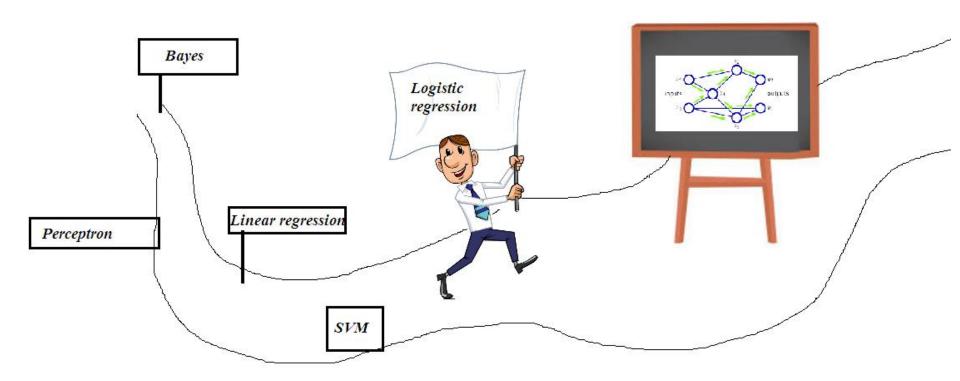
Logistic Regression

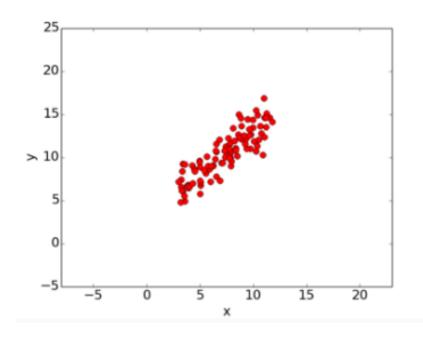
Sigmoid Activation in Perceptron



Overview

- Linear Regression Review
- Linear Regression as classifier Problem with outliers
- Logistic Regression Sigmoid
 - Classifier ?
 - Criterion used in logistic regression
 - Solution

Linear regression



$$y = mx + b$$

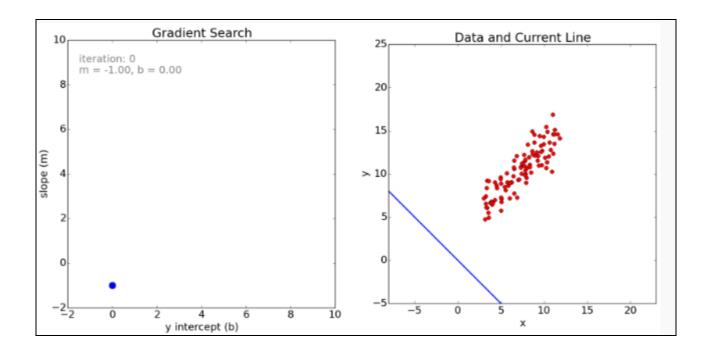
We want to fit a straight line (in 2D case). The sample we are given with is $\{(x_1, y_1), (x_2, y_2), ..., (x_N, y_N)\}.$

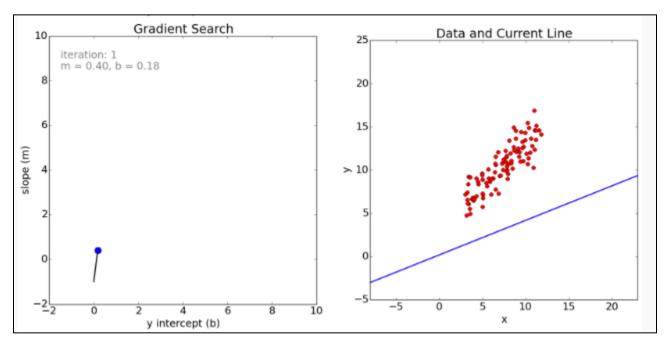
We want to find (m, b).

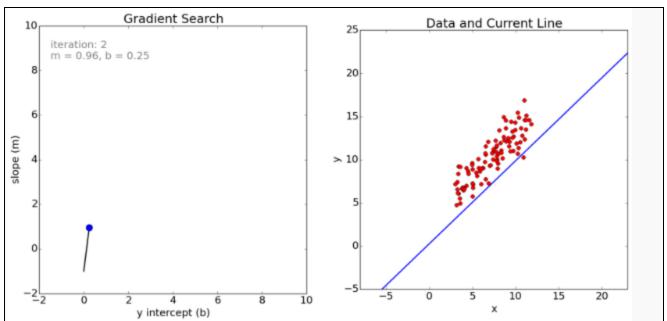
In the space (m, b) what is the function we are going to define? Minimum value of that function should be a solution for us.

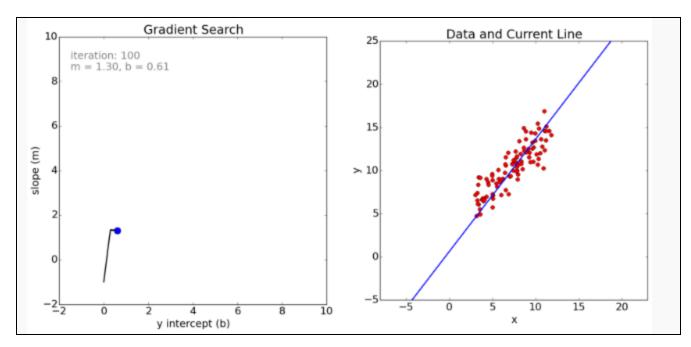
Error_(m,b) =
$$\frac{1}{N} \sum_{i=1}^{N} (y_i - (mx_i + b))^2$$

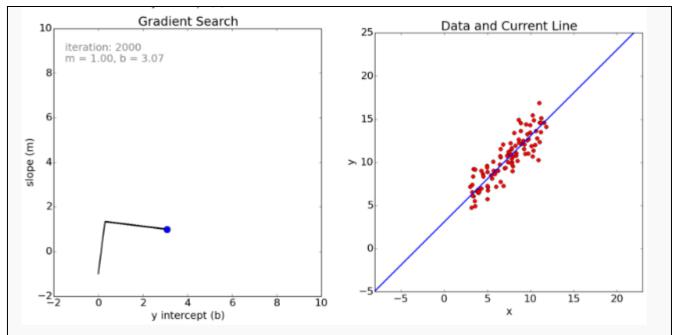
$$\frac{\partial}{\partial \mathbf{m}} = \frac{2}{N} \sum_{i=1}^{N} -x_i (y_i - (mx_i + b))$$
$$\frac{\partial}{\partial \mathbf{b}} = \frac{2}{N} \sum_{i=1}^{N} -(y_i - (mx_i + b))$$









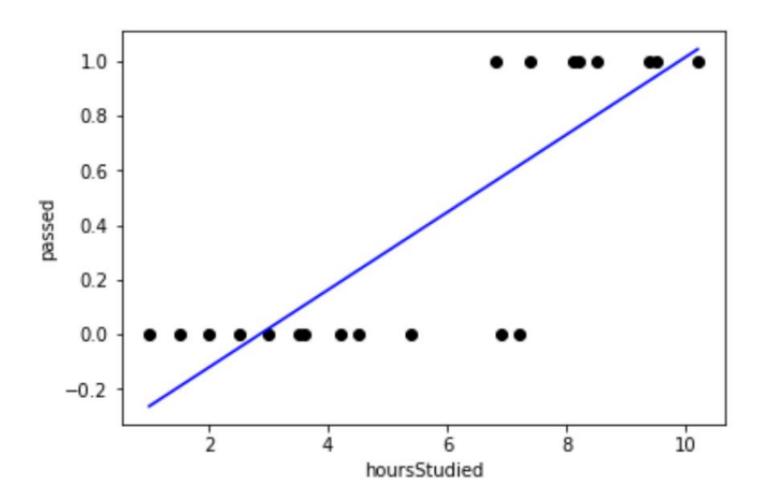


Closed form solution

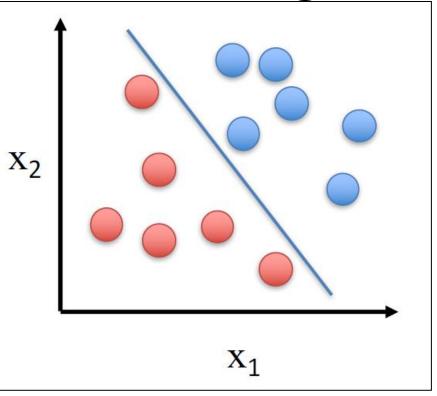
- Since the criterion that is minimized is quadratic, the linear regression problem must be having a closed form solution.
- This is nothing but applying the Newton's descent method.

Linear Regression for classification

Example with 1D data

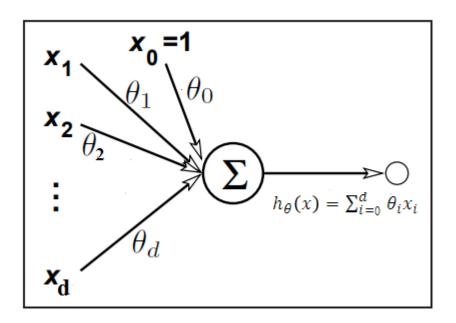


Linear Regression for classification



Example with 2D data

Direct attempt, in learning the linear discriminant



$$h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \dots + \theta_d x_d$$

The parameter vector θ is learnt from the data such that the sum of squared error

$$E(\theta) = \frac{1}{2} \sum_{i=1}^{n} (y^{(i)} - h_{\theta}(x^{(i)}))^{2}$$

Where the training set

$$D = \{ (x^{(i)}, y^{(i)}) | i = 1, \dots, n \}$$

 $E(\theta)$ is convex(also quadratic) \Rightarrow no local minima problem (closed form solution)

Training Procedure

•
$$\nabla_{\theta}(E) = \sum_{i=1}^{n} (y^{(i)} - h_{\theta}(x^{(i)}))(-x^{(i)})$$

Batch Method:

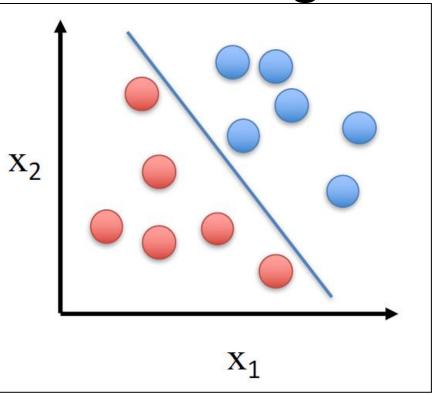
•
$$\theta_{new} = \theta + \eta \sum_{i=1}^{n} (y^{(i)} - h_{\theta}(x^{(i)})) x^{(i)}$$

Single Sample (Stochastic update)

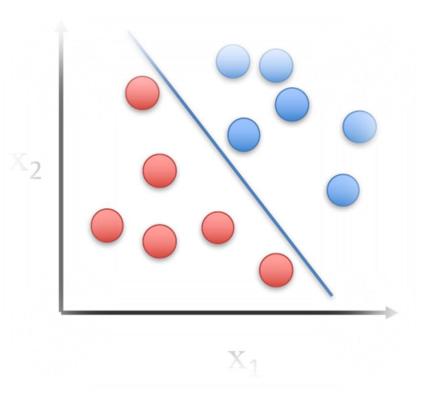
•
$$\theta_{new} = \theta + \eta (y^{(i)} - h_{\theta}(x^{(i)})) x^{(i)}$$

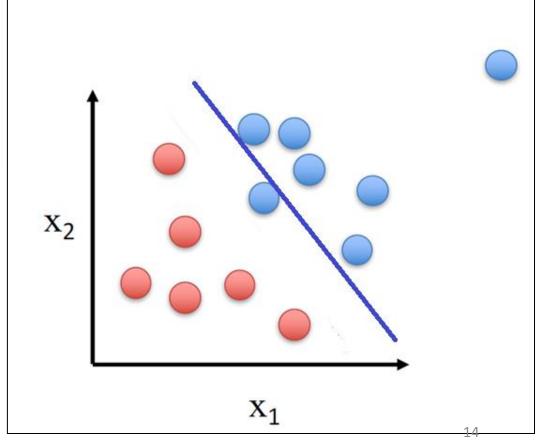
•
$$h_{\theta}(x^{(i)}) = \theta^T x^{(i)}$$

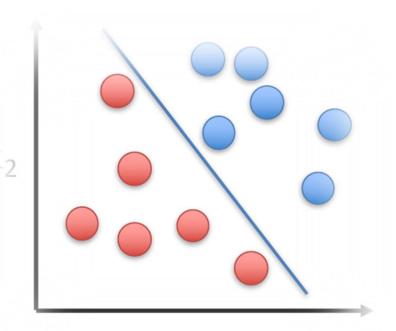
Linear Regression for classification



But, outliers can be a big problem.

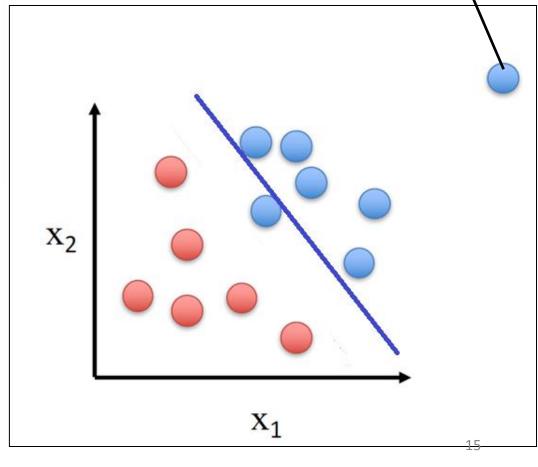






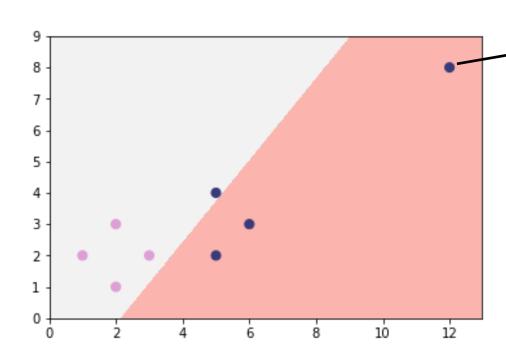
This is well within the blue class. This is a good training example.

Why this is causing us problem??



This is well within the blue class. This is a good training example.

Why this is causing us problem??



Note

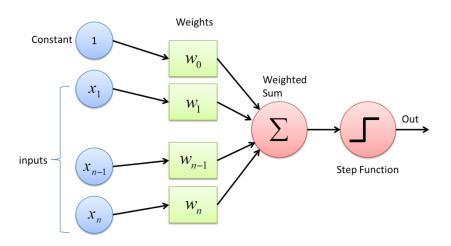
 Perceptron (Rosenblatt) does not have this problem (i.e., problem with seeming outliers).

Note

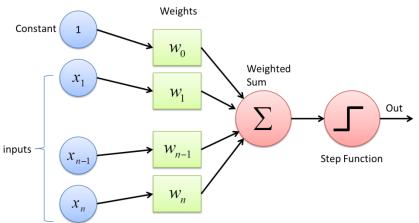
- Perceptron (Rosenblatt) does not have this problem (i.e., problem with seeming outliers).
- But works only for linearly separable data.

Note

- Perceptron (Rosenblatt) does not have this problem (i.e., problem with seeming outliers).
- But works only for linearly separable data.
- Actually, it is

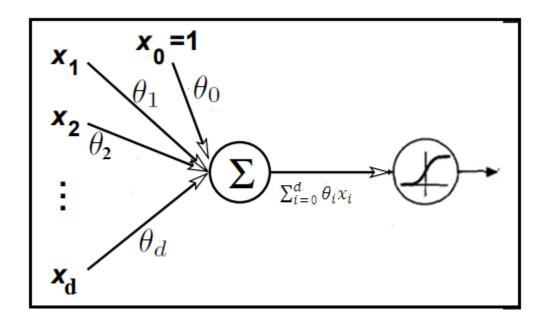


- Step (or Sign) function is not differentiable.
- So we can't employ gradient descent to get the minimum error (in this formulation) solution.

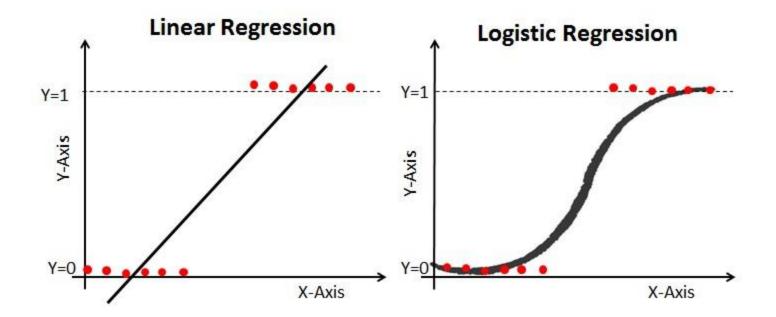




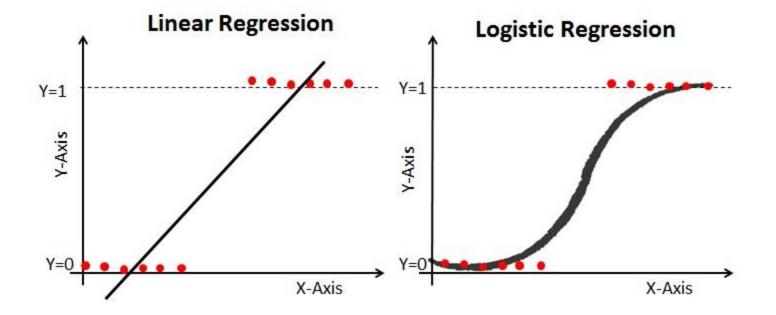
Logistic Regression



1D: what it does

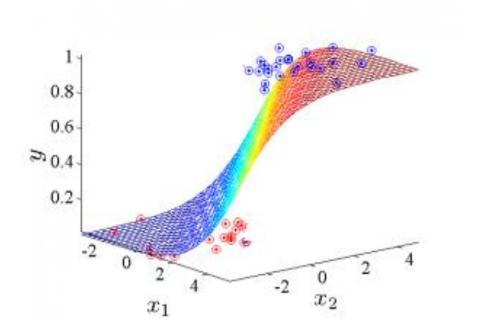


1D: what it does



See, the seeming outliers are indeed very good fits.

2D: what it does



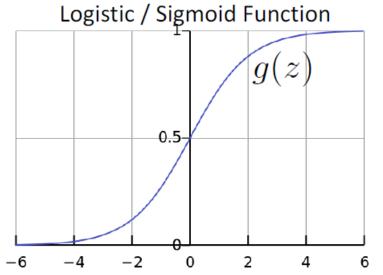
Notation used

•
$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix}$$
, $x = \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_d \end{bmatrix}$

Logistic regression model:

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g(\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x})$$
$$g(z) = \frac{1}{1 + e^{-z}}$$

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^{\mathsf{T}} \boldsymbol{x}}}$$



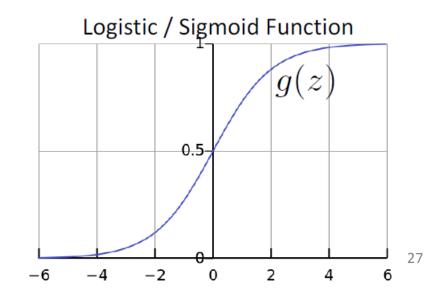
Notation used

• Given $\left\{\left(\boldsymbol{x}^{(1)}, y^{(1)}\right), \left(\boldsymbol{x}^{(2)}, y^{(2)}\right), \dots, \left(\boldsymbol{x}^{(n)}, y^{(n)}\right)\right\}$ where $\boldsymbol{x}^{(i)} \in \mathbb{R}^d, \ y^{(i)} \in \{0, 1\}$

Logistic regression model:

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g(\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x})$$
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$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^{\mathsf{T}} \boldsymbol{x}}}$$



Differentiation of the sigmoid

$$g'(z) = \frac{d}{dz} \frac{1}{1 + e^{-z}}$$

$$= \frac{1}{(1 + e^{-z})^2} (e^{-z})$$

$$= \frac{1}{(1 + e^{-z})} \cdot \left(1 - \frac{1}{(1 + e^{-z})}\right)$$

$$= g(z)(1 - g(z)).$$

Logistic Regression Objective Function

Can't just use squared loss as in linear regression:

$$J(\boldsymbol{\theta}) = \frac{1}{2n} \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right)^{2}$$

Using the logistic regression model

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^{\mathsf{T}} \boldsymbol{x}}}$$

results in a non-convex optimization

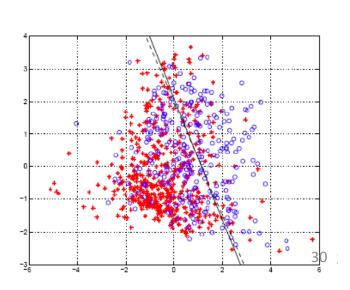
Classification Based on Probability

- Instead of just predicting the class, give the probability of the instance being that class
 - i.e., learn $p(y \mid \boldsymbol{x})$
- Comparison to perceptron:
 - Perceptron doesn't produce probability estimate

Recall that:

$$0 \le p(\text{event}) \le 1$$

 $p(\text{event}) + p(\neg \text{event}) = 1$



- Takes a probabilistic approach to learning discriminative functions (i.e., a classifier)
- $h_{\theta}(x)$ should give $p(y = 1 \mid x; \theta)$

- Want $0 \le h_{\boldsymbol{\theta}}(\boldsymbol{x}) \le 1$ -

Can't just use linear regression with a threshold

Interpretation of Hypothesis Output

$$h_{\boldsymbol{\theta}}(\boldsymbol{x})$$
 = estimated $p(y=1 \mid \boldsymbol{x}; \boldsymbol{\theta})$

Example: Cancer diagnosis from tumor size

$$\boldsymbol{x} = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ \text{tumorSize} \end{bmatrix}$$
 $h_{\boldsymbol{\theta}}(\boldsymbol{x}) = 0.7$

→ Tell patient that 70% chance of tumor being malignant

Note that: $p(y = 0 | x; \theta) + p(y = 1 | x; \theta) = 1$

Therefore, $p(y = 0 \mid x; \theta) = 1 - p(y = 1 \mid x; \theta)$

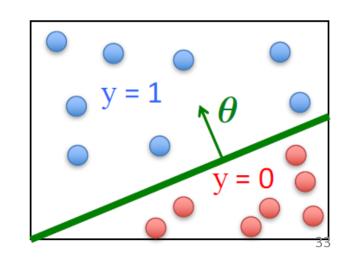
Logistic Regression

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g\left(\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}\right)$$

$$g(z) = \frac{1}{1 + e^{-z}}$$

$$\theta^{\mathsf{T}}\boldsymbol{x} \text{ should be large } \underbrace{\begin{array}{c} 0.5 \\ \text{negative} \\ \text{values for negative instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large } \underbrace{\begin{array}{c} \theta^{\mathsf{T}}\boldsymbol{x} \\ \text{values for positive instances} \end{array}}_{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}} \text{ should be large }$$

- Assume a threshold and...
 - Predict y = 1 if $h_{\theta}(x) \ge 0.5$
 - Predict y = 0 if $h_{\boldsymbol{\theta}}(\boldsymbol{x}) < 0.5$



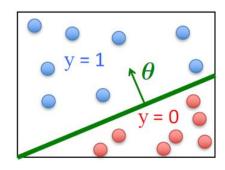
What we want ...??

We have

$$P(y = 1 \mid x; \theta) = h_{\theta}(x)$$

$$P(y = 0 \mid x; \theta) = 1 - h_{\theta}(x)$$

Given



• Find θ so that the data agrees to the maximum extent.

We can use maximum likelihood parameter estimation (MLE)

• Likelihood of data is given by: $l(\theta) = \prod_{i=1}^{n} p(y^{(i)} \mid \boldsymbol{x}^{(i)}; \boldsymbol{\theta})$

• So, looking for the heta that maximizes the likelihood

$$\boldsymbol{\theta}_{\text{MLE}} = \arg \max_{\boldsymbol{\theta}} l(\boldsymbol{\theta}) = \arg \max_{\boldsymbol{\theta}} \prod_{i=1} p(y^{(i)} \mid \boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

Can take the log without changing the solution:

$$\boldsymbol{\theta}_{\text{MLE}} = \arg \max_{\boldsymbol{\theta}} \log \prod_{i=1}^{n} p(y^{(i)} \mid \boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

$$= \arg \max_{\boldsymbol{\theta}} \sum_{i=1} \log p(y^{(i)} \mid \boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

$$P(y = 1 \mid x; \theta) = h_{\theta}(x)$$

$$P(y = 0 \mid x; \theta) = 1 - h_{\theta}(x)$$

Note that this can be written more compactly as

$$p(y \mid x; \theta) = (h_{\theta}(x))^{y} (1 - h_{\theta}(x))^{1-y}$$

Likelihood

$$L(\theta) = \prod_{i=1}^{n} p(y^{(i)} \mid x^{(i)}; \theta)$$

$$= \prod_{i=1}^{n} \left(h_{\theta}(x^{(i)}) \right)^{y^{(i)}} \left(1 - h_{\theta}(x^{(i)}) \right)^{1 - y^{(i)}}$$

Log-likelihood

$$\ell(\theta) = \log L(\theta)$$

$$= \sum_{i=1}^{n} y^{(i)} \log h(x^{(i)}) + (1 - y^{(i)}) \log(1 - h(x^{(i)}))$$

Find θ that maximizes $l(\theta)$

- $l(\theta)$ is taken to be the criterion, but, note this has to be maximized.
- We can employ gradient ascent method.
- We can show that, the negative of the log-likelihood, i.e., $-l(\theta)$ which should be minimized is convex (hence no local minima problem)
- For proof of this refer the link
 http://mathgotchas.blogspot.com/2011/10/why-is-error-function-minimized-in.html

•
$$\nabla_{\theta} l(\theta) = (y - h_{\theta}(x)) x$$

- Note, here x is a vector.
- This is for a single training example.

This we obtained from,

$$\begin{split} \frac{\partial}{\partial \theta_j} \ell(\theta) &= \left(y \frac{1}{g(\theta^T x)} - (1 - y) \frac{1}{1 - g(\theta^T x)} \right) \frac{\partial}{\partial \theta_j} g(\theta^T x) \\ &= \left(y \frac{1}{g(\theta^T x)} - (1 - y) \frac{1}{1 - g(\theta^T x)} \right) g(\theta^T x) (1 - g(\theta^T x)) \frac{\partial}{\partial \theta_j} \theta^T x \\ &= \left(y (1 - g(\theta^T x)) - (1 - y) g(\theta^T x) \right) x_j \\ &= \left(y - h_{\theta}(x) \right) x_j \end{split}$$

Stochastic or single sample update rule

•
$$\theta_{new}$$
 = $\theta + \eta \nabla_{\theta} l(\theta)$
= $\theta + \eta (y - h_{\theta}(x)) x$

Batch Method

$$\theta_{new} = \theta + \eta \sum_{i=1}^{n} (y^{(i)} - h_{\theta}(x^{(i)})) x^{(i)}$$

Stochastic or single sample update rule

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Batch Method

$$\theta_{new} = \theta + \eta \sum_{i=1}^{n} (y^{(i)} - h_{\theta}(x^{(i)})) x^{(i)}$$

This looks IDENTICAL to linear regression!!!

However, the form of the model is very different:

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^{\mathsf{T}} \boldsymbol{x}}}$$

• The End

Supplementary Material

•
$$h_{\theta}(x) = \sum_{i=1}^{d} \theta_i x_i$$