Logistic Regression

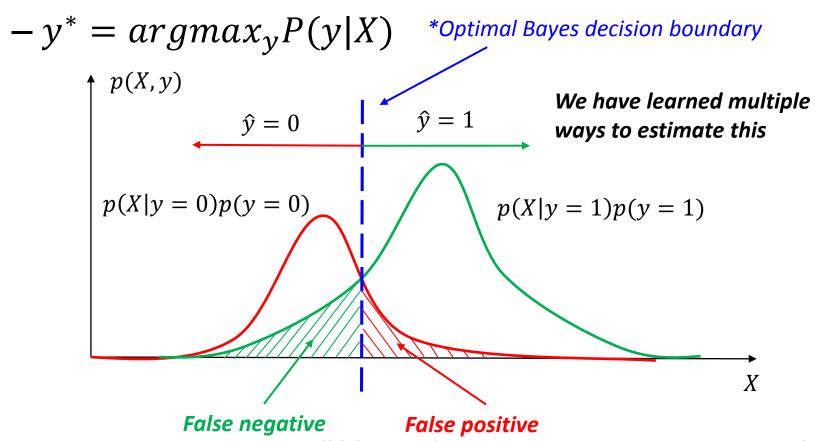
Hongning Wang CS@UVa

Today's lecture

- Logistic regression model
 - A discriminative classification model
 - Two different perspectives to derive the model
 - Parameter estimation

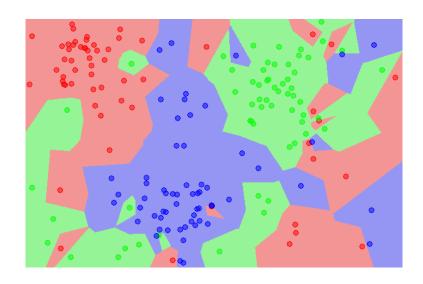
Review: Bayes risk minimization

Risk – assign instance to a wrong class



Instance-based solution

- k nearest neighbors
 - Approximate Bayes decision rule in a subset of data around the testing point



Instance-based solution

- k nearest neighbors
 - Approximate Bayes decision rule in a subset of data around the testing point
 - Let V be the volume of the m dimensional ball around x containing the k nearest neighbors for x, we have

$$p(x)V = \frac{k}{N} \implies p(x) = \frac{k}{NV} \qquad p(x|y=1) = \frac{k_1}{N_1V} \qquad p(y=1) = \frac{N_1}{N}$$
Total number of instances

$$p(x)V = \frac{k}{N} \implies p(x) = \frac{k}{NV} \qquad p(x|y=1) = \frac{k_1}{N_1V} \qquad p(y=1) = \frac{N_1}{N}$$

$$Total \ number \ of \ instances$$

$$With \ Bayes \ rule: \qquad \qquad \frac{N_1}{N} \times \frac{k_1}{N_1V} = \frac{k_1}{k} \qquad \qquad Total \ number \ of \ instances \ in \ class \ 1$$

$$p(y=1|x) = \frac{\frac{N_1}{N} \times \frac{k_1}{N_1V}}{\frac{k}{NV}} = \frac{k_1}{k} \qquad \qquad Counting \ the \ nearest$$

Counting the nearest neighbors from class1

Generative solution

Naïve Bayes classifier

$$-y^* = argmax_y P(y|X)$$

$$= argmax_y P(X|y)P(y)$$

$$= argmax_y \prod_{i=1}^{|d|} P(x_i|y) P(y)$$
By independence assumption

Estimating parameters

Maximial likelihood estimator

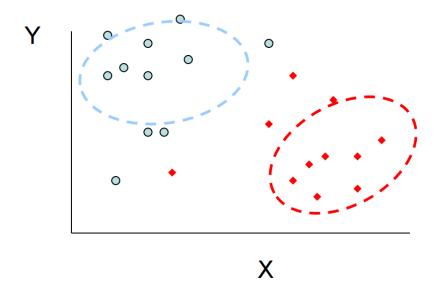
$$-P(x_i|y) = \frac{\sum_d \sum_j \delta(x_d^j = x_i, y_d = y)}{\sum_d \delta(y_d = y)}$$
$$-P(y) = \frac{\sum_d \delta(y_d = y)}{\sum_d 1}$$

	text	information	identify	mining	mined	is	useful	to	from	apple	delicious	Y
D1	1	1	1	1	0	1	1	1	0	0	0	1
D2	1	1	0	0	1	1	1	0	1	0	0	1
D3	0	0	0	0	0	1	0	0	0	1	1	0

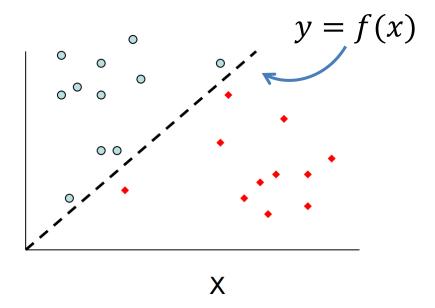
Discriminative v.s. generative models

All instances are considered for probability density estimation

Generative model



Discriminative model



More attention will be put onto the boundary points

Parametric form of decision boundary in Naïve Bayes

For binary case

$$-f(X) = sgn(\log P(y=1|X) - \log P(y=0|X))$$

$$= sgn\left(\log \frac{P(y=1)}{P(y=0)} + \sum_{i=1}^{|d|} c(x_i, d) \log \frac{P(x_i|y=1)}{P(x_i|y=0)}\right)$$

$$= sgn(w^T \overline{X})$$
where
$$w = \left(\log \frac{P(y=1)}{P(y=1)} \log \frac{P(x_1|y=1)}{P(x_1|y=1)}\right)$$

$$w = \left(\log \frac{P(y=1)}{P(y=0)}, \log \frac{P(x_1|y=1)}{P(x_1|y=0)}, \dots, \log \frac{P(x_v|y=1)}{P(x_v|y=0)}\right)$$

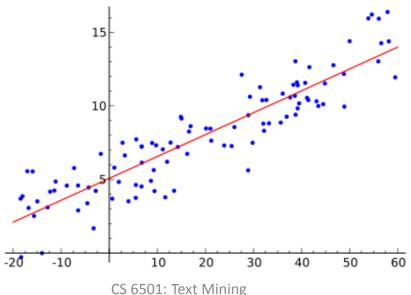
$$\bar{X} = (1, c(x_1, d), \dots, c(x_v, d))$$

Regression for classification?

Linear regression

$$-y \leftarrow w^T X$$

Relationship between a <u>scalar</u> dependent variable
 y and one or more explanatory variables

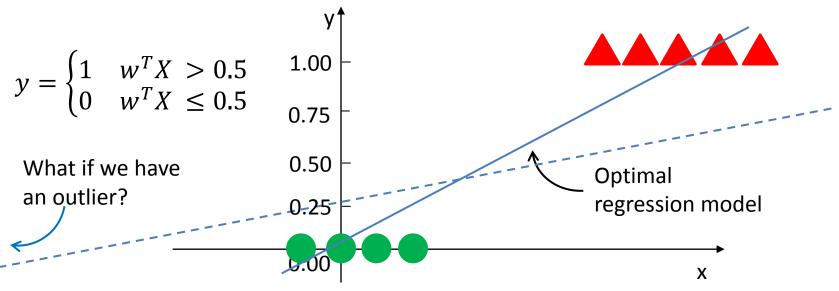


Regression for classification?

- Linear regression
 - $-y \leftarrow w^T X$

Y is discrete in a classification problem!

Relationship between a <u>scalar</u> dependent variable
 y and one or more explanatory variables



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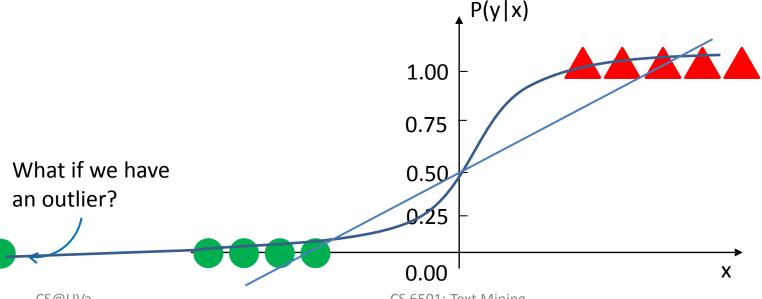
Regression for classification?

Logistic regression

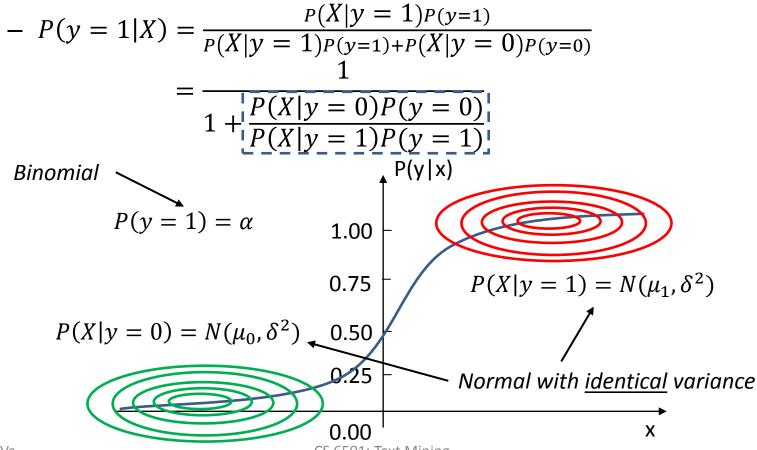
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$$-p(y|x) = \sigma(w^T X) = \frac{1}{1 + \exp(-w^T X)}$$

Directly modeling of class posterior



Why sigmoid function?



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Why sigmoid function?

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

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

$$= \frac{1}{1 + \exp\left(-\ln\frac{P(X|y=1)P(y=1)}{P(X|y=0)P(y=0)}\right)}$$

Why sigmoid function?

$$P(x|y) = \frac{1}{\delta\sqrt{2\pi}}e^{-\frac{(x-\mu)^2}{2\delta^2}}$$

■
$$\ln \frac{P(X|y=1)P(y=1)}{P(X|y=0)P(y=0)} = \ln \frac{P(y=1)}{P(y=0)} + \sum_{i=1}^{V} \ln \frac{P(x_i|y=1)}{P(x_i|y=0)}$$

$$= \ln \frac{\alpha}{1-\alpha} + \sum_{i=1}^{V} \left(\frac{\mu_{1i} - \mu_{0i}}{\delta_i^2} x_i - \frac{\mu_{1i}^2 - \mu_{0i}^2}{2\delta_i^2} \right)$$

$$= w_0 + \sum_{i=1}^{V} \frac{\mu_{1i} - \mu_{0i}}{\delta_i^2} x_i$$
Origin of the name:
$$= w_0 + w^T X$$

$$= \overline{w}^T \overline{X}$$

Why sigmoid function?

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

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

$$= \frac{1}{1 + \exp\left(-\frac{\ln\frac{P(X|y = 1)P(y = 1)}{P(X|y = 0)P(y = 0)}\right)}$$

$$= \frac{1}{1 + \exp(-\overline{w}^T \overline{X})}$$
Generalized Linear Model

Note: it is still a linear relation among the features!

For multi-class categorization

$$-P(y = k|X) = \frac{\exp(w_k^T X)}{\sum_{j=1}^K \exp(w_j^T X)}$$

$$-P(y=k|X) \propto \exp(w_k^T X)$$

Warning: redundancy in model parameters,

When K=2,

$$P(y = 1|X) = \frac{\exp(w_1^T X)}{\exp(w_1^T X) + \exp(w_0^T X)}$$
$$= \frac{1}{1 + \exp(-(w_1 - w_0)^T X)}$$
 \bar{w}

Decision boundary for binary case

$$-\hat{y} = \begin{cases} 1, p(y=1|X) > 0.5\\ 0, & otherwise \end{cases}$$

$$p(y=1|X) = \frac{1}{1 + \exp(-w^T X)} > 0.5$$
i.f.f.
$$\exp(-w^T X) < 1$$
i.f.f.
$$w^T X > 0$$

$$-\hat{y} = \begin{cases} 1, & w^T x > 0\\ 0, & otherwise \end{cases}$$
A linear model!

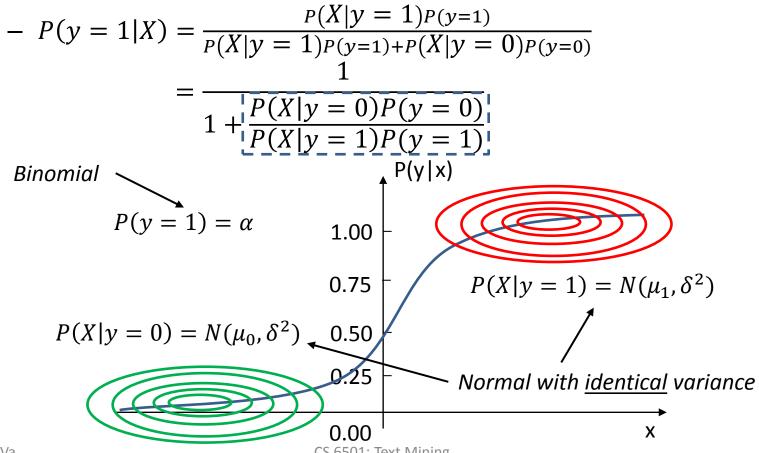
Decision boundary in general

$$-\hat{y} = argmax_{y}p(y|X)$$

$$= argmax_{y} \exp(w_{y}^{T}X)$$

$$= argmax_{y}w_{y}^{T}X$$
A linear model!

Summary



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Imagine we have the following

Documents

Sentiment

"happy", "good", "purchase", "item", "indeed"

positive

$$p(x = \text{"happy"}, y = 1) + p(x = \text{"good"}, y = 1) + p(x = \text{"purchase"}, y = 1) + p(x = \text{"item"}, y = 1) + p(x = \text{"indeed"}, y = 1) = 1$$

Question: find a distribution p(x, y) that satisfies this observation.

Answer1: p(x = "item", y = 1) = 1, and all the others 0

Answer2: p(x = "indeed", y = 1) = 0.5, p(x = "good", y = 1) = 0.5, and all the others 0

We have too little information to favor either one of them.

Occam's razor

- A problem-solving principle
 - "among competing hypotheses that predict equally well, the one with the fewest assumptions should be selected."
 - William of Ockham (1287–1347)
 - Principle of Insufficient Reason: "when one has no information to distinguish between the probability of two events, the best strategy is to consider them equally likely"
 - Pierre-Simon Laplace (1749–1827)

Imagine we have the following

Documents Sentiment "happy", "good", "purchase", "item", "indeed" positive

$$p(x = \text{"happy"}, y = 1) + p(x = \text{"good"}, y = 1) + p(x = \text{"purchase"}, y = 1) + p(x = \text{"item"}, y = 1) + p(x = \text{"indeed"}, y = 1) = 1$$

Question: find a distribution p(x, y) that satisfies this observation.

As a result, a *safer* choice would be:

$$p(x = "\cdot", y = 1) = 0.2$$

Equally favor every possibility

Imagine we have the following

Observations Sentiment "happy", "good", "purchase", "item", "indeed" positive 30% of time "good", "item" positive

$$p(x = \text{"happy"}, y = 1) + p(x = \text{"good"}, y = 1) + p(x = \text{"purchase"}, y = 1) + p(x = \text{"item"}, y = 1) + p(x = \text{"indeed"}, y = 1) = 1$$
 $p(x = \text{"good"}, y = 1) + p(x = \text{"item"}, y = 1) = 0.3$

Question: find a distribution p(x, y) that satisfies this observation.

Again, a safer choice would be:

$$p(x = "good", y = 1) = p(x = "item", y = 1) = 0.15$$
, and all the others $\frac{7}{30}$

Equally favor every possibility

Imagine we have the following

```
Observations Sentiment "happy", "good", "purchase", "item", "indeed" positive 30\% of time "good", "item" positive 50\% of time "good", "happy" positive p(x = \text{"happy"}, y = 1) + p(x = \text{"good"}, y = 1) + p(x = \text{"purchase"}, y = 1) + p(x = \text{"item"}, y = 1) + p(x = \text{"indeed"}, y = 1) = 1 p(x = \text{"good"}, y = 1) + p(x = \text{"item"}, y = 1) = 0.3 p(x = \text{"good"}, y = 1) + p(x = \text{"happy"}, y = 1) = 0.5
```

Question: find a distribution p(x, y) that satisfies this observation.

Time to think about:

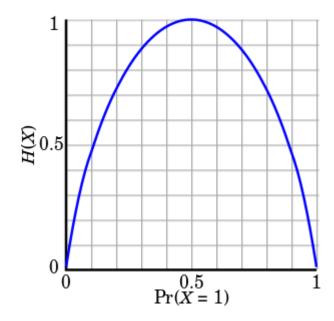
- 1) what do we mean by equally/uniformly favoring the models?
- 2) given all these constraints, how could we find the most preferred model?

Maximum entropy modeling

A measure of uncertainty of random events

$$-H(X) = E[I(X)] = -\sum_{x \in X} P(x) \log P(x)$$

Maximized when P(X) is uniform distribution





Question 1 is answered, then how about question 2?

- Indicator function
 - E.g., to express the observation that word 'good' occurs in a positive document

•
$$f(x,y) = \begin{cases} 1 & \text{if } y = 1 \text{ and } x = \text{`good'} \\ 0 & \text{otherwise} \end{cases}$$

Usually referred as feature function

 Empirical expectation of feature function over a corpus

$$-E[\tilde{p}(f)] = \sum_{x,y} \tilde{p}(x,y) f(x,y)$$
 where $\tilde{p}(x,y) = \frac{c(f(x,y))}{N}$ i.e., frequency of observing $f(x,y)$ in a given collection.

Expectation of feature function under a given statistical model

$$-E[p(f)] = \sum_{x,y} \tilde{p}(x) p(y|x) f(x,y)$$

Empirical distribution of x in the same collection.

Model's estimation of conditional distribution.

 When a feature is important, we require our preferred statistical model to accord with it

$$-C := \{ p \in P | E[p(f_i)] = E[\tilde{p}(f_i)], \forall i \in \{1, 2, ..., n\} \}$$

$$-E[p(f_i)] = E[\tilde{p}(f_i)]$$

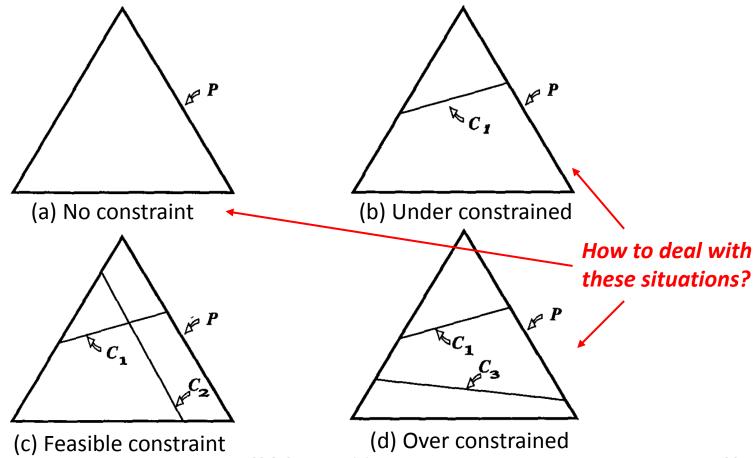
$$\sum_{x,y} \tilde{p}(x,y) f_i(x,y) = \sum_{x,y} \tilde{p}(x) p(y|x) f_i(x,y)$$



We only need to specify this in our preferred model!

Is Question 2 answered?

Let's visualize this



• To select a model from a set C of allowed probability distributions, choose the model $p^* \in C$ with maximum entropy H(p)

$$p^* = argmax_{p \in C} H(p)$$

$$p(y|x)$$

Both questions are answered!

 Let's solve this constrained optimization problem with Lagrange multipliers

Primal:

$$p^* = argmax_{p \in C}H(p)$$

Lagrangian:

a strategy for finding the local maxima and minima of a function subject to equality constraints

$$L(p,\lambda) = H(p) + \sum_{i} \lambda_{i}(p(f_{i}) - \tilde{p}(f_{i}))$$

 Let's solve this constrained optimization problem with Lagrange multipliers

Lagrangian:

$$L(p,\lambda) = H(p) + \sum_{i} \lambda_{i}(p(f_{i}) - \tilde{p}(f_{i}))$$
Dual:
$$p_{\lambda}(y|x) = \frac{1}{Z_{\lambda}(x)} \exp\left(\sum_{i} \lambda_{i} f_{i}(x,y)\right)$$

$$\Psi(\lambda) = -\sum_{x} \tilde{p}(x) \log Z_{\lambda}(x) + \sum_{i} \lambda_{i} \, \tilde{p}(f_{i})$$

 Let's solve this constrained optimization problem with Lagrange multipliers

Dual:

$$\Psi(\lambda) = -\sum_{x} \tilde{p}(x) \log Z_{\lambda}(x) + \sum_{i} \lambda_{i} \, \tilde{p}(f_{i})$$
where
$$Z_{\lambda} = \sum_{y} \exp\left(\sum_{i} \lambda_{i} f_{i}(x, y)\right)$$

Primal: maximum entropy

$$-p^* = argmax_{p \in C}H(p)$$

Dual: logistic regression

$$-p_{\lambda}(y|x) = \frac{1}{Z_{\lambda}(x)} \exp(\sum_{i} \lambda_{i} f_{i}(x, y))$$

where
$$Z_{\lambda} = \sum_{y} \exp\left(\sum_{i} \lambda_{i} f_{i}(x, y)\right)$$

 λ^* is determined by $\Psi(\lambda)$

Let's take a close look at the dual function

$$\Psi(\lambda) = -\sum_{x} \tilde{p}(x) \log Z_{\lambda}(x) + \sum_{i} \lambda_{i} \, \tilde{p}(f_{i})$$
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Maximum entropy principle

Let's take a close look at the dual function

$$\Psi(\lambda) = -\sum_{x} \tilde{p}(x) \log Z_{\lambda}(x) + \sum_{x} \tilde{p}(x) \sum_{i} \lambda_{i} \tilde{p}(f_{i})$$

$$= \sum_{x} \tilde{p}(x) \log \frac{\exp(\sum_{i} \lambda_{i} \tilde{p}(f_{i}))}{Z_{\lambda}(x)}$$

$$= \sum_{x} \tilde{p}(x) \log p(y|x)$$

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Maximum likelihood estimator!

Summary

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

$$= \frac{1}{1 + \frac{P(X|y = 0)P(y = 0)}{P(X|y = 1)P(y = 1)}}$$
Binomial
$$P(y = 1) = \alpha$$

$$0.75$$

$$P(X|y = 0) = N(\mu_0, \delta^2)$$

$$0.50$$

$$0.25$$
Normal with identical variance and variance of the property of the

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Why sigmoid function?

$$P(x|y) = \frac{1}{\delta\sqrt{2\pi}}e^{-\frac{(x-\mu)^2}{2\delta^2}}$$

$$\ln \frac{P(X|y=1)P(y=1)}{P(X|y=0)P(y=0)} = \ln \frac{P(y=1)}{P(y=0)} + \sum_{i=1}^{V} \ln \frac{P(x_i|y=1)}{P(x_i|y=0)}$$

$$= \ln \frac{\alpha}{1-\alpha} + \sum_{i=1}^{V} \left(\frac{\mu_{1i} - \mu_{0i}}{\delta_i^2} x_i - \frac{\mu_{1i}^2 - \mu_{0i}^2}{2\delta_i^2}\right)$$

$$= w_0 + \sum_{i=1}^{V} \frac{\mu_{1i} - \mu_{0i}}{\delta_i^2} x_i$$
Origin of the name:
$$= w_0 + w^T X$$

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Decision boundary for binary case

$$-\hat{y} = \begin{cases} 1, p(y=1|X) > 0.5\\ 0, & otherwise \end{cases}$$

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$$\exp(-w^T X) < 1$$
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$$-\hat{y} = \begin{cases} 1, & w^T x > 0\\ 0, & otherwise \end{cases}$$
A linear model!

Recap: Occam's razor

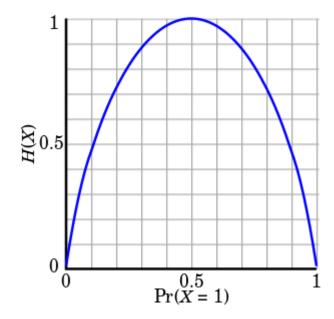
- A problem-solving principle
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Recap: maximum entropy principle

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Recap: maximum entropy principle

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Dual: logistic regression

$$-p_{\lambda}(y|x) = \frac{1}{Z_{\lambda}(x)} \exp(\sum_{i} \lambda_{i} f_{i}(x, y))$$

where
$$Z_{\lambda} = \sum_{y} \exp\left(\sum_{i} \lambda_{i} f_{i}(x, y)\right)$$

 λ^* is determined by $\Psi(\lambda)$

Questions haven't been answered

- Class conditional density
 - Why it should be Gaussian with equal variance?
- Model parameters
 - What is the relationship between w and λ ?
 - How to estimate them?

Maximum entropy principle

Let's take a close look at the dual function

$$\Psi(\lambda) = -\sum_{x} \tilde{p}(x) \log Z_{\lambda}(x) + \sum_{x} \tilde{p}(x) \sum_{i} \lambda_{i} \tilde{p}(f_{i})$$

$$= \sum_{x} \tilde{p}(x) \log \frac{\exp(\sum_{i} \lambda_{i} \tilde{p}(f_{i}))}{Z_{\lambda}(x)}$$

$$= \sum_{x} \tilde{p}(x) \log p(y|x)$$
Maximum likelihood estimator!

Maximum entropy principle

 The maximum entropy model subject to the constraints C has the parametric solution $p_{\lambda}^{*}(y|x)$ where the parameter values λ^{*} can be determined by maximizing the likelihood function of $p_{\lambda}(y|x)$ over a training set



Features follow

With a Gaussian distribution, differential entropy is maximized for a given variance. Maximum entropy Gaussian distribution

Logistic regression

Why sigmoid function?

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Maximum entropy principle

 Let's solve this constrained optimization problem with Lagrange multipliers

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$$L(p,\lambda) = H(p) + \sum_{i} \lambda_{i}(p(f_{i}) - \tilde{p}(f_{i}))$$

- Maximum likelihood estimation
 - $L(w) = \sum_{d \in D} y_d \log p(y_d = 1|X_d) + (1 y_d) \log p(y_d = 0|X_d)$
 - Take gradient of L(w) with respect to w

$$\frac{\partial L(w)}{\partial w} = \sum_{d \in D} y_d \frac{\partial \log p(y_d = 1|X_d)}{\partial w} + (1 - y_d) \frac{\partial \log p(y_d = 0|X_d)}{\partial w}$$

Maximum likelihood estimation

$$\frac{\partial \log p(y_d=1|X_d)}{\partial w} = -\frac{\partial \log(1+\exp(-w^T X_d))}{\partial w}$$

$$= \frac{\exp(-w^T X_d)}{1+\exp(-w^T X_d)} X_d$$

$$= (1-p(y_d=1|X_d)) X_d$$

$$\frac{\partial \log p(y_d=0|X_d)}{\partial w} = (0-p(y_d=1|X_d)) X_d$$

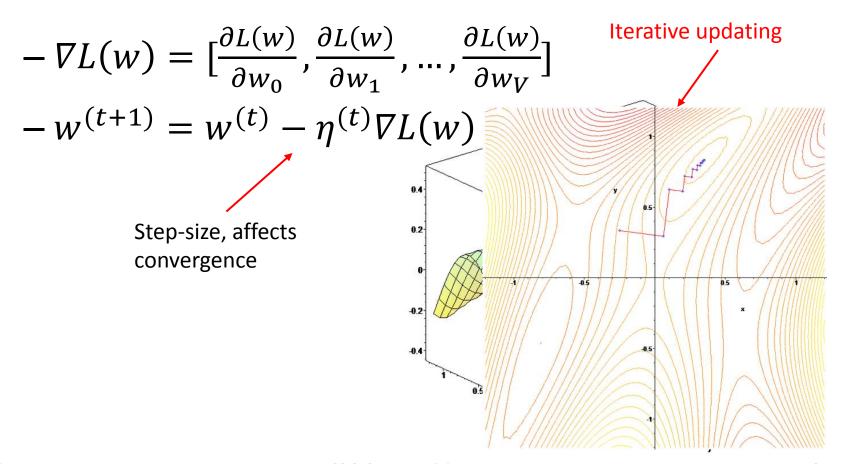
- Maximum likelihood estimation
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 - Take gradient of L(w) with respect to w

$$\begin{split} \frac{\partial L(w)}{\partial w} &= \sum_{d \in D} y_d \boxed{\frac{\partial \log p(y_d = 1|X_d)}{\partial w}} + (1 - y_d) \boxed{\frac{\partial \log p(y_d = 0|X_d)}{\partial w}} \\ &= \sum_{d \in D} y_d \Big(1 - p(y_d = 1|X_d)\Big) X_d + (1 - y_d) \Big(0 - p(y_d = 1|X_d)\Big) X_d \\ &= \sum_{d \in D} \underbrace{\Big(y_d - p(y = 1|X_d)\Big) X_d}_{\text{Concave function for } w} \boxed{\frac{\text{Good news: neat format, concave function for } w}{\text{Bad news: no close form solution}} \end{split}$$

Can be easily generalized to multi-class case

Gradient-based optimization

Gradient descent



Stochastic gradient descent

while not converge

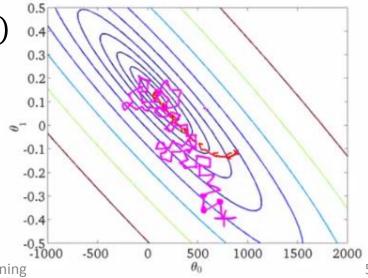
randomly choose $d \in D$

$$\nabla L_d(w) = \left[\frac{\partial L_d(w)}{\partial w_0}, \frac{\partial L_d(w)}{\partial w_1}, \dots, \frac{\partial L_d(w)}{\partial w_V}\right]$$

$$w^{(t+1)} = w^{(t)} - \eta^{(t)} \nabla L_d(w)$$

$$\eta^{(t+1)} = a\eta^{(t)}$$

Gradually shrink the step-size



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Batch gradient descent

while not converge

Compute gradient w.r.t. all training instances

$$\nabla L_D(w) = \left[\frac{\partial L_D(w)}{\partial w_0}, \frac{\partial L_D(w)}{\partial w_1}, \dots, \frac{\partial L_D(w)}{\partial w_V}\right]$$
Compute step size $\eta^{(t)}$

$$w^{(t+1)} = w^{(t)} - \eta^{(t)} \nabla L_d(w)$$

Line search is required to ensure sufficient decent

First order method

Second order methods, e.g., quasi-Newton method and conjugate gradient, provide faster convergence

Model regularization

- Avoid over-fitting
 - We may not have enough samples to well estimate model parameters for logistic regression
 - Regularization
 - Impose additional constraints over the model parameters
 - E.g., sparsity constraint enforce the model to have more zero parameters

Model regularization

- L2 regularized logistic regression
 - Assume the model parameter w is drawn from Gaussian: $w \sim N(0, \sigma^2)$
 - $-p(y_d, w|X_d) \propto p(y_d|X_d, w)p(w)$

$$-L(w) = \sum_{d \in D} [y_d \log p(y_d = 1 | X_d) + (1 - y_d) \log p(y_d = 0 | X_d)] - \frac{w^T w}{2\sigma^2}$$

$$L2\text{-norm of } w$$

Generative V.S. discriminative models

Generative

- Specifying joint distribution
 - Full probabilistic specification for all the random variables
- Dependence assumption has to be specified for p(X|y) and p(y)
- Flexible, can be used in unsupervised learning

Discriminative

- Specifying conditional distribution
 - Only explain the target variable
- Arbitrary features can be incorporated for modeling p(y|X)
- Need labeled data, only suitable for (semi-) supervised learning

Naïve Bayes V.S. Logistic regression

Naive Bayes

- Conditional independence
 - $p(X|y) = \prod_i p(x_i|y)$
- Distribution assumption of $p(x_i|y)$
- # parameters

$$- k(V + 1)$$

- Model estimation
 - Closed form MLE
- Asymptotic convergence rate

$$- \epsilon_{NB,n} \le \epsilon_{NB,\infty} + O(\sqrt{\frac{\log V}{n}})$$

Logistic Regression

- No independence assumption
- Functional form assumption of $p(y|X) \propto \exp(w_y^T X)$
- # parameters

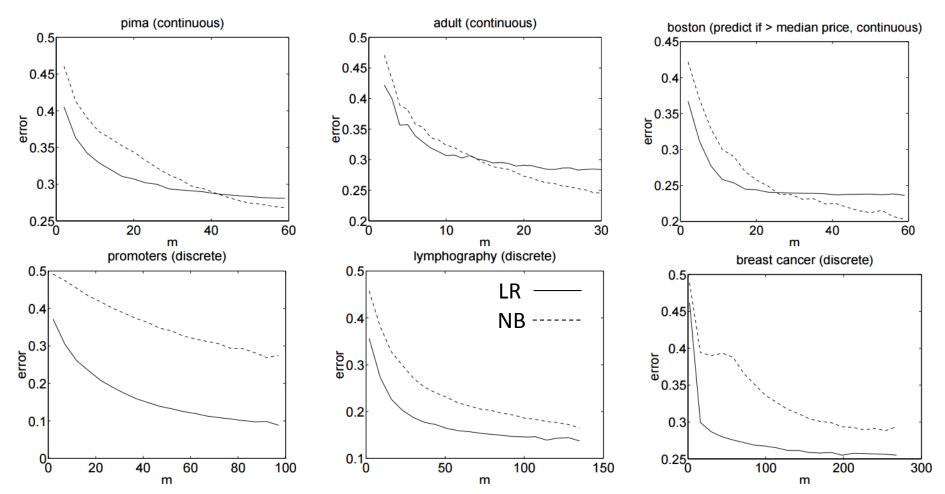
$$-(k-1)(V+1)$$

- Model estimation
 - Gradient-based MLE
- Asymptotic convergence rate

$$-\epsilon_{LR,n} \le \epsilon_{LR,\infty} + O(\sqrt{\frac{v}{n}})$$

Need more training data

Naïve Bayes V.S. Logistic regression



"On discriminative vs. generative classifiers: A comparison of logistic regression and naive bayes." – Ng, Jordan NIPS 2002, UCI Data set

What you should know

- Two different derivations of logistic regression
 - Functional form from Naïve Bayes assumptions
 - p(X|y) follows equal variance Gaussian
 - Sigmoid function
 - Maximum entropy principle
 - Primal/dual optimization
 - Generalization to multi-class
- Parameter estimation
 - Gradient-based optimization
 - Regularization
- Comparison with Naïve Bayes

Today's reading

- Speech and Language Processing
 - Chapter 6: Hidden Markov and Maximum Entropy
 Models
 - 6.6 Maximum entropy models: background
 - 6.7 Maximum entropy modeling