

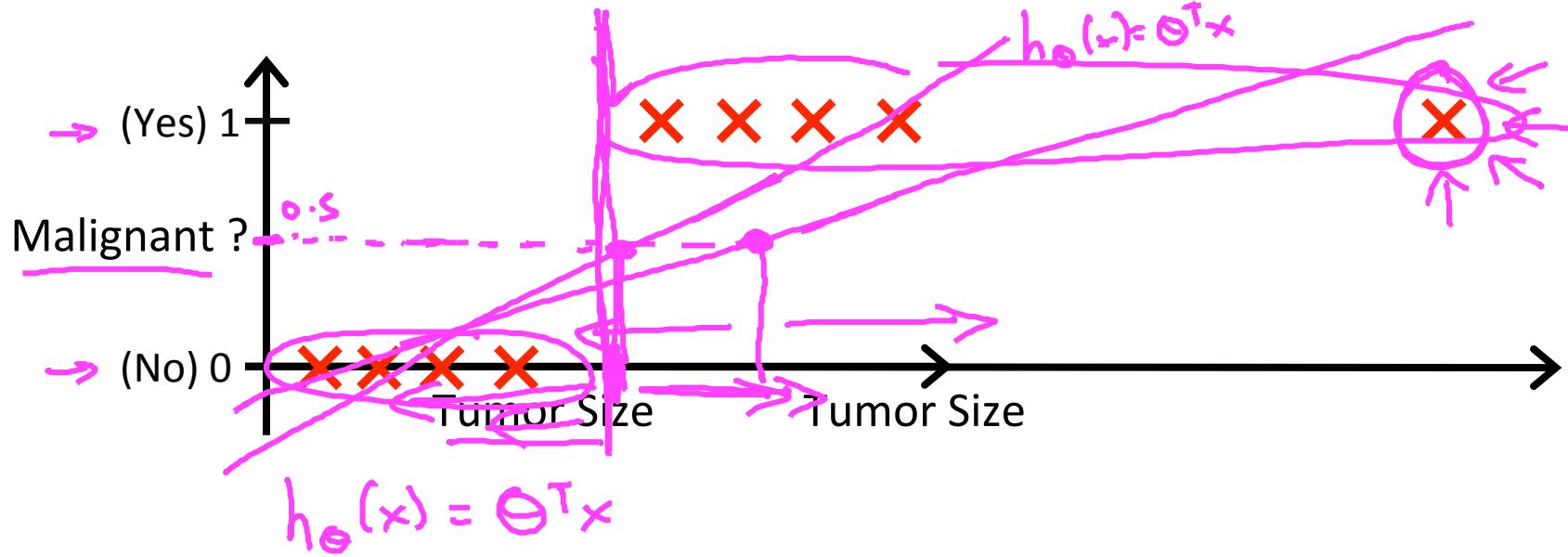
Machine Learning

Logistic Regression

Classification

Classification

- Email: Spam / Not Spam?
 - Online Transactions: Fraudulent (Yes / No)?
 - Tumor: Malignant / Benign ?
- $y \in \{0, 1\}$
- 0: “Negative Class” (e.g., benign tumor)
- 1: “Positive Class” (e.g., malignant tumor)
- $y \in \{0, 1, 2, 3\}$



→ Threshold classifier output $h_{\theta}(x)$ at 0.5:

→ If $h_{\theta}(x) \geq 0.5$, predict "y = 1"

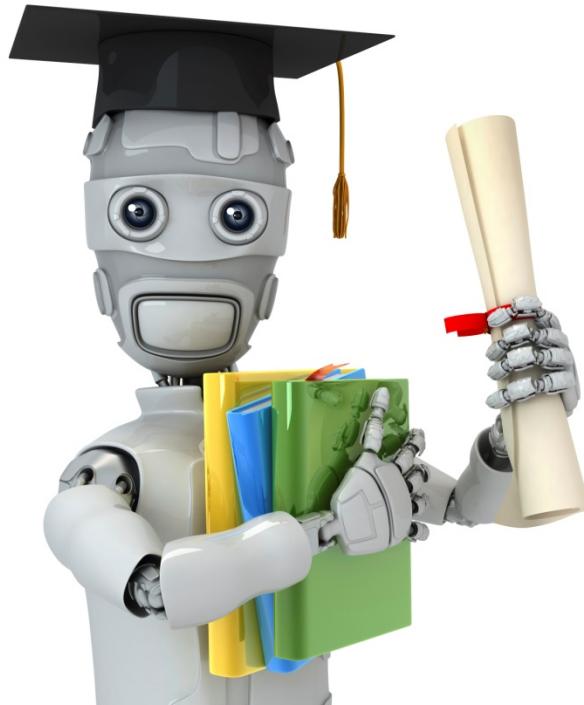
If $h_{\theta}(x) < 0.5$, predict "y = 0"

Classification: $y = 0 \text{ or } 1$

$h_\theta(x)$ can be $\underline{> 1}$ or $\underline{< 0}$

Logistic Regression: $0 \leq h_\theta(x) \leq 1$

(Classification)



Machine Learning

Logistic Regression

Hypothesis Representation

Logistic Regression Model

Want $0 \leq h_\theta(x) \leq 1$

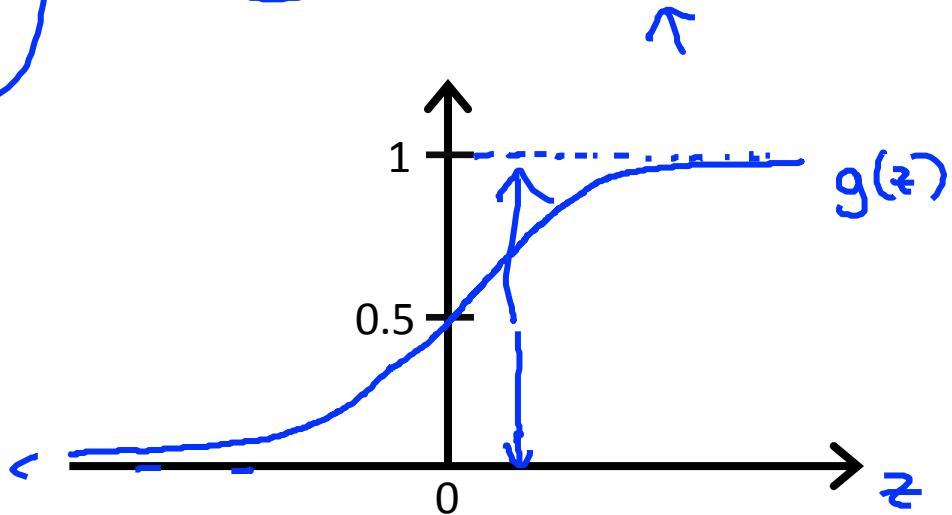
$$h_\theta(x) = g(\theta^T x)$$

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

$\theta^T x$

- Sigmoid function
- Logistic function

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



Parameters $\underline{\theta}$

Interpretation of Hypothesis Output

$$h_{\theta}(x)$$

$h_{\theta}(x)$ = estimated probability that $y = 1$ on input x

Example: If $x = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ \text{tumorSize} \end{bmatrix}$

$h_{\theta}(x) = 0.7$ $y=1$

Tell patient that 70% chance of tumor being malignant

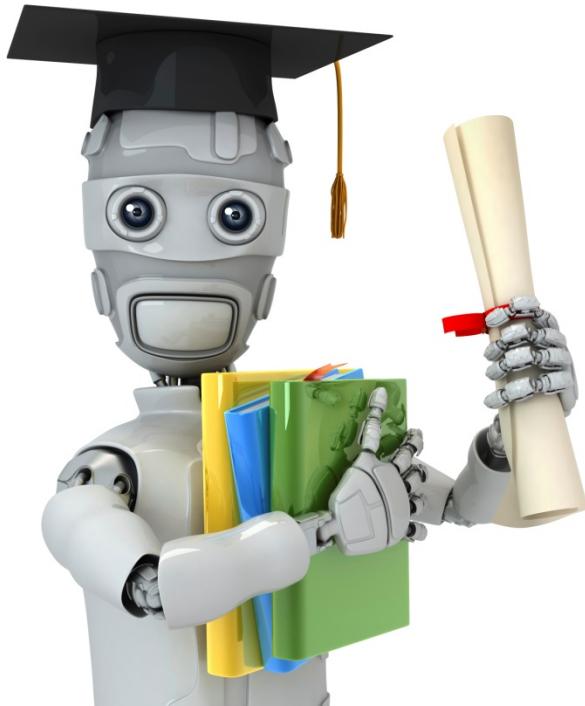
$$h_{\theta}(x) = \underline{P(y=1|x; \theta)}$$

“probability that $y = 1$, given x , parameterized by θ ”

$y = 0$ or 1

$$\rightarrow P(y = 0|x; \theta) + P(y = 1|x; \theta) = 1$$

$$\rightarrow P(y = 0|x; \theta) = 1 - P(y = 1|x; \theta)$$



Machine Learning

Logistic Regression

Decision boundary

Logistic regression

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

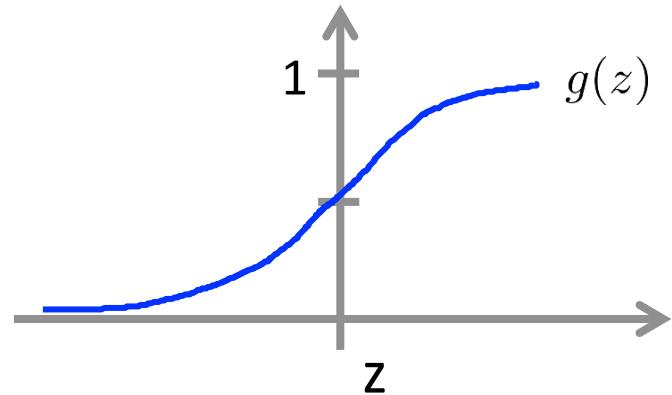
$$g(z) = \frac{1}{1+e^{-z}}$$

Suppose predict " $y = 1$ " if $h_{\theta}(x) \geq 0.5$

$$\theta^T x \geq 0$$

predict " $y = 0$ " if $h_{\theta}(x) < 0.5$

$$\theta^T x < 0$$



$$g(z) \geq 0.5$$

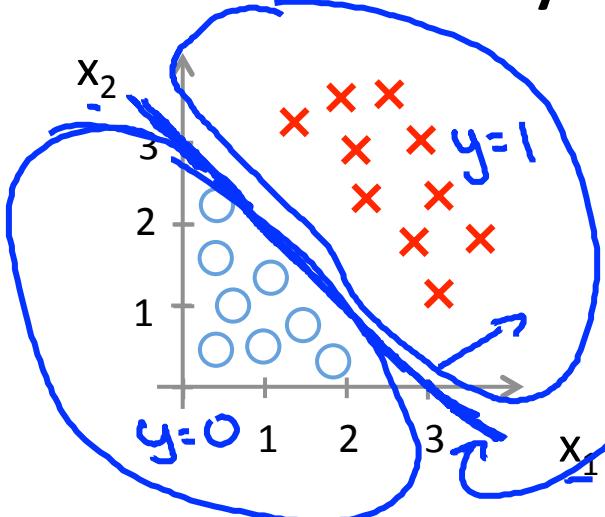
when $z \geq 0$

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

$$g(z) < 0.5$$

when $z < 0$

Decision Boundary



$$\Theta = \begin{bmatrix} -3 \\ 1 \\ 1 \end{bmatrix} \leftarrow$$

$$h_{\theta}(x) = g(\theta_0 + \underline{\theta_1 x_1} + \underline{\theta_2 x_2})$$

Decision boundary

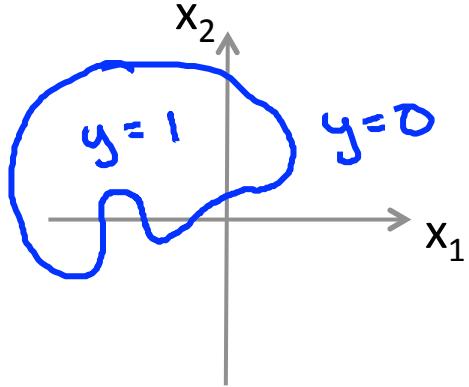
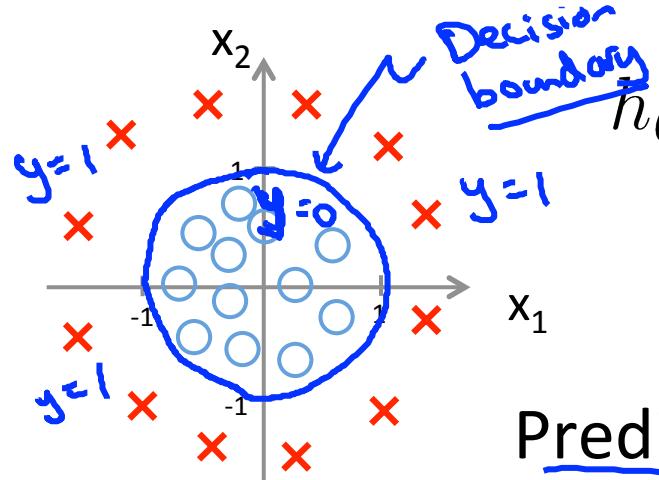
Predict " $y = 1$ " if $\underline{-3 + x_1 + x_2 \geq 0}$
 $\Theta^T x$

$$\underline{x_1 + x_2 \geq 3}$$

$$\begin{array}{l} x_1 + x_2 < 3 \\ \rightarrow y = 0 \end{array}$$

$$\begin{array}{l} x_1, x_2 \\ \rightarrow h_{\theta}(x) = 0.5 \\ x_1 + x_2 = 3 \end{array}$$

Non-linear decision boundaries



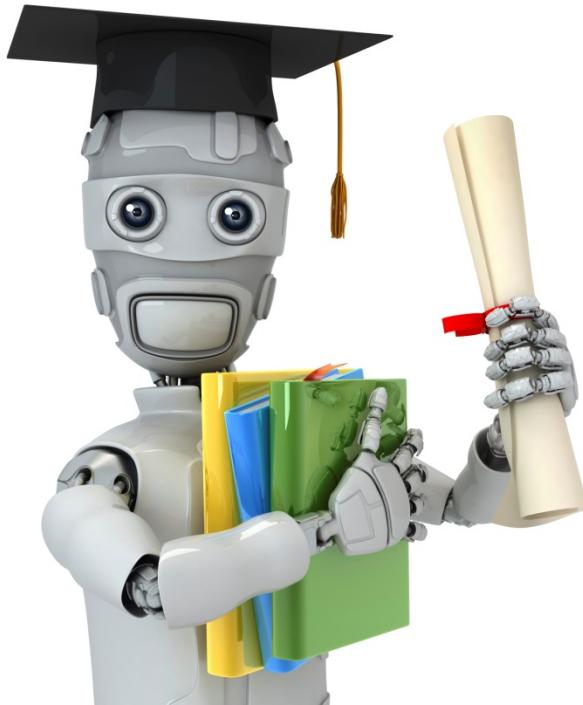
$$h_{\theta}(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2)$$

$$\theta = \begin{bmatrix} -1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Predict " $y = 1$ " if $\boxed{x_1^2 + x_2^2 \geq 1}$

$$\boxed{x_1^2 + x_2^2 \geq 1}$$

$$h_{\theta}(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 \underline{x_1^2} + \theta_4 \underline{x_1^2 x_2} + \theta_5 \underline{x_1^2 x_2^2} + \theta_6 \underline{x_1^3 x_2} + \dots)$$



Machine Learning

Logistic Regression

Cost function

Training set:

m examples

$$x \in \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix} \quad \mathbb{R}^{n+1}$$

$x_0 = 1, y \in \{0, 1\}$

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

How to choose parameters θ ?

Cost function

→ Linear regression:

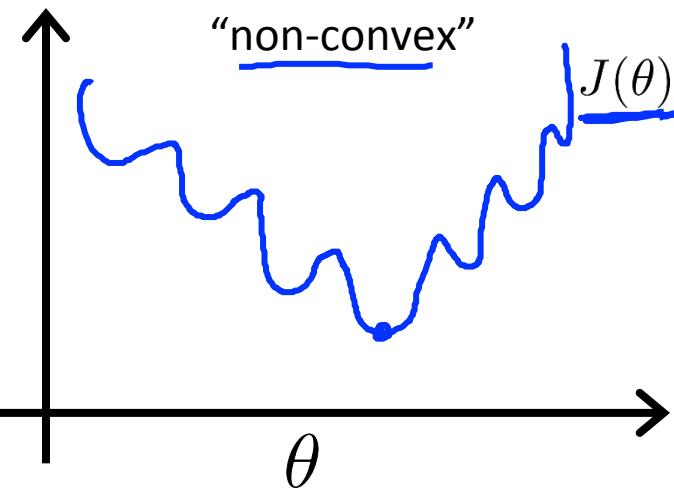
logistic

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

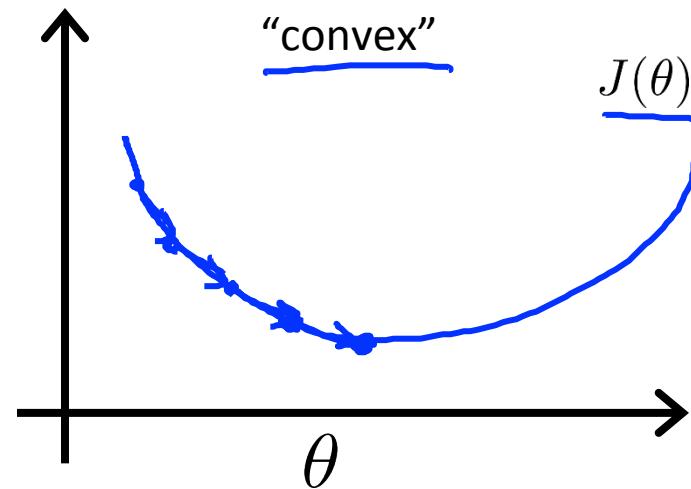
cost($h_\theta(x^{(i)})$, $y^{(i)}$)

$$\text{Cost}(h_\theta(x^{(i)}), y^{(i)}) = \frac{1}{2} (h_\theta(x^{(i)}) - y^{(i)})^2$$

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



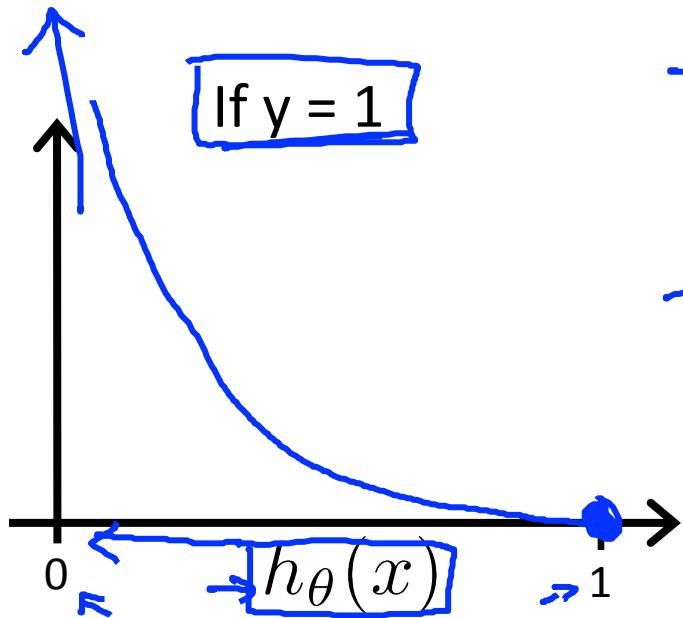
"non-convex"



"convex"

Logistic regression cost function

$$\text{Cost}(h_\theta(x), y) = \begin{cases} -\log(h_\theta(x)) & \text{if } y = 1 \\ -\log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$

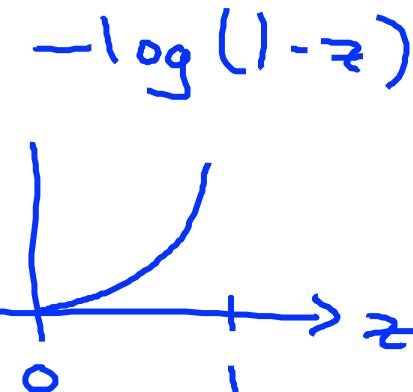
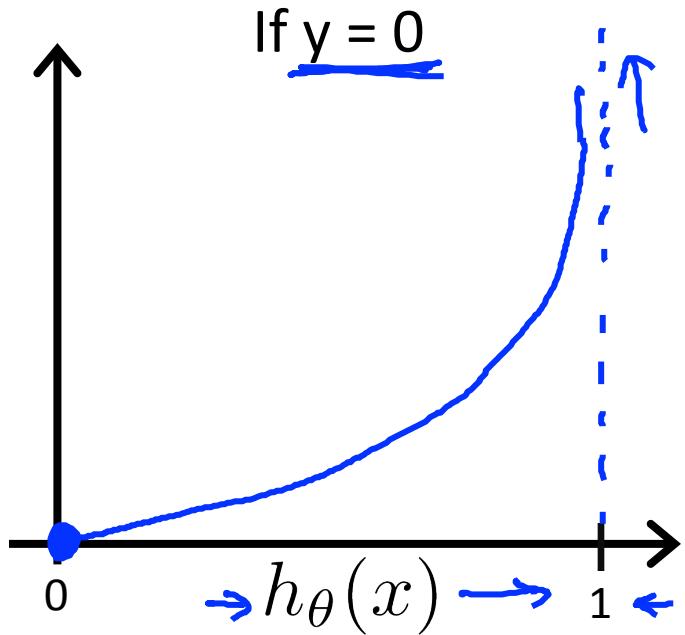


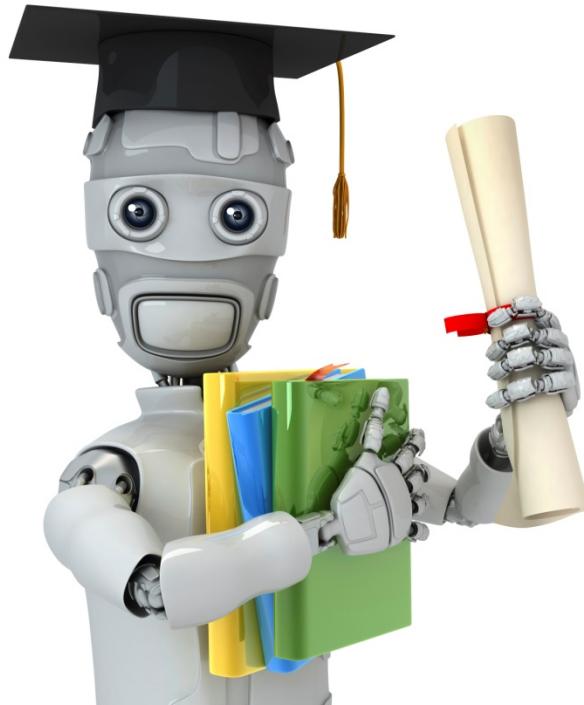
→ Cost = 0 if $y = 1, h_\theta(x) = 1$
But as $h_\theta(x) \rightarrow 0$
 $\text{Cost} \rightarrow \infty$

→ Captures intuition that if $h_\theta(x) = 0$,
(predict $P(y = 1|x; \theta) = 0$), but $y = 1$,
we'll penalize learning algorithm by a very
large cost.

Logistic regression cost function

$$\text{Cost}(h_\theta(x), y) = \begin{cases} -\log(h_\theta(x)) & \text{if } y = 1 \\ -\log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$





Machine Learning

Logistic Regression

Simplified cost function
and gradient descent

Logistic regression cost function

$$\rightarrow J(\theta) = \frac{1}{m} \sum_{i=1}^m \text{Cost}(h_\theta(x^{(i)}), y^{(i)})$$

$$\rightarrow \text{Cost}(h_\theta(x), y) = \begin{cases} -\log(h_\theta(x)) & \text{if } y = 1 \\ -\log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$

Note: $y = 0$ or 1 always

$$\rightarrow \text{Cost}(h_\theta(x), y) = -y \log(h_\theta(x)) - (1-y) \log(1-h_\theta(x))$$

If $y=1$: $\text{Cost}(h_\theta(x), y) = -\log h_\theta(x)$

If $y=0$: $\text{Cost}(h_\theta(x), y) = -\log(1-h_\theta(x))$

Logistic regression cost function

$$\begin{aligned} J(\theta) &= \frac{1}{m} \sum_{i=1}^m \text{Cost}(h_\theta(x^{(i)}), y^{(i)}) \\ &= -\frac{1}{m} \left[\sum_{i=1}^m y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_\theta(x^{(i)})) \right] \end{aligned}$$

To fit parameters θ :

$$\min_{\theta} J(\theta)$$

Get $\underline{\theta}$

To make a prediction given new x :

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

$p(y=1 | x; \theta)$

Gradient Descent

$$\rightarrow J(\theta) = -\frac{1}{m} \left[\sum_{i=1}^m y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_\theta(x^{(i)})) \right]$$

Want $\min_{\theta} J(\theta)$:

Repeat {

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

}

(simultaneously update all θ_j)

$$\frac{\partial}{\partial \theta_j} J(\theta) = \underline{\frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}}$$

Gradient Descent

$$J(\theta) = -\frac{1}{m} \left[\sum_{i=1}^m y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_\theta(x^{(i)})) \right]$$

Want $\min_{\theta} J(\theta)$:

Repeat {

$$\rightarrow \theta_j := \theta_j - \alpha \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

}

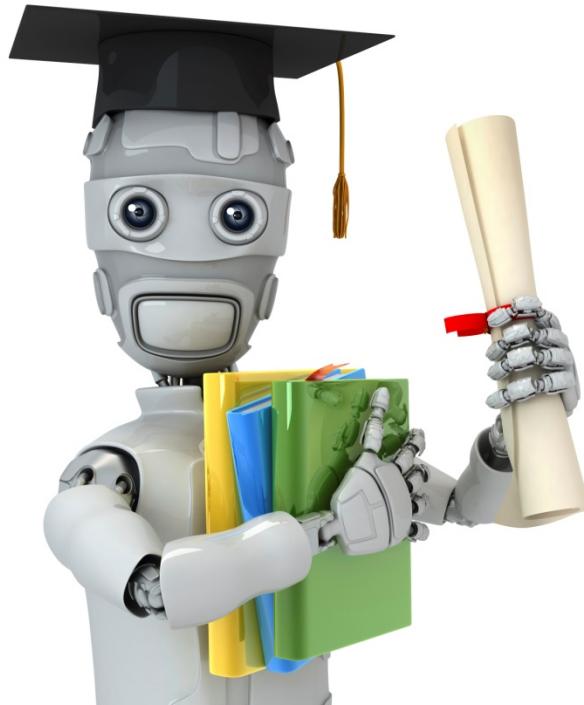
(simultaneously update all θ_j)

$$\Theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix} \quad \text{for } i=0 \dots n$$

$$h_\theta(x) = \theta^T x$$

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

Algorithm looks identical to linear regression!



Machine Learning

Logistic Regression

Advanced optimization

Optimization algorithm

Cost function $J(\theta)$. Want $\min_{\theta} J(\theta)$.

Given θ , we have code that can compute

$$\begin{aligned} \rightarrow & - J(\theta) \\ \rightarrow & - \frac{\partial}{\partial \theta_j} J(\theta) \quad (\text{for } j = 0, 1, \dots, n) \end{aligned}$$

Gradient descent:

Repeat {

$$\rightarrow \theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

}

Optimization algorithm

Given θ , we have code that can compute

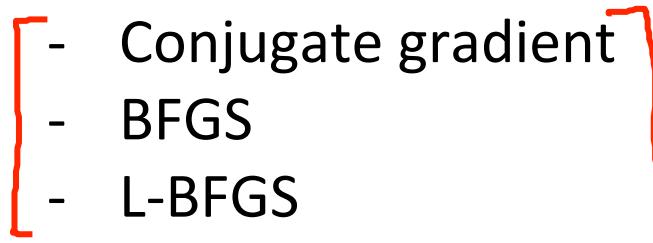
- $J(\theta)$
- $\frac{\partial}{\partial \theta_j} J(\theta)$



(for $j = 0, 1, \dots, n$)

Optimization algorithms:

- - Gradient descent
- Conjugate gradient
- BFGS
- L-BFGS



Advantages:

- No need to manually pick α
- Often faster than gradient descent.

Disadvantages:

- More complex



Example: $\min_{\theta} J(\theta)$

$$\rightarrow \theta = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} \quad \theta_1 = 5, \theta_2 = 5.$$

$$\rightarrow J(\theta) = (\theta_1 - 5)^2 + (\theta_2 - 5)^2$$

$$\rightarrow \frac{\partial}{\partial \theta_1} J(\theta) = 2(\theta_1 - 5)$$

$$\rightarrow \frac{\partial}{\partial \theta_2} J(\theta) = 2(\theta_2 - 5)$$

```
→ options = optimset('GradObj', 'on', 'MaxIter', '100');  
→ initialTheta = zeros(2,1);  
[optTheta, functionVal, exitFlag] ...  
= fminunc(@costFunction, initialTheta, options);
```

↑ ↑

$\theta \in \mathbb{R}^2 \quad d \geq 2$.

```
function [jVal, gradient]  
= costFunction(theta)  
jVal = (theta(1)-5)^2 + ...  
      (theta(2)-5)^2;  
gradient = zeros(2,1);  
gradient(1) = 2*(theta(1)-5);  
gradient(2) = 2*(theta(2)-5);
```

theta = $\begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix}$ theta(1) ←
theta(2)
theta(n+1)

function [jVal gradient] = costFunction(theta)

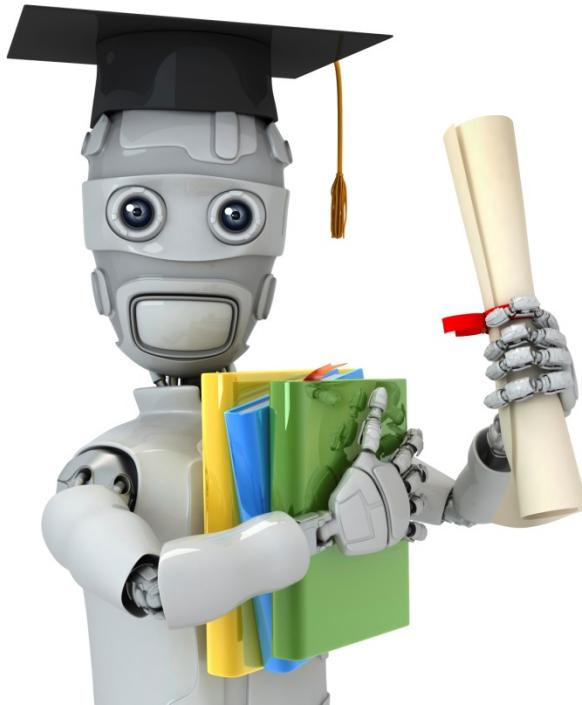
jVal = [code to compute $J(\theta)$];

gradient(1) = [code to compute $\frac{\partial}{\partial \theta_0} J(\theta)$];

gradient(2) = [code to compute $\frac{\partial}{\partial \theta_1} J(\theta)$];

⋮

gradient(n+1) = [code to compute $\frac{\partial}{\partial \theta_n} J(\theta)$];



Machine Learning

Logistic Regression

Multi-class classification:
One-vs-all

Multiclass classification

Email foldering/tagging: Work, Friends, Family, Hobby

$$y=1 \quad y=2 \quad y=3 \quad y=4$$

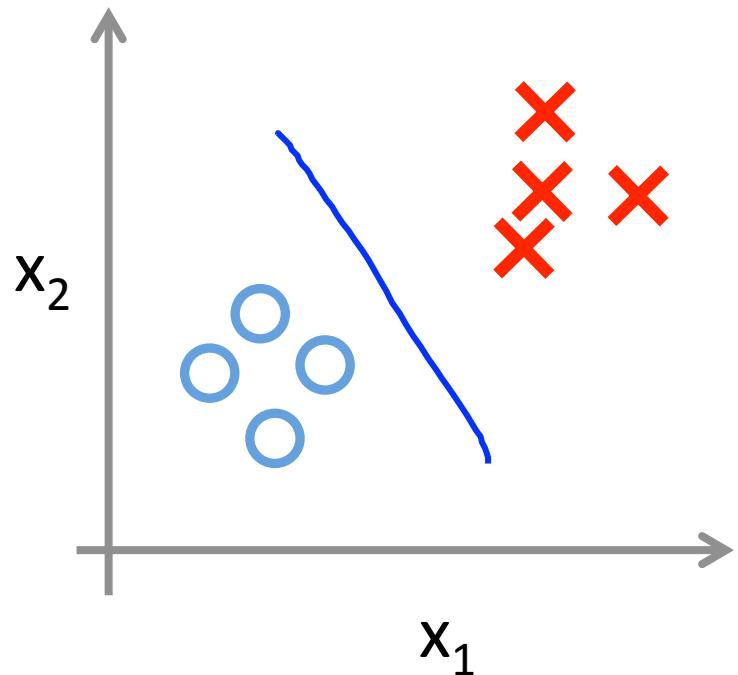
Medical diagrams: Not ill, Cold, Flu

$$y=1 \quad 2 \quad 3$$

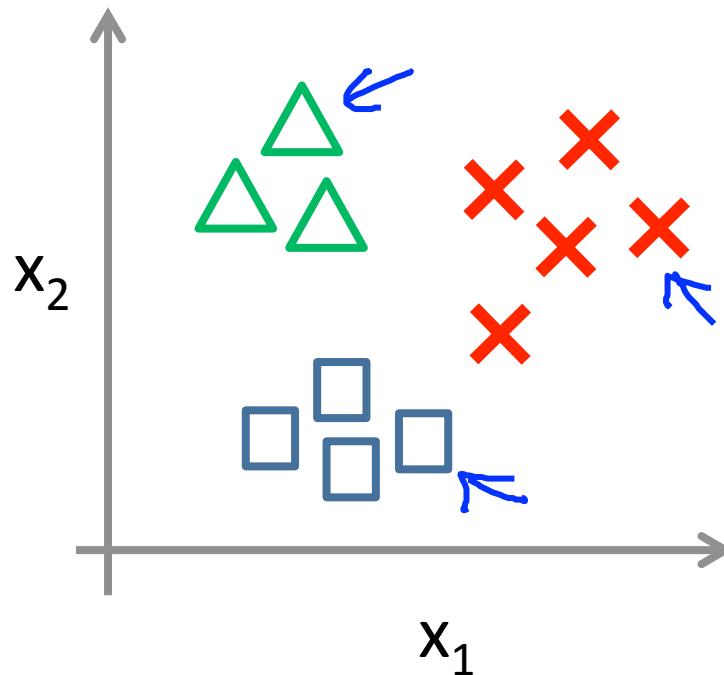
Weather: Sunny, Cloudy, Rain, Snow



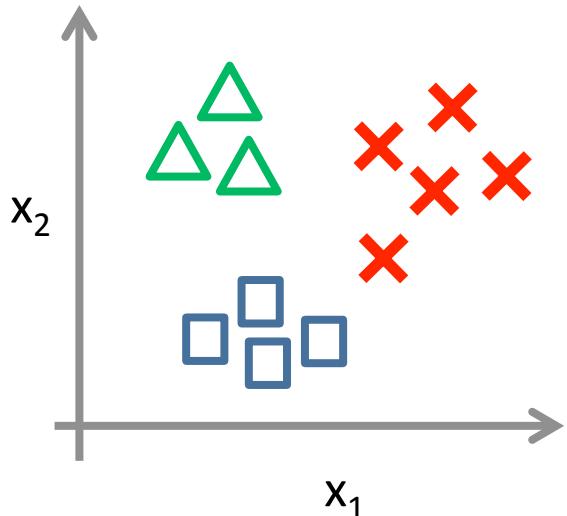
Binary classification:



Multi-class classification:



One-vs-all (one-vs-rest):

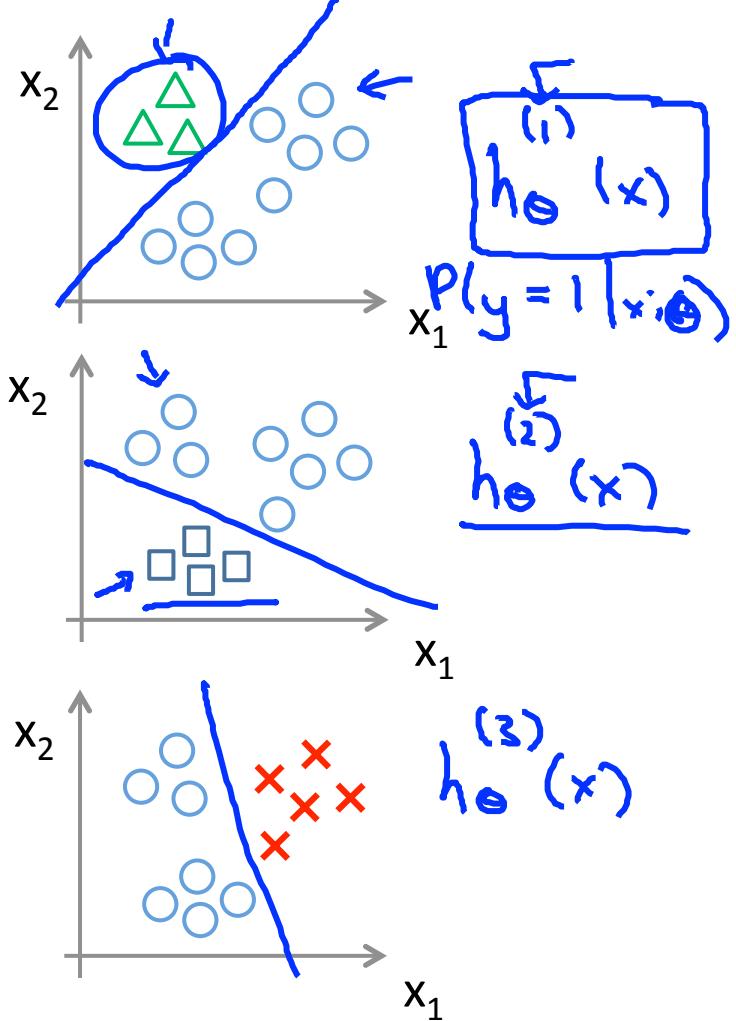


Class 1:

Class 2:

Class 3:

$$h_{\theta}^{(i)}(x) = P(y = i|x; \theta) \quad (i = 1, 2, 3)$$



One-vs-all

Train a logistic regression classifier $\underline{h_{\theta}^{(i)}(x)}$ for each class \underline{i} to predict the probability that $\underline{y = i}$.

On a new input \underline{x} , to make a prediction, pick the class i that maximizes

$$\max_i \underline{\underline{h_{\theta}^{(i)}(x)}}$$