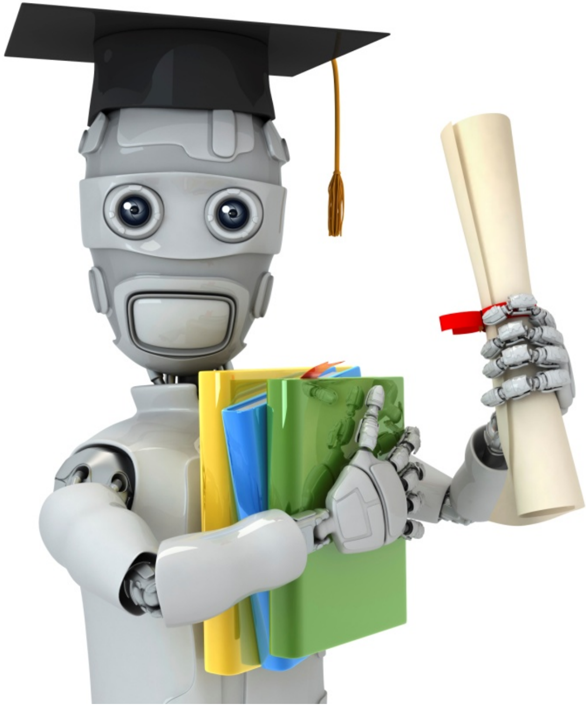


Machine Learning

Logistic Regression

one of the most popular and widely used learning algorithm today.

Classification

output y is discrete value

Classification

examples

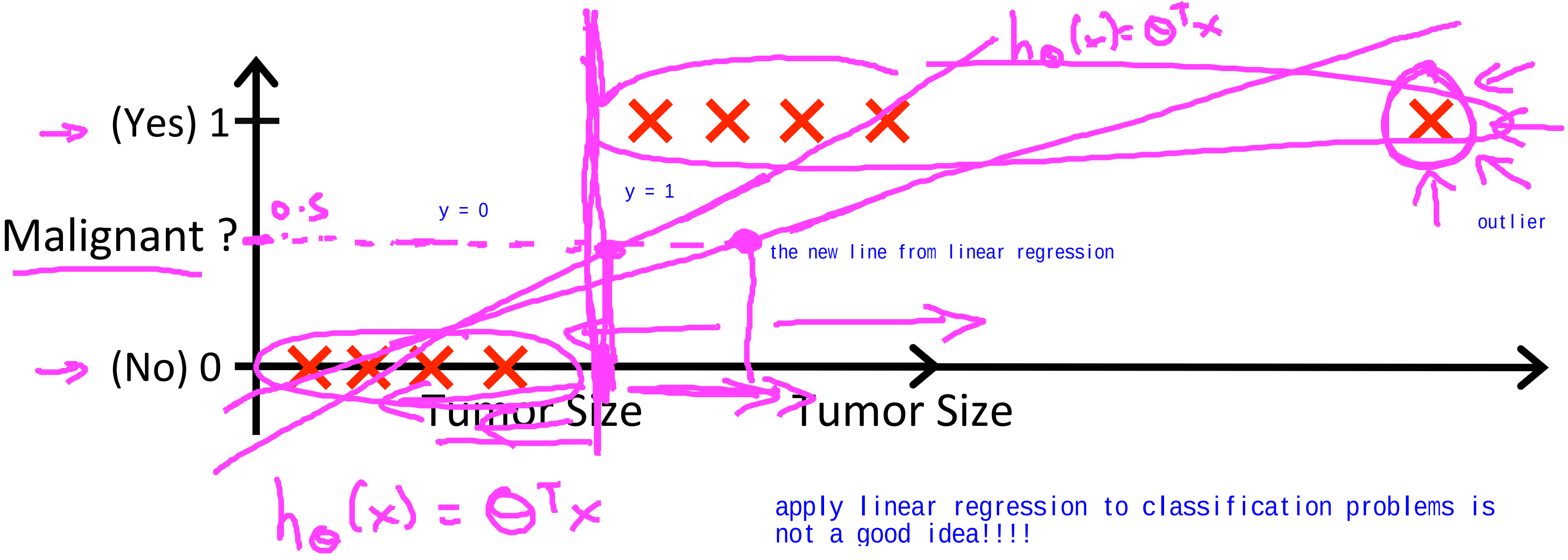
- Email: Spam / Not Spam?
- Online Transactions: Fraudulent (Yes / No)?
- Tumor: Malignant / Benign ?

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

0: "Negative Class" (e.g., benign tumor)

1: "Positive Class" (e.g., malignant tumor)

$y \in \{0, 1, 2, 3\}$ later we will talk about multi-classification problem`



one method to do this using linear regression

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"

Andrew Ng

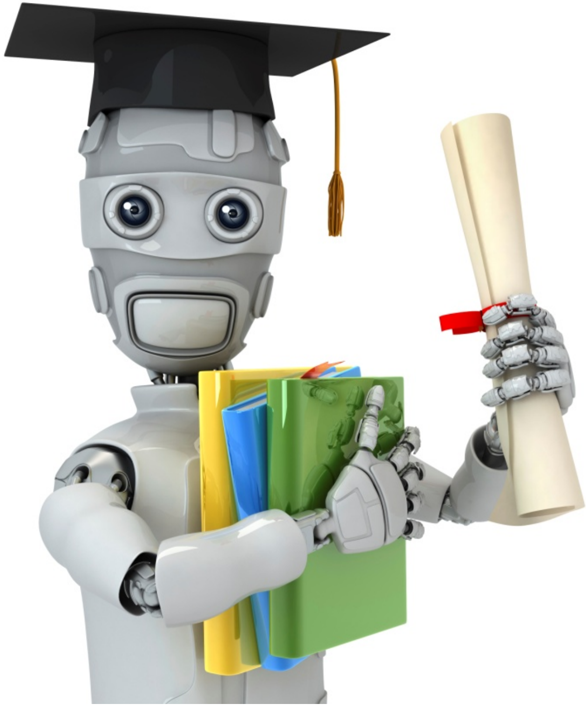
Classification: $\boxed{y = 0 \text{ or } 1}$

$h_\theta(x)$ can be > 1 or < 0 if we use linear regression method

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

logistic regression has this property
output is bounded by [0,1]

Classification



Machine Learning

Logistic Regression

Hypothesis Representation

we want our function to satisfy this property

Logistic Regression Model

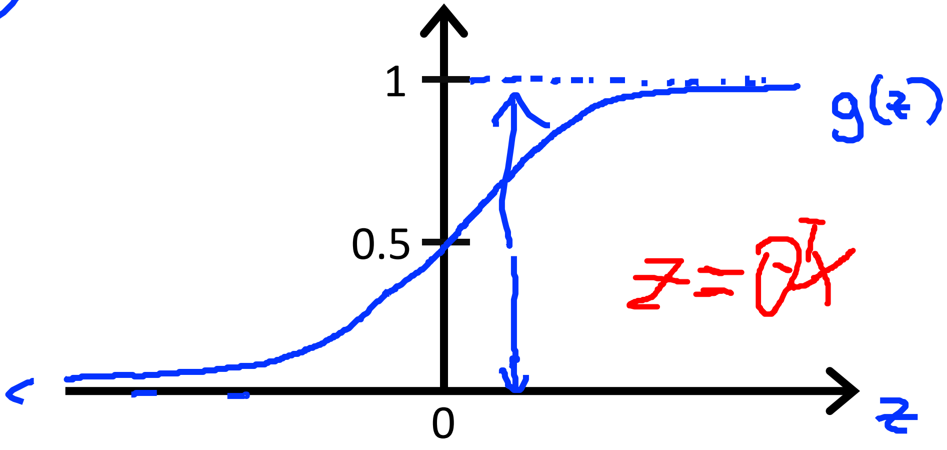
Want $\boxed{0 \leq h_\theta(x) \leq 1}$

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

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

$\theta^T x$

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



Sigmoid function

Logistic function alternative names

Parameters θ - objective: fitting parameter theta

Interpretation of Hypothesis Output

$h_\theta(x)$

hypothesis function

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

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

$$h_\theta(x) = 0.7$$

$y=1$

interpretation of the output value

Tell patient that 70% chance of tumor being malignant

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

written formally

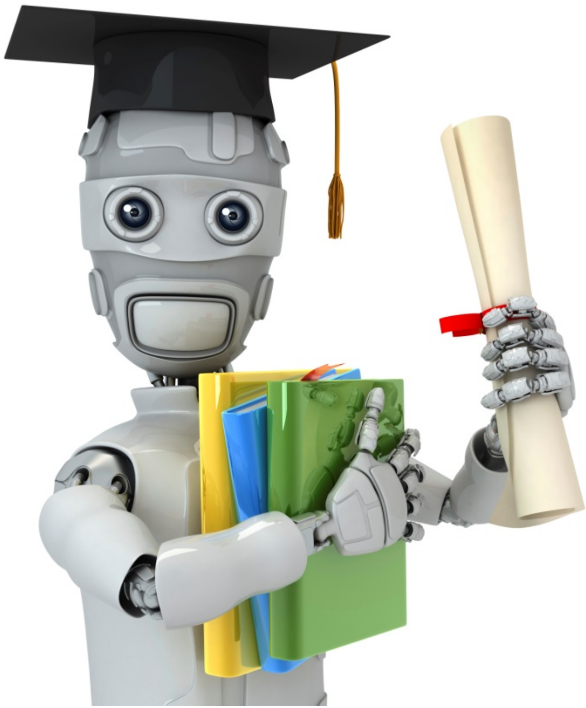
“probability that y = 1, given x, parameterized by θ”

$y = 0$ or 1

only value y can take is 1 or 0

$$P(y=0|\cancel{x;}\theta) + \boxed{P(y=1|\cancel{x;}\theta)} = 1$$

$$P(y=0|x;\theta) = 1 - \boxed{P(y=1|x;\theta)}$$



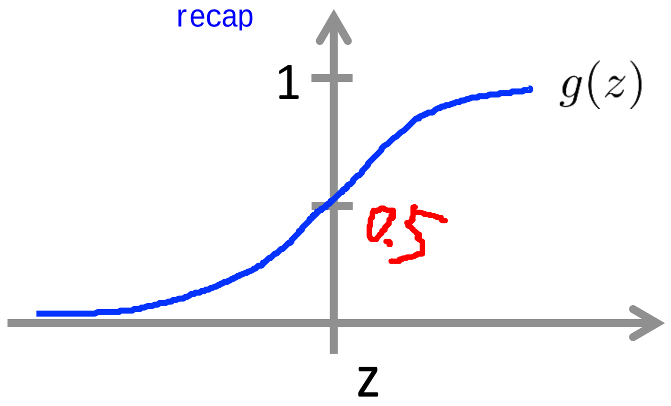
Logistic Regression

Decision boundary

Machine Learning

Logistic regression

$$\boxed{\begin{aligned} h_\theta(x) &= g(\theta^T x) \\ g(z) &= \frac{1}{1+e^{-z}} \end{aligned}}$$ $= P(y=1|x;\theta)$



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 $z \geq 0$

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

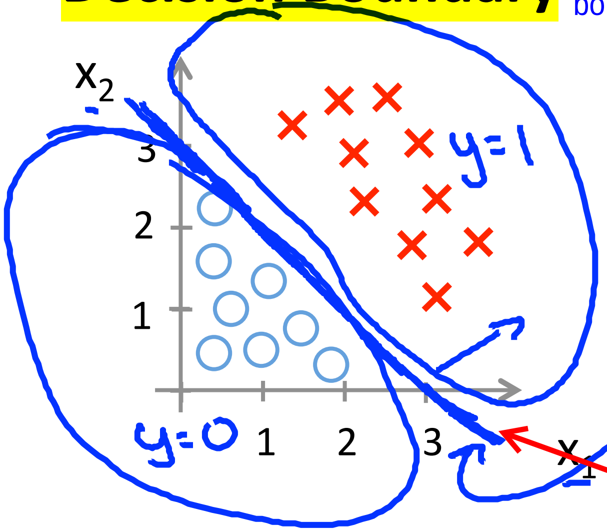
whenever theta'*x >=0

$g(z) < 0.5$

when $z < 0$

Decision Boundary

linear decision boundary



suppose we choose this parameter set

$$\theta = \begin{bmatrix} -3 \\ 1 \\ 1 \end{bmatrix}$$

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

$$\theta_0 = -3, \quad \theta_1 = 1, \quad \theta_2 = 1$$

$\boxed{\text{Decision boundary}}$

This line is called the decision boundary

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

$\rightarrow x_1 + x_2 \geq 3$

x_1, x_2

$\rightarrow h_\theta(x) = 0.5$

$\boxed{x_1 + x_2 = 3}$

$x_1 + x_2 < 3$

$\rightarrow y = 0$

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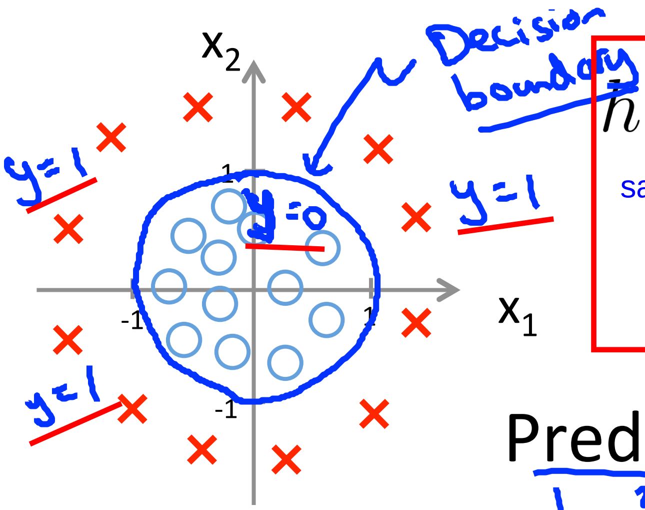
Non-linear decision boundaries



$$h_\theta(x) = g(\underbrace{\theta_0}_{-1} + \underbrace{\theta_1}_{0} x_1 + \underbrace{\theta_2}_{0} x_2 + \underbrace{\theta_3}_{1} x_1^2 + \underbrace{\theta_4}_{1} x_2^2)$$

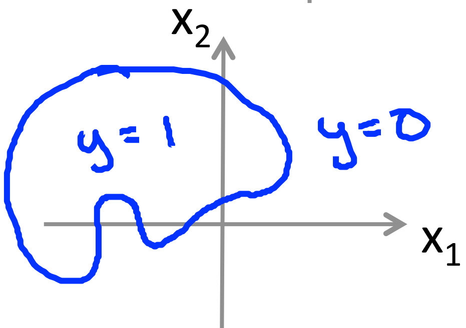
same as the polynomial fit

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

suppose we have this data set

Predict "$y = 1$" if $\underbrace{-1 + x_1^2 + x_2^2 \geq 0}_{x_1^2 + x_2^2 \geq 1}$

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



More complicate examples

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

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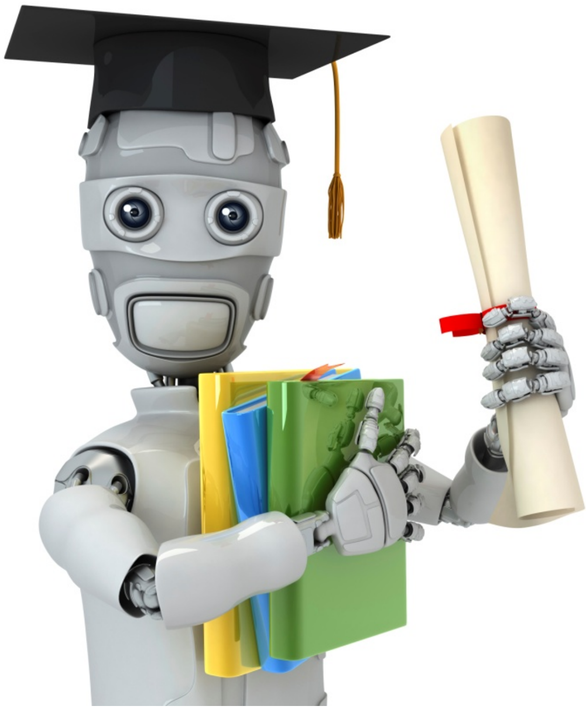


Machine Learning

Logistic Regression

Cost function

Training set:

$$\underline{\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \cdots, (x^{(m)}, y^{(m)})\}}$$

m examples

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

n features

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

as usual

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

my hypothesis

How to choose parameters θ ?

Andrew Ng

Cost function

→ ~~Linear~~ regression: $J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \cancel{\frac{1}{2}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2}$

Logistic

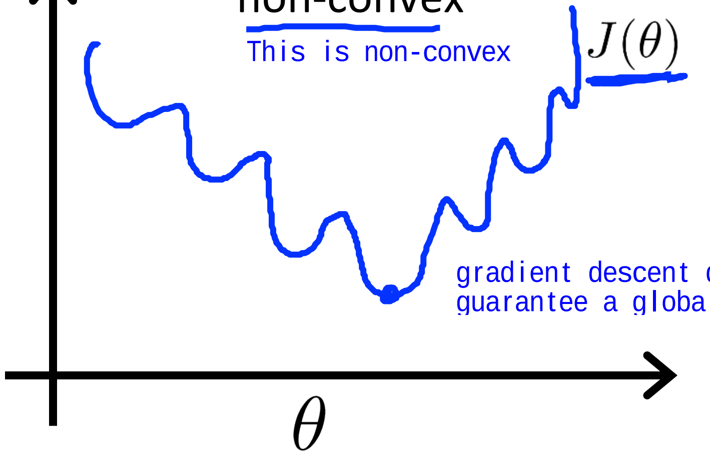
$\to \mathrm{cost}(h_\theta(x^{(i)}), y)$

we want to minimize a cost function

$$\to \mathrm{Cost}(h_\theta(x^{(i)}), y^{(i)}) = \boxed{\frac{1}{2}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2} \leftarrow \boxed{\frac{1}{1+e^{-\theta^T x}}}$$

"non-convex"

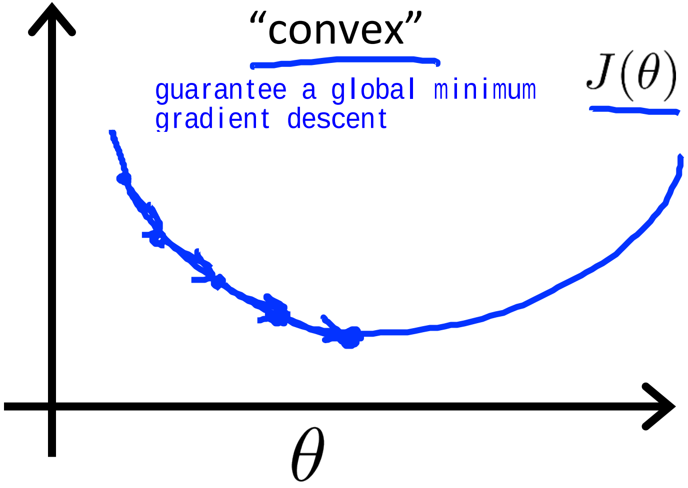
This is non-convex



gradient descent does not guarantee a global minimum

"convex"

guarantee a global minimum
gradient descent



Logistic regression cost function

cost function is linear regression for logistic regression is not convex, we have to define a new cost function so that it can be convex!

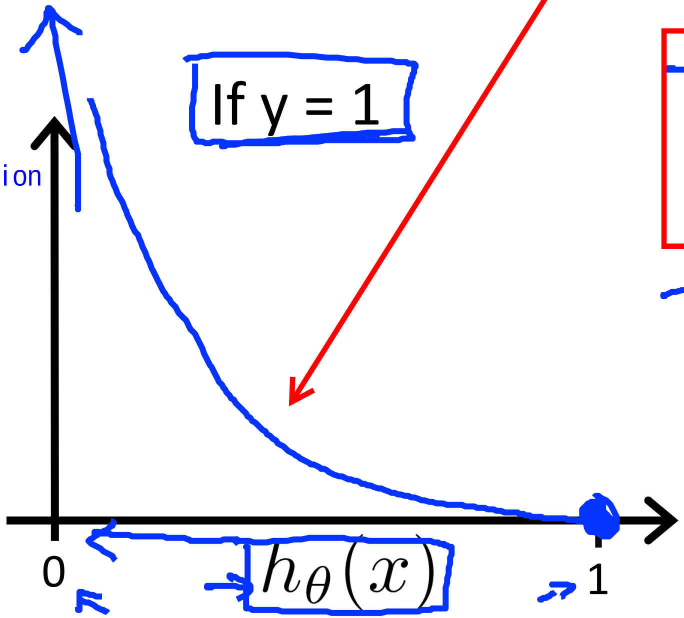
predicted value

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

actual value

when cost=0, if y=1, the predicted is 1
if the predicted approaches 0, the cost approaches infinity!!!

cost function
y = 1



→ $\mathrm{Cost} = 0$ if $y = 1, h_\theta(x) = 1$

But as $h_\theta(x) \to 0$
$Cost \to \infty$

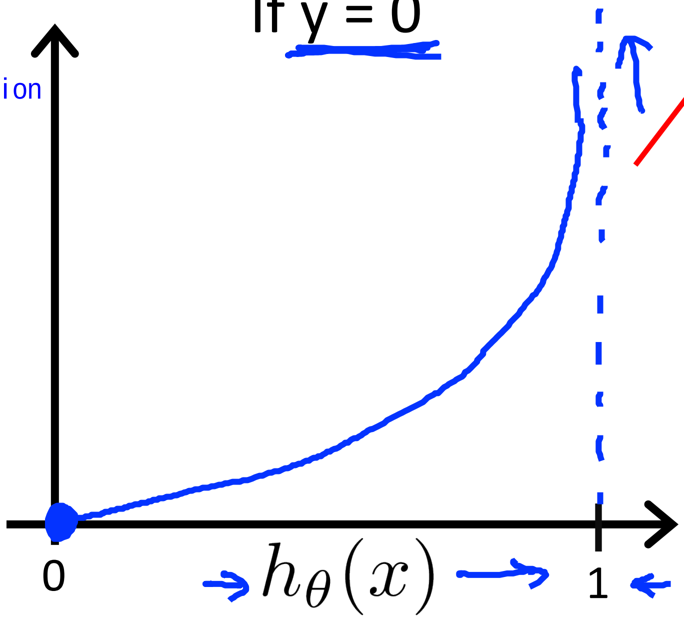
→ Captures intuition that if $h_\theta(x) = 0$, (predict $P(y = 1|x; \theta) = 0$), but $\boxed{y = 1,}$ we'll penalize learning algorithm by a very large cost.

Logistic regression cost function

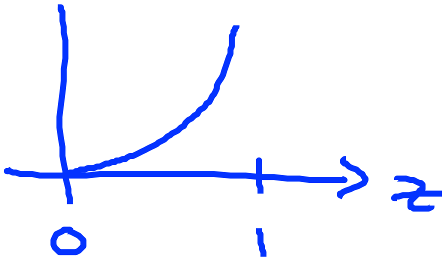
$$\mathrm{Cost}(h_\theta(x), y) = \begin{cases} -\log(h_\theta(x)) & \text{if } y = 1 \\ \boxed{-\log(1 - h_\theta(x))} & \text{if } y = 0 \end{cases}$$

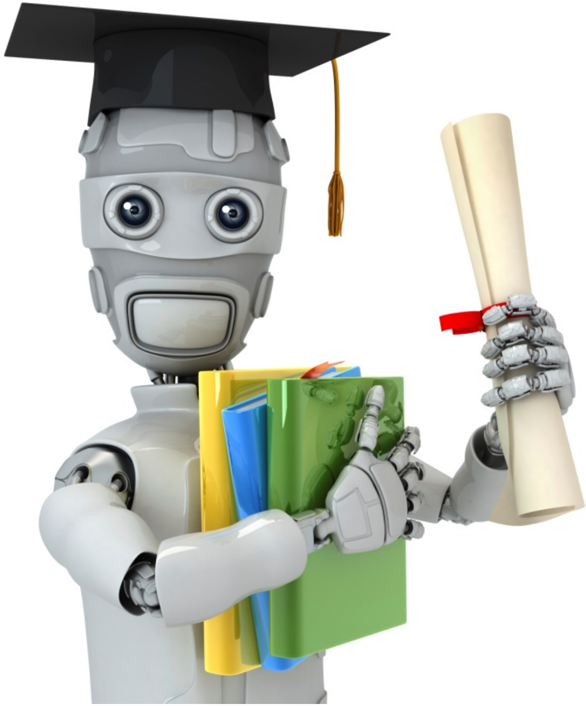
If y = 0

cost function
y = 0



$-\log(1-z)$





Machine Learning

Logistic Regression

Simplified cost function and gradient descent

Logistic regression cost function

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

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

Note: $y = \boxed{0}$ or $\boxed{1}$ always

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

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

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

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

To fit parameters θ :

$$\min_\theta J(\theta)$$

Get θ

To make a prediction given new x :

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

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

Gradient Descent

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

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

Repeat $\{$

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

$\}$

(simultaneously update all θ_j)

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

Gradient Descent

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

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

$$\Theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix}$$

for i=0 to n

Repeat $\{$

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

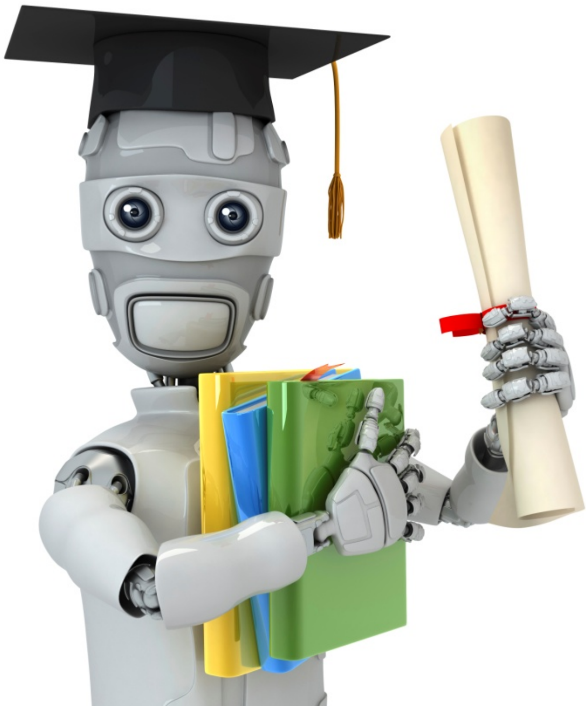
$h_\theta(x) = \theta^T x$

(simultaneously update all θ_j)

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

$\}$

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

- $\boxed{J(\theta)}$
- $\boxed{\frac{\partial}{\partial\theta_j} J(\theta)}$ (for $j = 0, 1, \ldots, n$)

Gradient descent:

Repeat $\{$

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

$\}$

Optimization algorithm

Given θ, we have code that can compute

- $J(\theta)$
- $\frac{\partial}{\partial\theta_j} J(\theta)$ (for $j = 0, 1, \ldots, n$)

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

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

$$\boxed{J(\theta) = (\theta_1 - 5)^2 + (\theta_2 - 5)^2}$$

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

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

```
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);
```

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

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

$$\texttt{theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix}$$

theta(1)

theta(2)

theta(n+1)

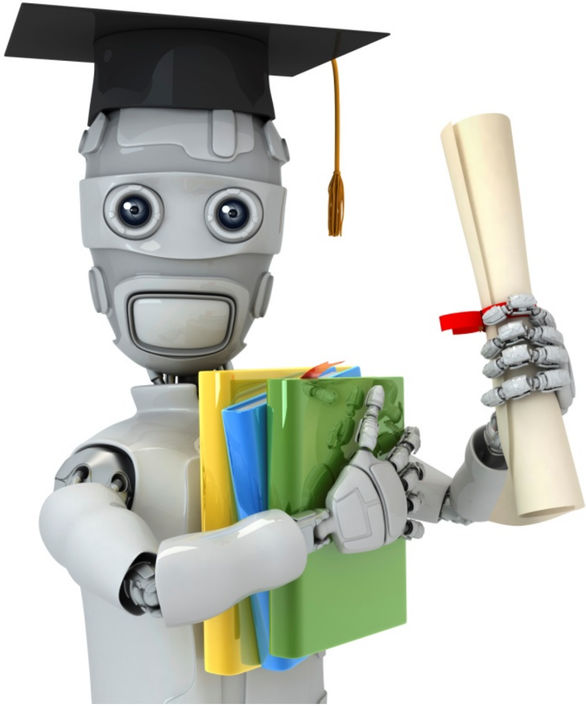
```
function [jVal, gradient] = costFunction(theta)

    jVal = [code to compute J(θ)];

    gradient(1) = [code to compute ∂/∂θ0 J(θ)];

    gradient(2) = [code to compute ∂/∂θ1 J(θ)];
      ⋮
    gradient(n+1) = [code to compute ∂/∂θn J(θ)];
```

Where the code to compute is $J(\theta)$, $\frac{\partial}{\partial\theta_0}J(\theta)$, $\frac{\partial}{\partial\theta_1}J(\theta)$, …, $\frac{\partial}{\partial\theta_n}J(\theta)$.



Logistic Regression

Multi-class classification: One-vs-all

Machine Learning

Multiclass classification

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

$y=1$ $y=2$ $y=3$ $y=4$

Medical diagrams: Not ill, Cold, Flu

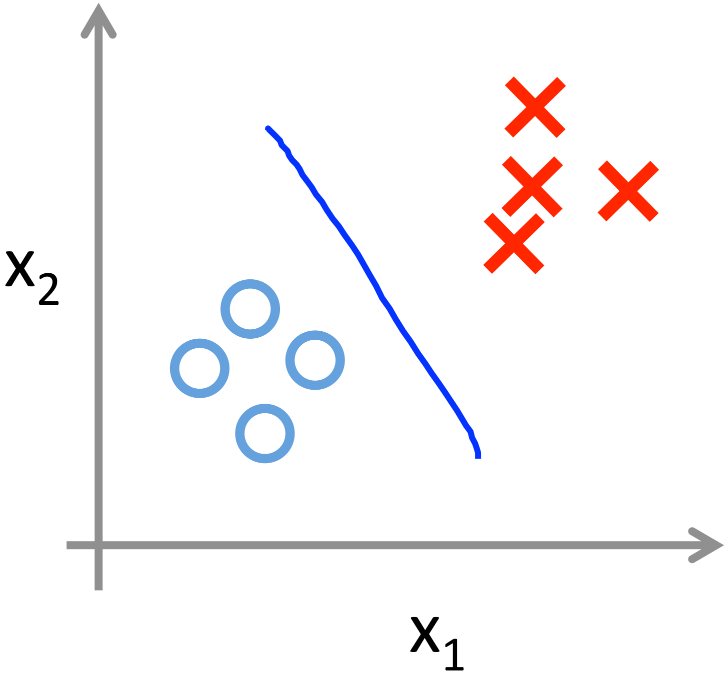
$y=1$ 2 3

Weather: Sunny, Cloudy, Rain, Snow

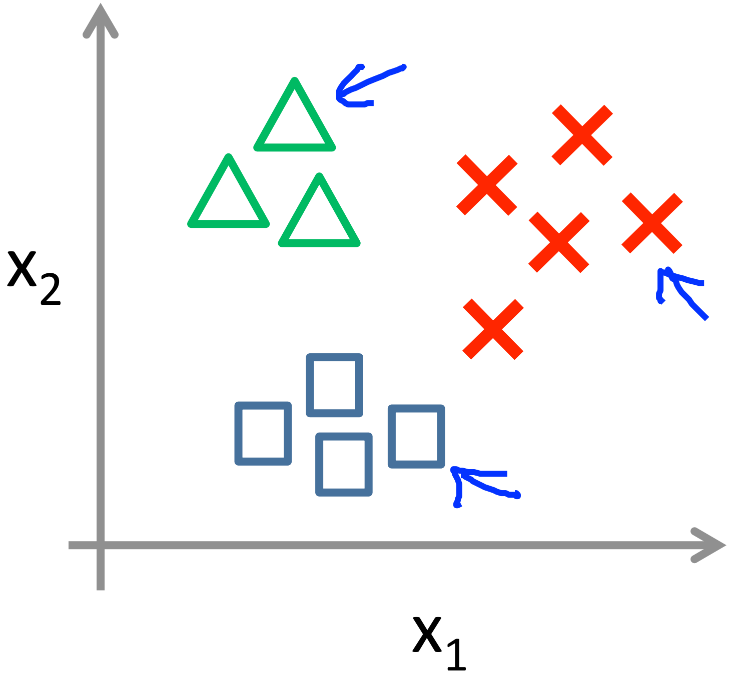
$y=1$ 2 3 4

0 1 2 3

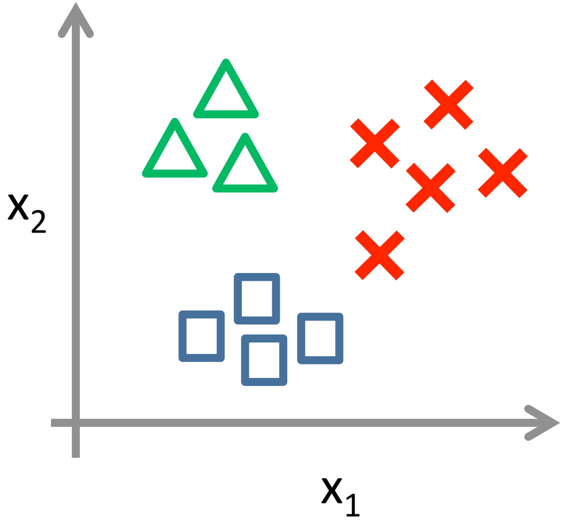
Binary classification:

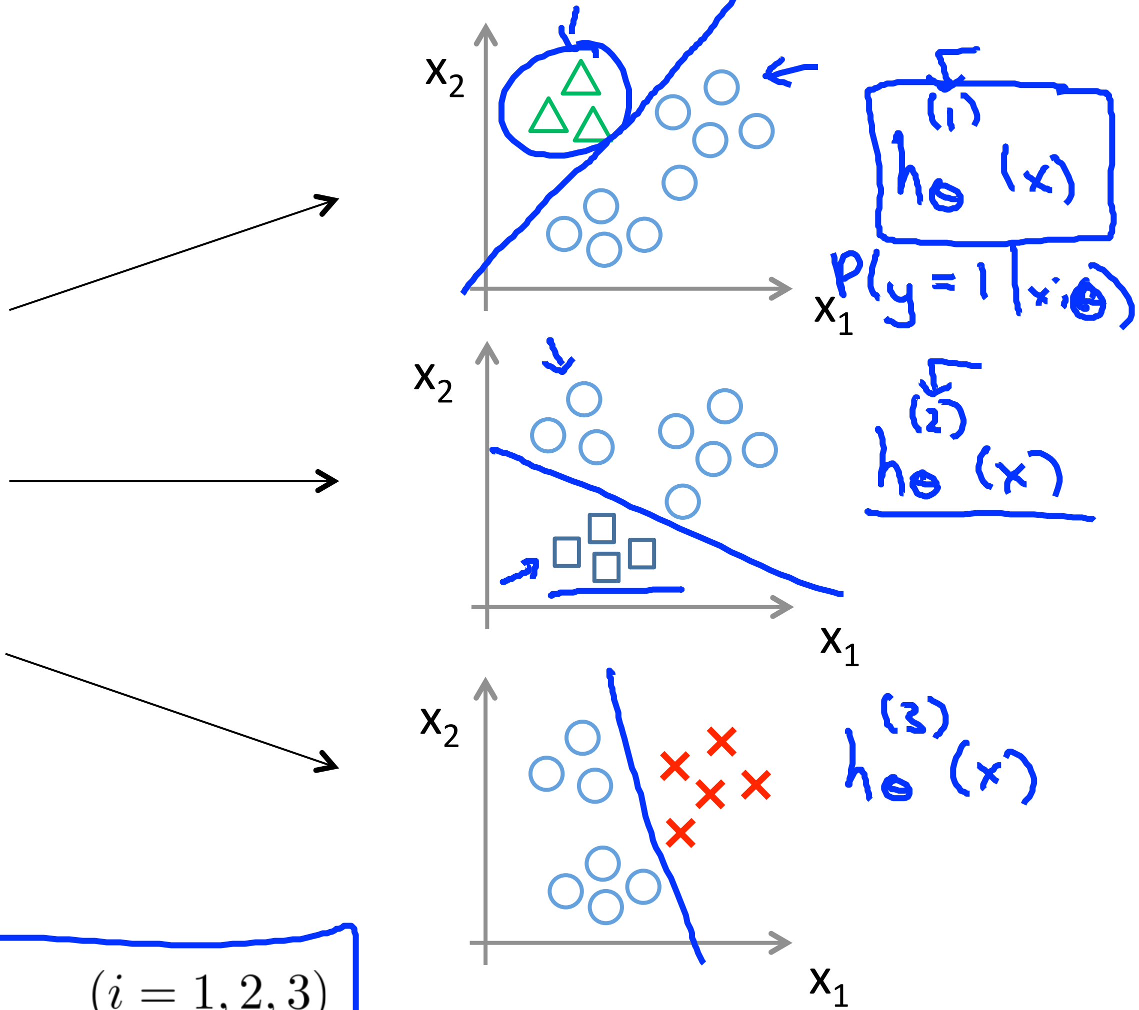


Multi-class classification:



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





Class 1: △

Class 2: □

Class 3: ×

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

One-vs-all

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

On a new input x, to make a prediction, pick the class i that maximizes

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