Logistic Regression

Machine Learning 10-601

Many of these slides are derived from Tom Mitchell, William Cohen, Eric Xing. Thanks!

Logistic Regression

Idea:

- Naïve Bayes allows computing P(Y|X) by learning P(Y) and P(X|Y)
  - Essentially learns P(Y)P(X|Y) = P(Y,X)

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

- Consider learning f: X → Y, where
  - Problem set-up:
    - X is a vector of real-valued features, < X_1 … X_n >
    - Y is boolean
  - Naïve Bayes assumption: 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 continuous X_i

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

Bayes rule

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

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

Conditional Independence

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

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

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

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

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

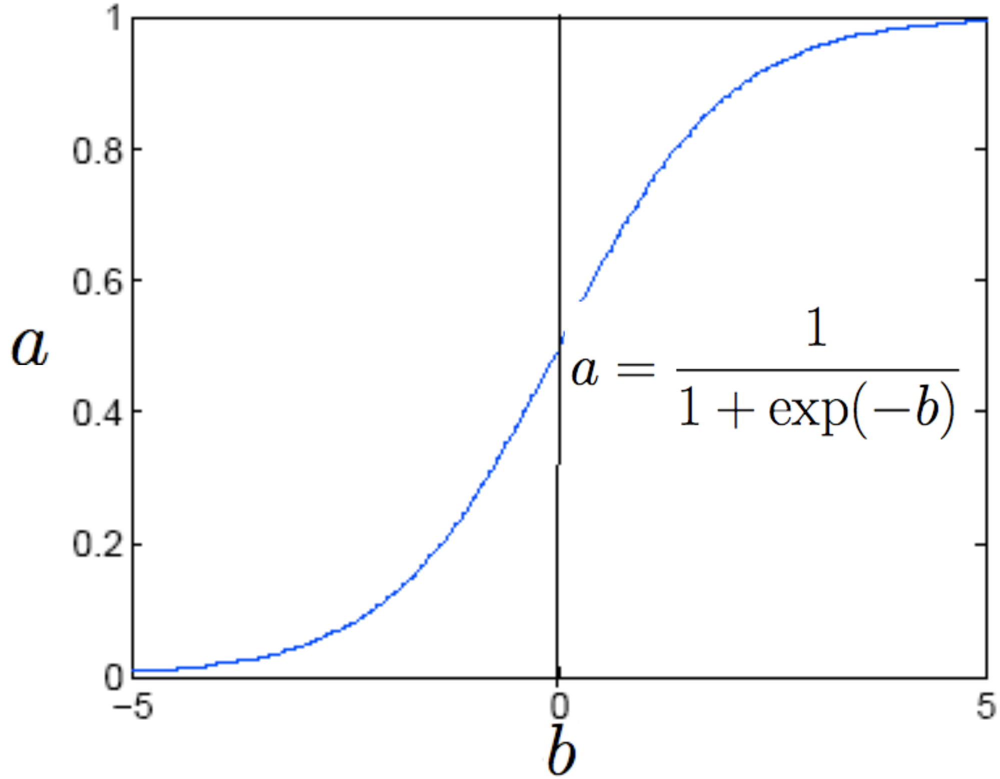
$$\frac{P(Y=0|X)}{P(Y=1|X)} = exp(w_0+\sum_i w_i X_i)$$

linear classification rule!

implies

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

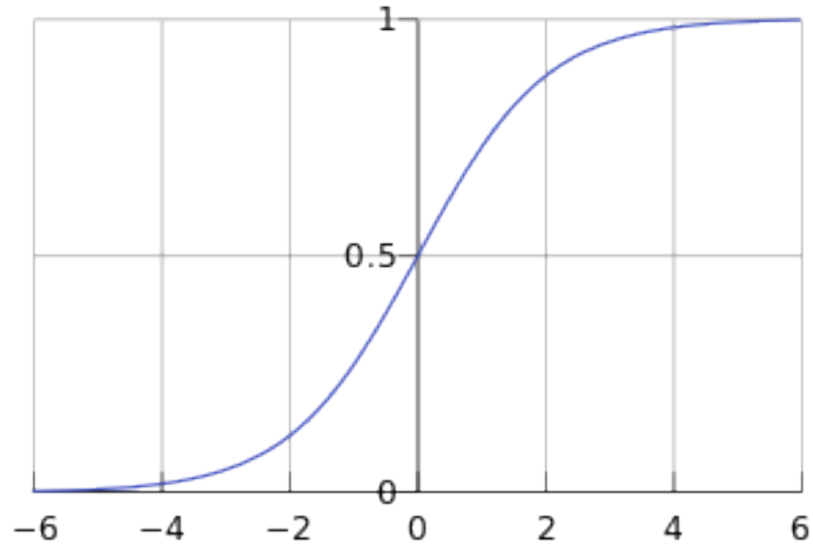
Logistic function

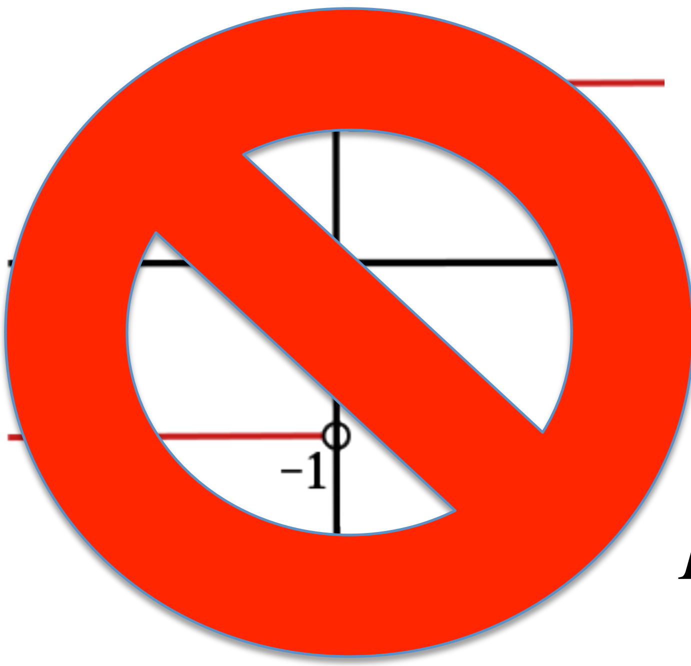


$$\underbrace{P(Y=1|X)}_{a} = \frac{1}{1+\exp(\underbrace{w_0+\sum_{i=1}^{n} w_i X_i}_{-b})}$$

Logistic function for classifiers

1. Replace sign(**x•w**) with something differentiable: e.g. the logistic**(x•w)**





$$\text{logistic}(u) \equiv \frac{1}{1+e^{-u}}$$

$$P(Y=1 \mid X=\mathbf{x}) \equiv \frac{1}{1+e^{-\mathbf{x}\cdot\mathbf{w}}}$$

Logistic regression more generally

- Logistic regression when Y not boolean (but still discrete-valued).
- Now $y \in \{y_1 \dots y_R\}$: 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: Maximum Conditional Likelihood Estimation (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

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

- maximum <u>conditional </u>likelihood estimate

Training Logistic Regression: MCLE

- Choose parameters $W = \langle w_0, \ldots w_n \rangle$ 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

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

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

$$l(W) \;=\; \sum_l \underline{Y^l \ln P(Y^l=1|X^l, W)} + \underline{(1-Y^l) \ln P(Y^l=0|X^l, W)}$$

For the samples with Y^l=1

For the samples with Y^l=0

Expressing Conditional Log Likelihood

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

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

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

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

Expressing Conditional Log Likelihood

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

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

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

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

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)*

Learning Logistic Regression with Gradient Descent

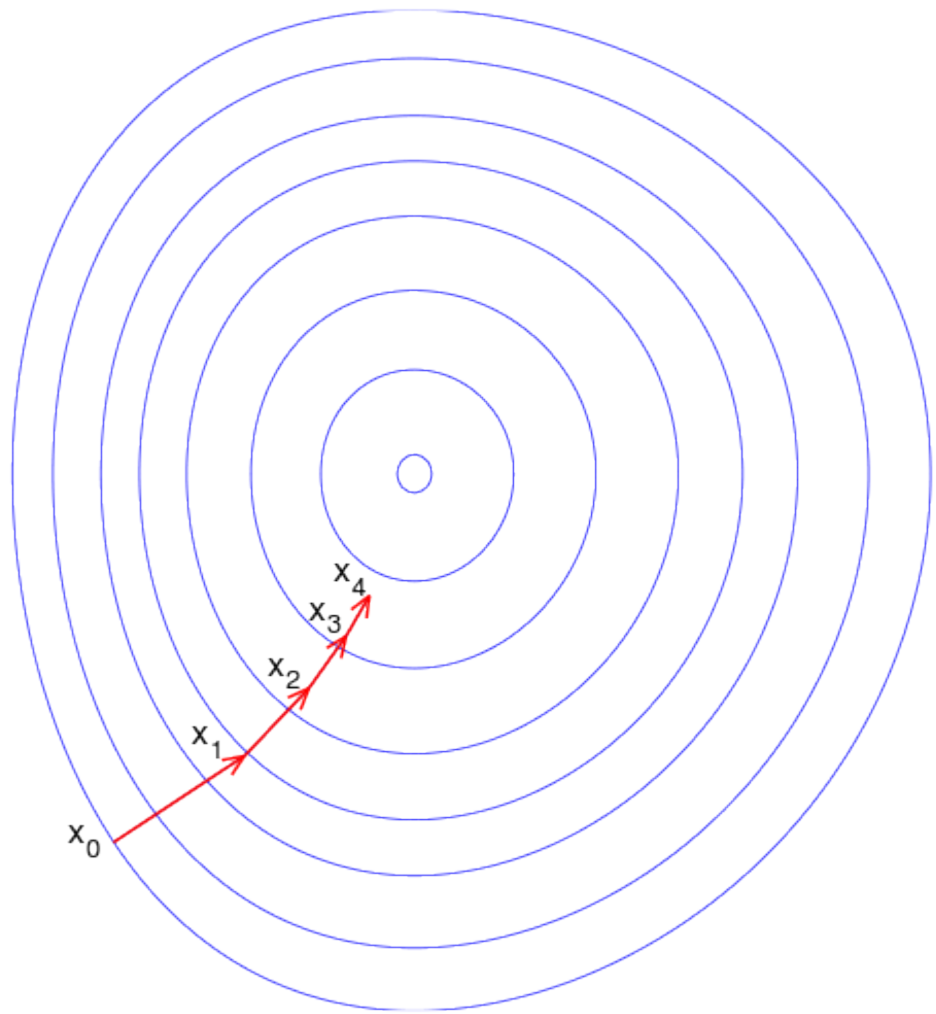
Learning as optimization: general procedure

- Goal: Learn the parameter **w** of …
- Dataset: $D=\{(x_1,y_1),\ldots,(x_n , y_n)\}$
- Write down a loss function
  - $\text{Loss}_D(\mathbf{w})$ = ….
- Set **w** to minimize Loss
  - Usually we use numeric methods to find the optimum
  - i.e., **gradient descent**: repeatedly take a small step in the direction of the gradient

Gradient descent

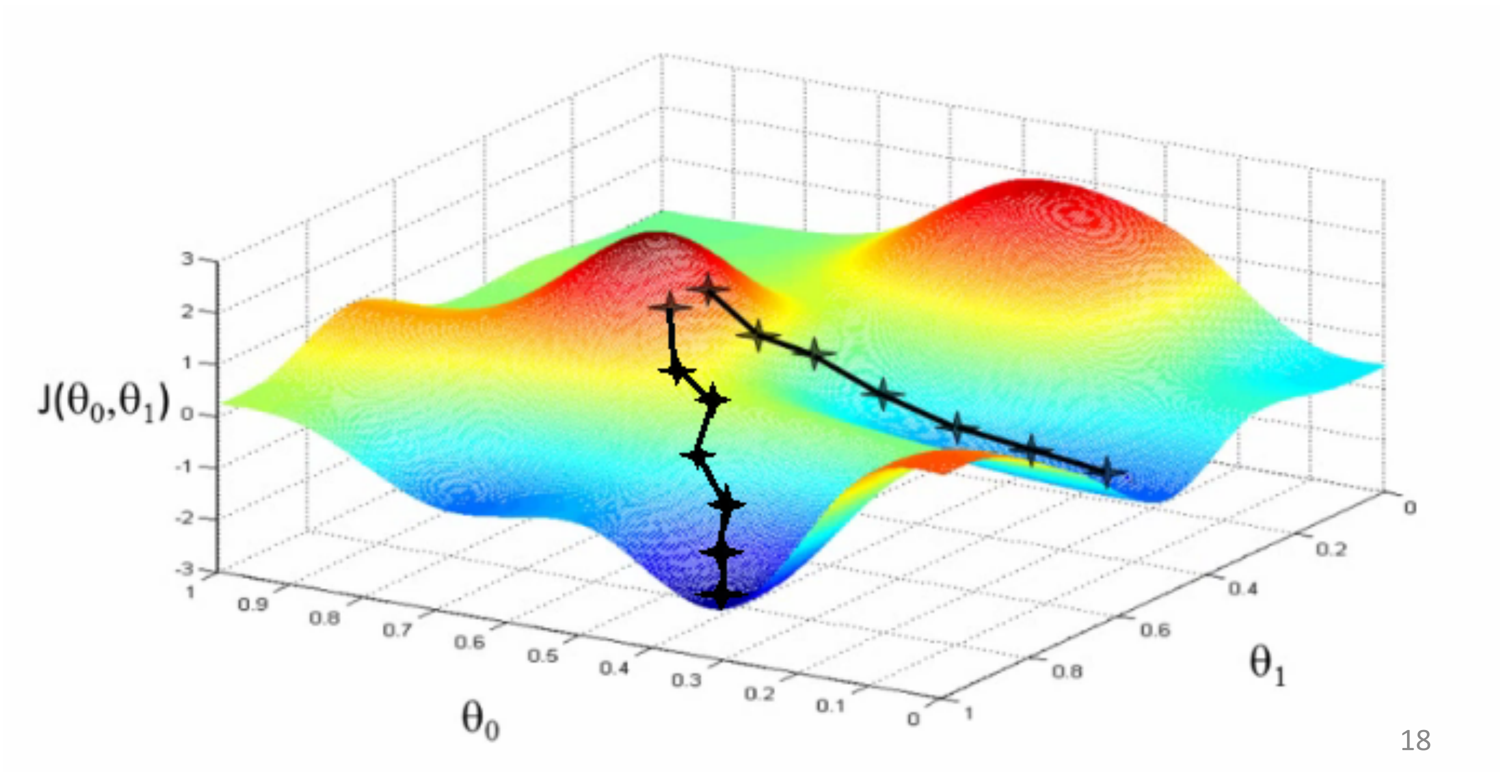
To find $\text{argmin}_{\mathbf{x}}\, f(\mathbf{x})$:

- Start with $\mathbf{x}_0$
- For t=1….
    - $\mathbf{x}_{t+1} = \mathbf{x}_t + \lambda f'(\mathbf{x}_t)$
    where λ is small



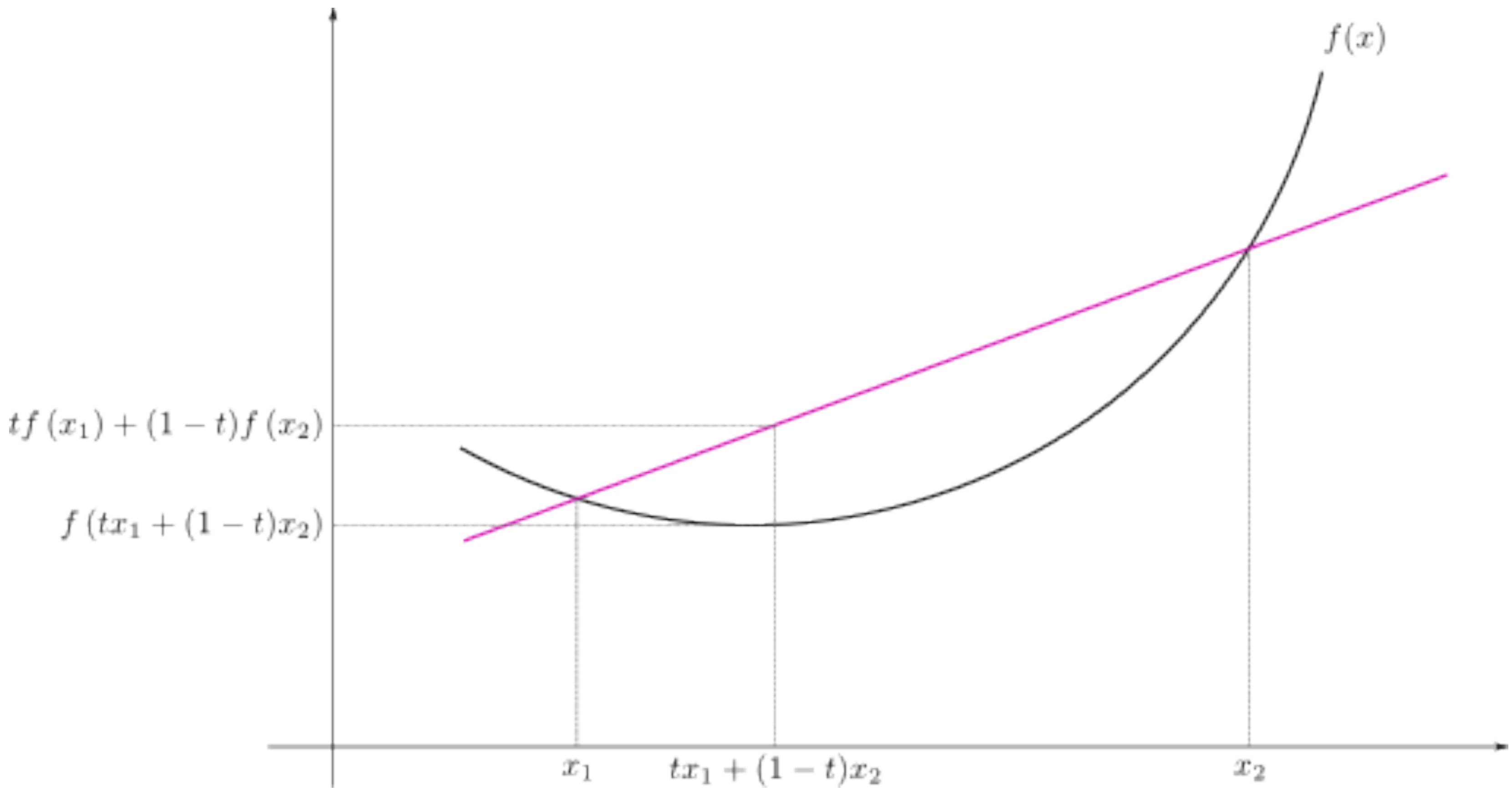
Pros and cons of gradient descent

- Simple and often quite effective on ML tasks
- Only applies to smooth functions (differentiable)
- Might find a local minimum, rather than a global one



Pros and cons of gradient descent

There is only one local optimum if the function is *convex*



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

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

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

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

Maximize Conditional Log Likelihood: Gradient Ascent

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

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

$$
(\log f)' = \frac{1}{f} f'
$$

$$
(e^f)' = e^f f'
$$

Gradient ascent algorithm: iterate until change < ε

For all i, repeat

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

MAP Estimation with Regularization

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

- MAP estimate

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

- One common approach is to define priors on W
  - Normal distribution, zero mean, identity covariance

- Helps avoid very large weights and overfitting

- let's assume Gaussian prior: W ~ N(0, $\sigma^2\mathbf{I}$) = 1/Z $(w^j)^{-2}$ (where Z is a constant)

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,σ^2I)

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

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

$\lambda = 1/(2\sigma^2)$

MAP Estimates and Regularization

- Maximum a posteriori estimate with prior W~N(0,σ²I)

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

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

called a "<u>regularization</u>" term
• helps reduce overfitting, 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 (π)

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

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

Generative vs. Discriminative Classifier

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) (i.e., P(X,Y))
- Estimate parameters of P(X|Y), P(X) directly from training data
- Use Bayes rule to calculate $P(Y|X= x_i)$

> - Find $\boldsymbol{\theta} = \text{argmax}_{\mathbf{w}}\ \boldsymbol{\Pi}_{\mathbf{i}}\ \Pr(y_i,x_i|\boldsymbol{\theta})$
> - Different assumptions about *generative process* for the data: Pr(X,Y), priors on **θ,…**

Discriminative classifiers (e.g., Logistic regression)

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

> - Find $\boldsymbol{\theta} = \text{argmax}_{\mathbf{w}}\ \boldsymbol{\Pi}_{\mathbf{i}}\ \Pr(y_i|x_i,\boldsymbol{\theta})$
> - Different assumptions about conditional probability: Pr(Y|X), priors on θ, …

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, $X=<X_1 \dots X_n>$

Number of parameters:

- NB: 4n +1 (3n+1 if we assume $\sigma_{ik}=\sigma_i$)
- LR: n+1

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

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

Estimation method:

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

G.Naïve Bayes vs. Logistic Regression

[Ng & Jordan, 2002]

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) -- decision surface can be non-linear

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

•LR -- decision surface linear, trained differently

Which method works better if we have <u>*infinite*</u> 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

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

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

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

•(1) is satisfied, but not (2) :

G.Naïve Bayes vs. Logistic Regression

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

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

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

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

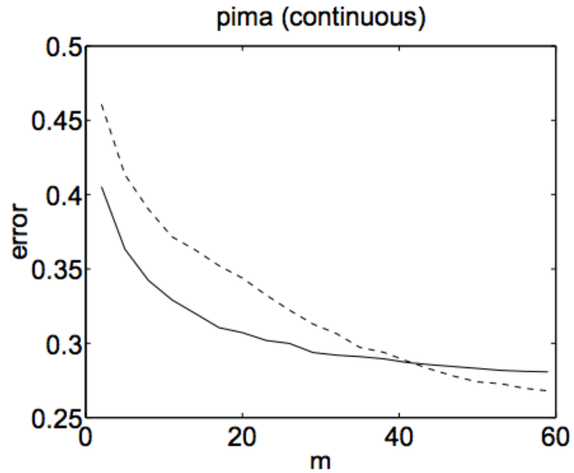
Let $\epsilon_{A,n}$ refer to expected error of learning algorithm A after *n* training examples

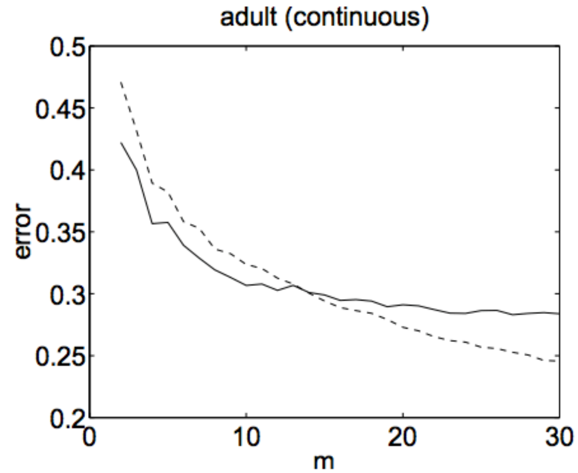
Let *d* be the number of features: <X_1 … X_d>

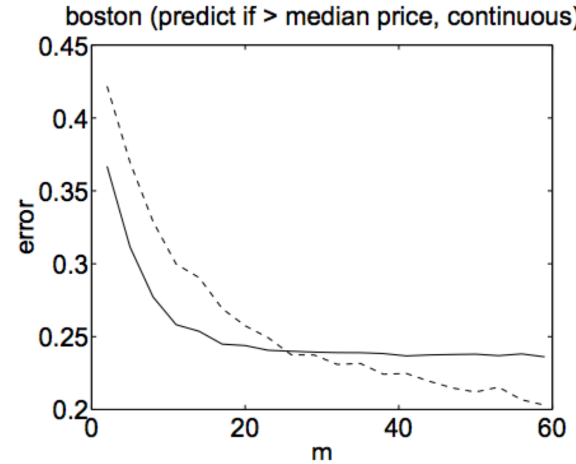
$$\epsilon_{LR,n} \leq \epsilon_{LR,\infty} + O\left(\sqrt{\frac{d}{n}}\right)$$

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

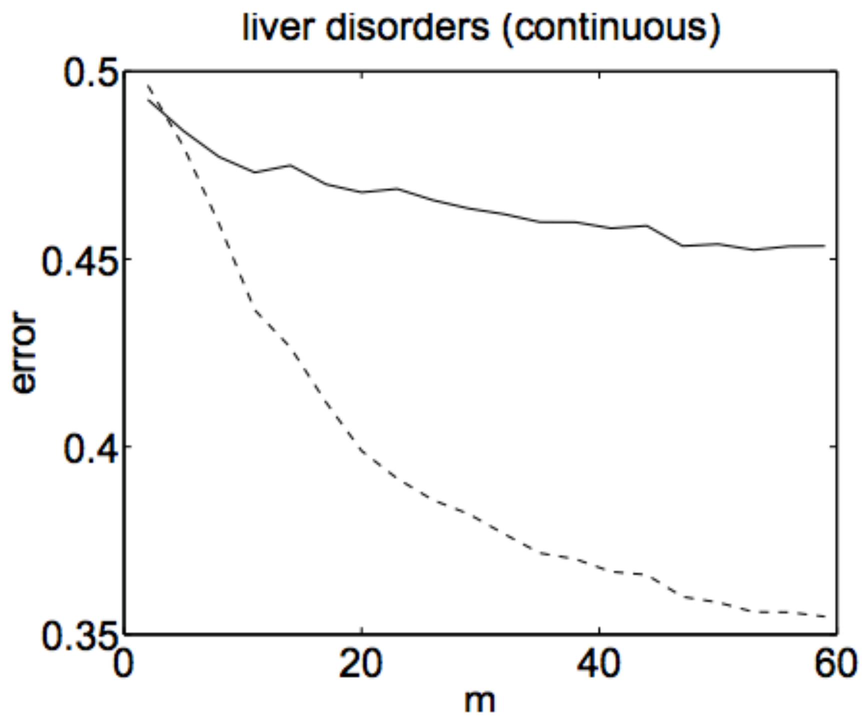
So, GNB requires n = O(log d) to converge, but LR requires n = O(d)

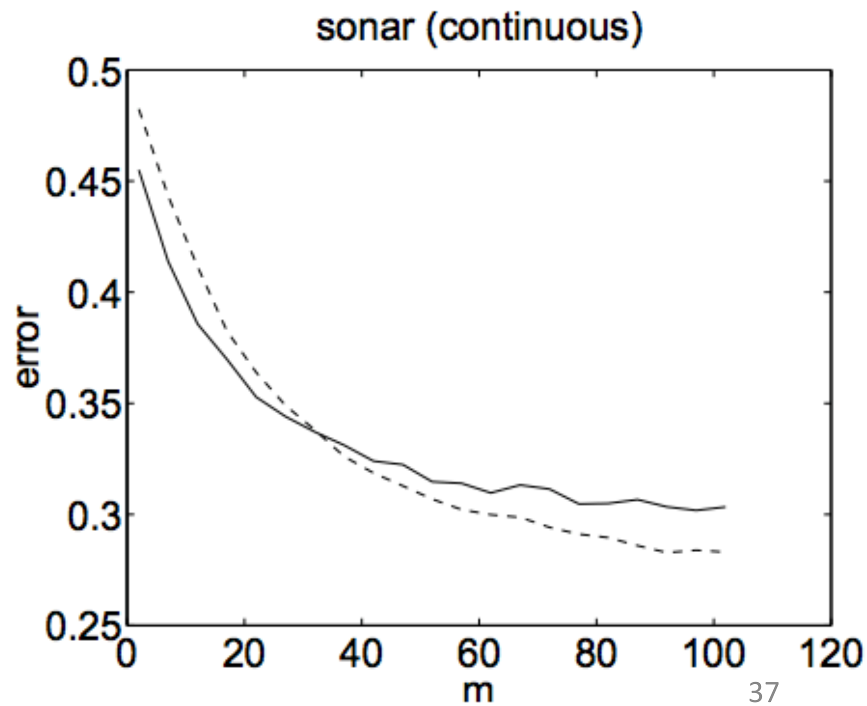


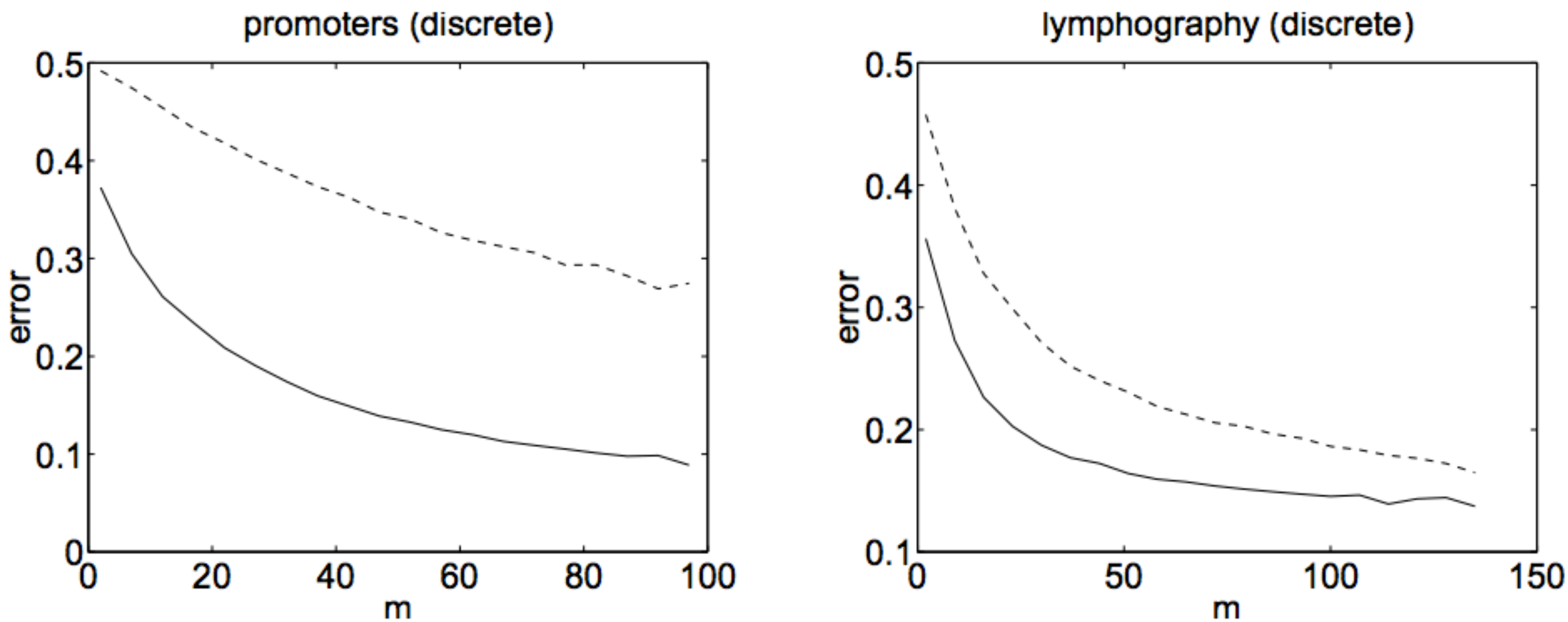




solid: NB dashed: LR







Naïve Bayes makes stronger assumptions about the data but needs fewer examples to estimate the parameters

"On Discriminative vs Generative Classifiers: …." Andrew Ng and Michael Jordan, NIPS 2001.

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 beat 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