Non-asymptotic analysis* (see [Ng & Jordan, 2002] )
  - convergence rate of parameter estimates – how many training examples needed to assure good estimates?
    - GNB order log n  (where n = # of attributes in X)
    - LR order n

GNB converges more quickly to its (perhaps less accurate) asymptotic estimates

Informally: because LR's parameter estimates are coupled, but GNB's are not




## 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.

## Summary: Naïve Bayes and Logistic Regression

- Modeling assumptions
  - Naïve Bayes more biased (cond. indep)
  - Both learn linear decision surfaces
- Convergence rate (n=number training examples)
  - Naïve Bayes ~ O(log n)
  - Logistic regression ~O(n)
- Bottom line
  - Naïve Bayes converges faster to its (potentially too restricted) final hypothesis

## 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 the conditional independence assumption
  - MLE training: pick W to maximize P(Y | X, W)
  - MAP training: pick W to maximize P(W | X,Y)
    - regularization: e.g., P(W) ~ N(0,σ)
    - helps reduce overfitting
- Gradient ascent/descent
  - General approach when closed-form solutions for MLE, MAP are unavailable
- Generative vs. Discriminative classifiers
  - Bias vs. variance tradeoff