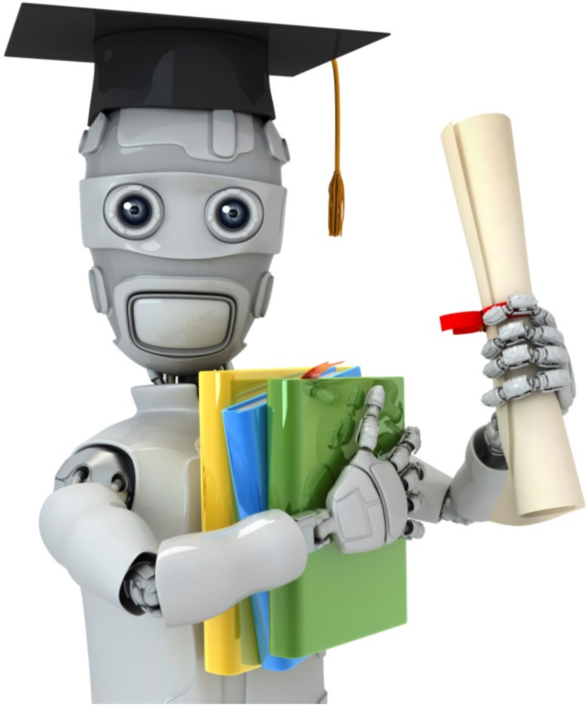


Machine Learning

Logistic Regression

Classification

Classification

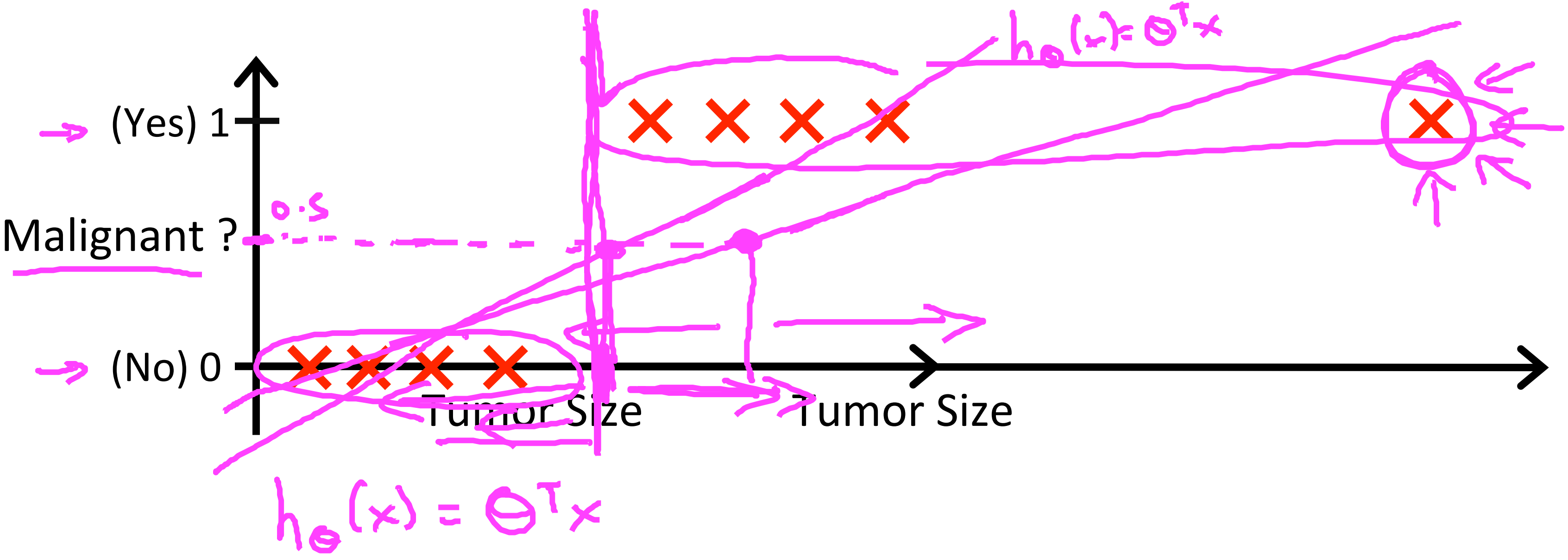
- Email: Spam / Not Spam?
- Online Transactions: Fraudulent (Yes / No)?
- Tumor: Malignant / Benign ?

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

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"

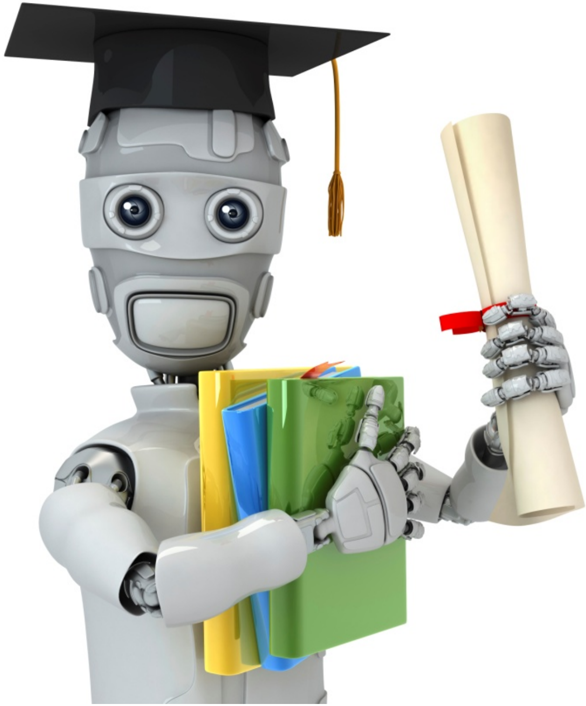
Andrew Ng

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

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

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

Classification



Machine Learning

Logistic Regression

Hypothesis Representation

Logistic Regression Model

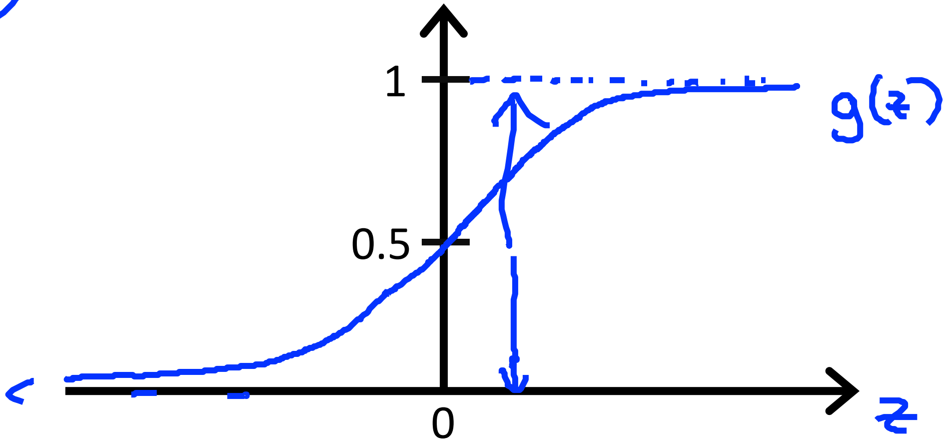
Want $\boxed{0 \le h_\theta(x) \le 1}$

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

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

$\theta^T x$

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



→ Sigmoid function

→ Logistic function

Parameters θ.

$h_\theta(x)$

Interpretation of Hypothesis Output

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

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

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

$y=1$

Tell patient that 70% chance of tumor being malignant

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

$y = 0$ or 1

"probability that y = 1, given x, parameterized by θ"

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

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

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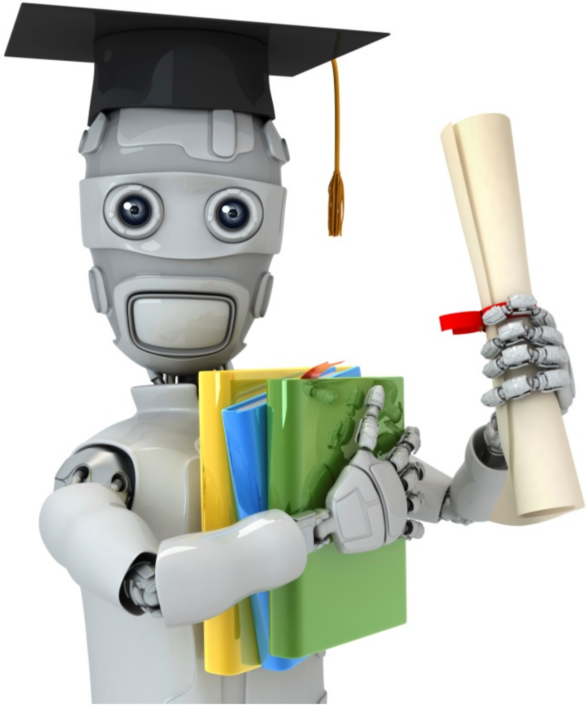


Machine Learning

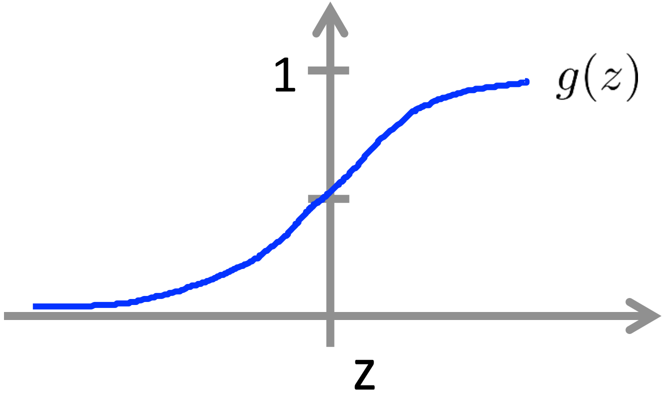
Logistic Regression

Decision boundary

Logistic regression

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

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



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

$\theta^T x \geq 0$

$g(z) \geq 0.5$

when $z \geq 0$

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

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

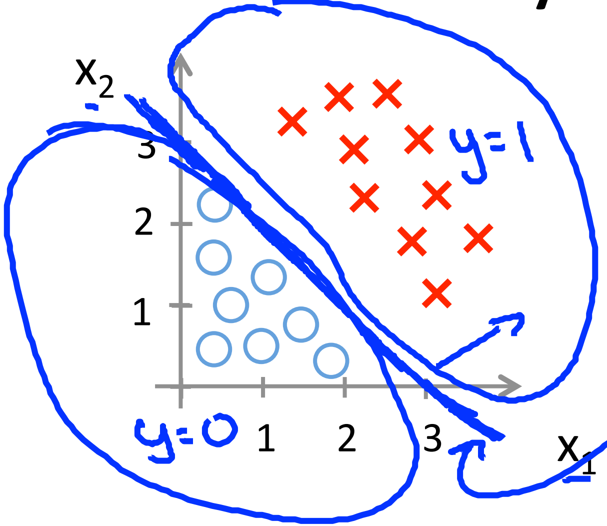
$\theta^T x < 0$

$g(z) < 0.5$

when $z < 0$

Decision Boundary

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



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

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

Decision boundary

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

$\to x_1 + x_2 \geq 3$

x_1, x_2

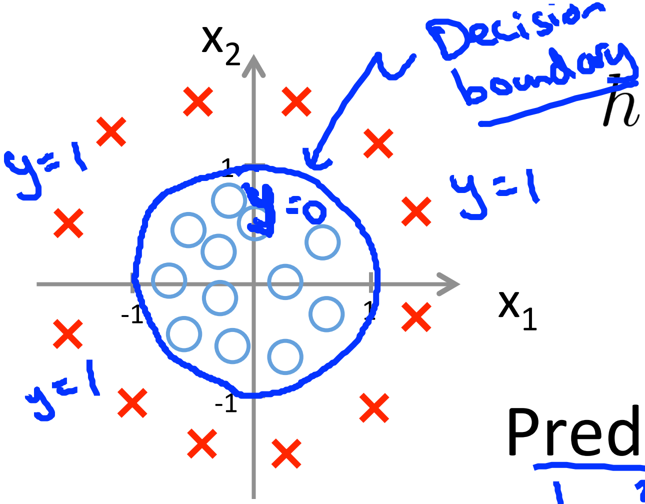
$\to h_\theta(x) = 0.5$

$\boxed{x_1 + x_2 = 3}$

$x_1 + x_2 < 3$

$\to y = 0$

Non-linear decision boundaries

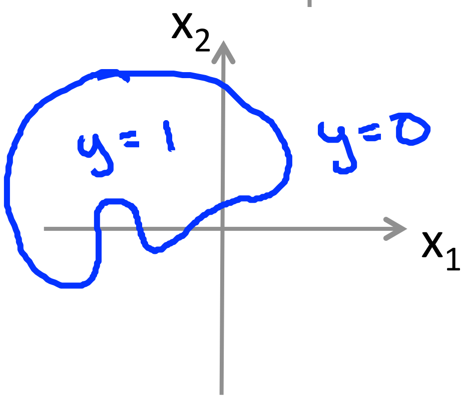


$$h_\theta(x) = g(\overset{=-1}{\theta_0} + \overset{=0}{\theta_1} x_1 + \overset{=0}{\theta_2} x_2 + \underset{=1}{\theta_3} x_1^2 + \underset{=1}{\theta_4} x_2^2)$$

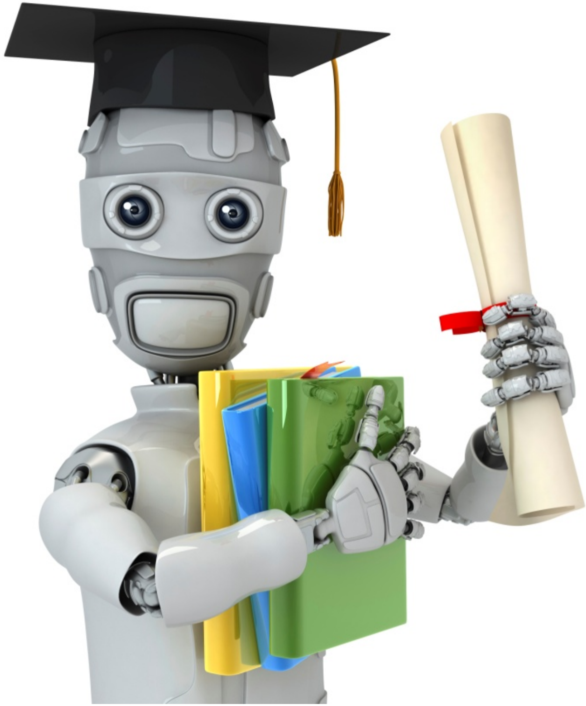
$$\theta = \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$$

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

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



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



Machine Learning

Logistic Regression

Cost function

Training set: $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \cdots, (x^{(m)}, y^{(m)})\}$

m examples

$$x \in \underbrace{\begin{bmatrix} x_0 \\ x_1 \\ \dots \\ x_n \end{bmatrix}}_{}\ \mathbb{R}^{n+1} \qquad x_0 = 1, y \in \{0, 1\}$$

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

How to choose parameters θ ?

Cost function

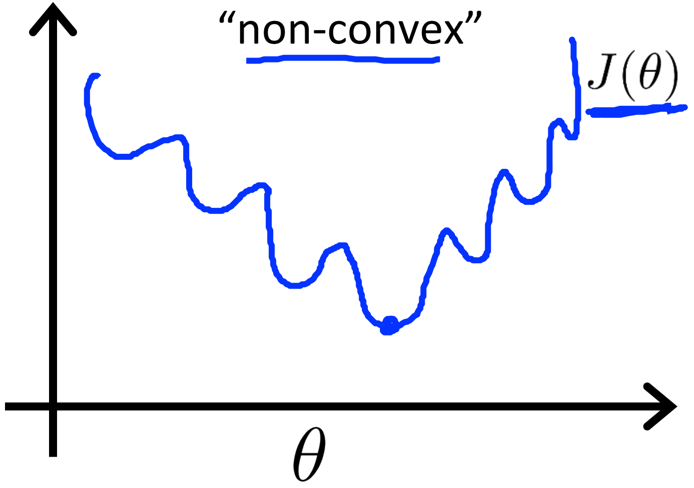
→ ~~Linear~~ regression: $J(\theta) = \boxed{\frac{1}{m}\sum_{i=1}^{m} \cancel{\frac{1}{2}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2}}$

Logistic

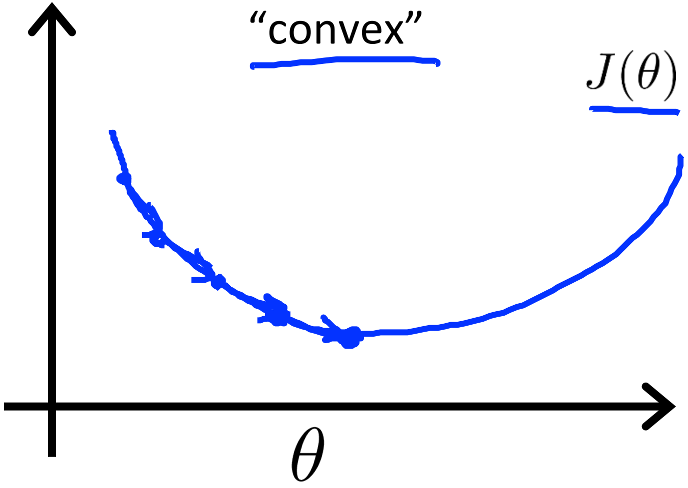
$\mathrm{cost}(h_\theta(x^{(i)}), y)$

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

"non-convex"

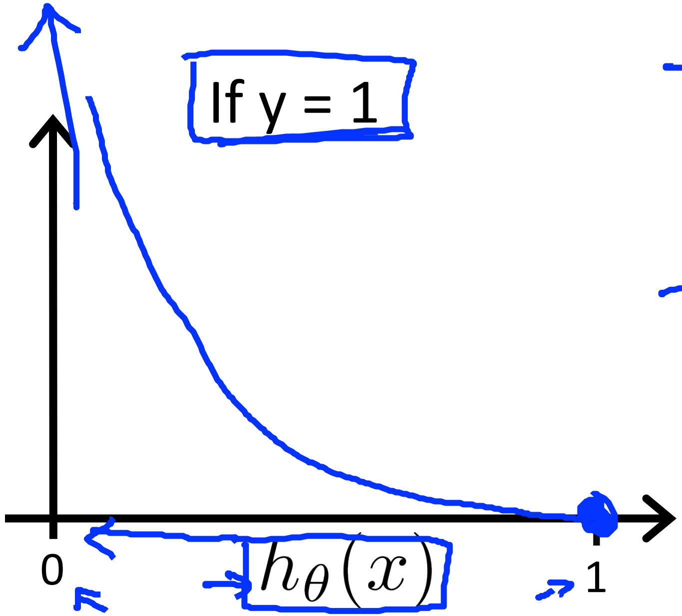


"convex"



Logistic regression cost function

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



Cost $= 0$ if $y = 1, h_\theta(x) = 1$

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

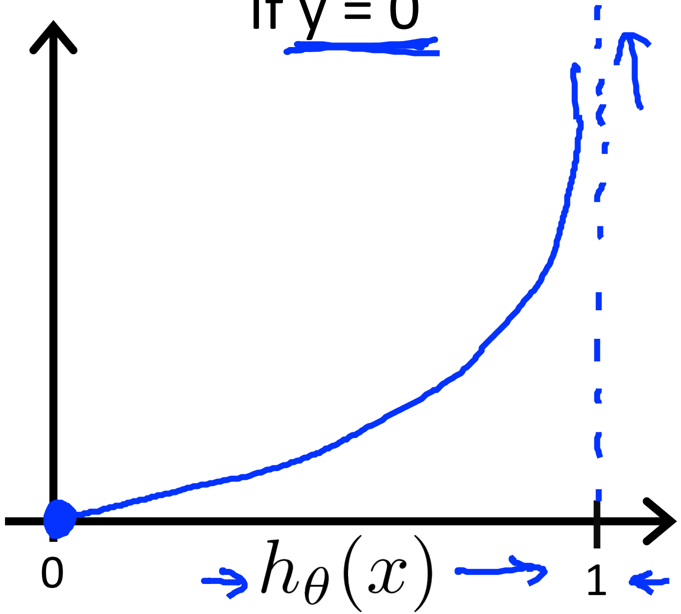
$Cost \to \infty$

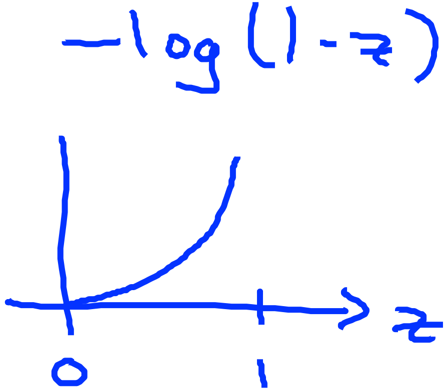
Captures intuition that if $h_\theta(x) = 0$, (predict $P(y = 1|x;\theta) = 0$), but $y = 1$, we'll penalize learning algorithm by a very large cost.

Logistic regression cost function

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

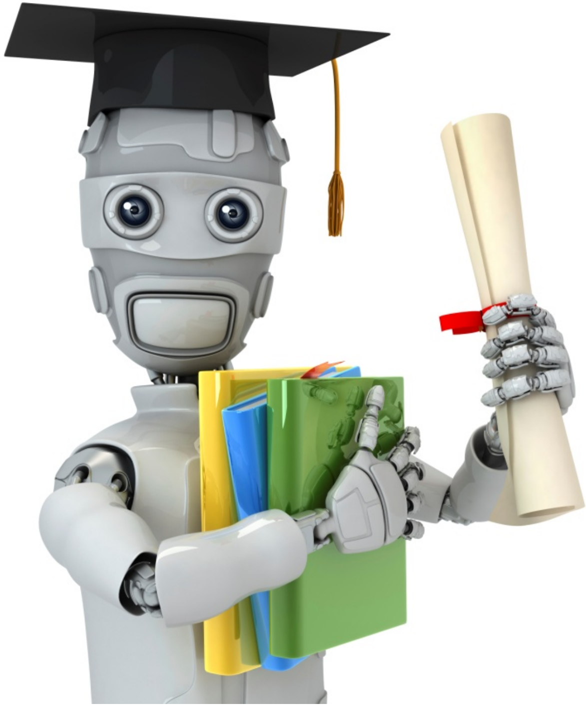
If y = 0





Logistic Regression

Simplified cost function and gradient descent



Machine Learning

Logistic regression cost function

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

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

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

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

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

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

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 :

$$\boxed{\min_\theta J(\theta) \quad \text{Get } \theta}$$

To make a prediction given new x:

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

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

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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

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

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

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

Repeat $\{$

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

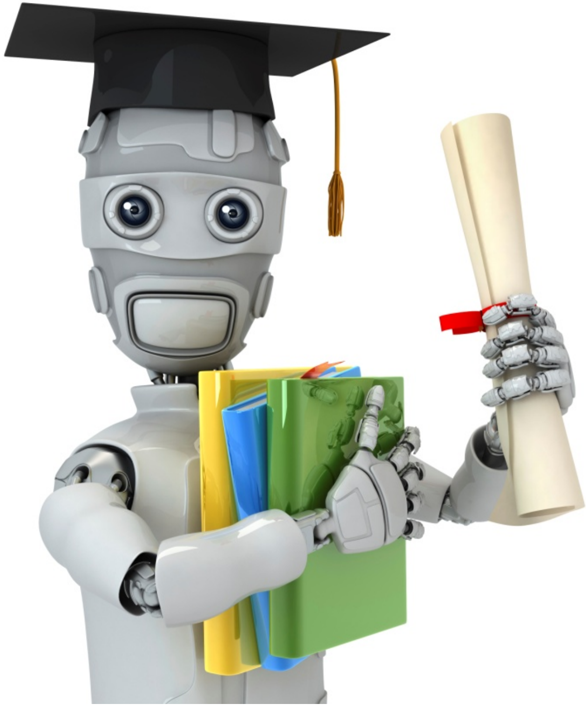
(simultaneously update all θ_j)

$\}$

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

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

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

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

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

$$\texttt{theta} = \begin{array}{cl} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix} & \begin{array}{l} \texttt{theta(1)} \\ \texttt{theta(2)} \\ \\ \texttt{theta(n+1)} \end{array} \end{array}$$

function [jVal, gradient] = costFunction(theta)

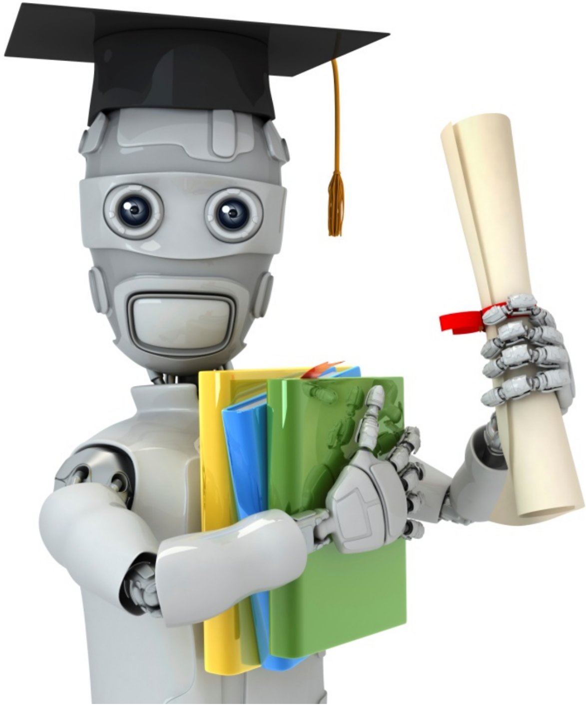
  jVal = [code to compute $J(\theta)$**];**

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

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

  $\vdots$

  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

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

Medical diagrams: Not ill, Cold, Flu

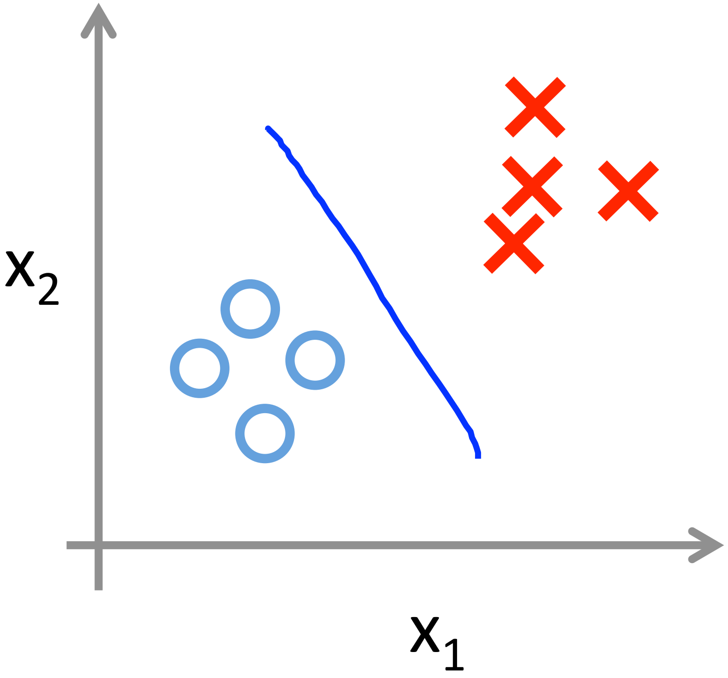
$y=1$ 2 3

Weather: Sunny, Cloudy, Rain, Snow

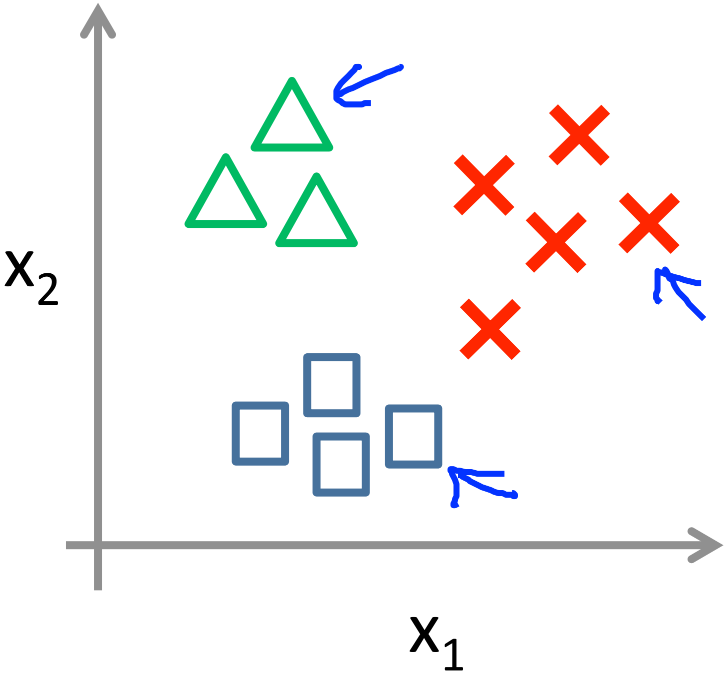
$y=1$ 2 3 4

0 1 2 3

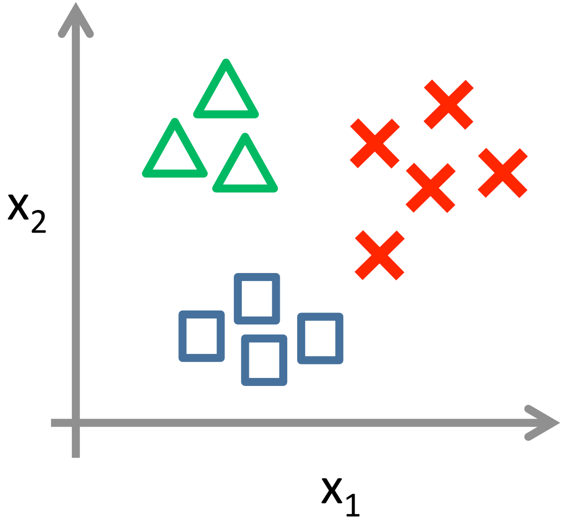
Binary classification:



Multi-class classification:

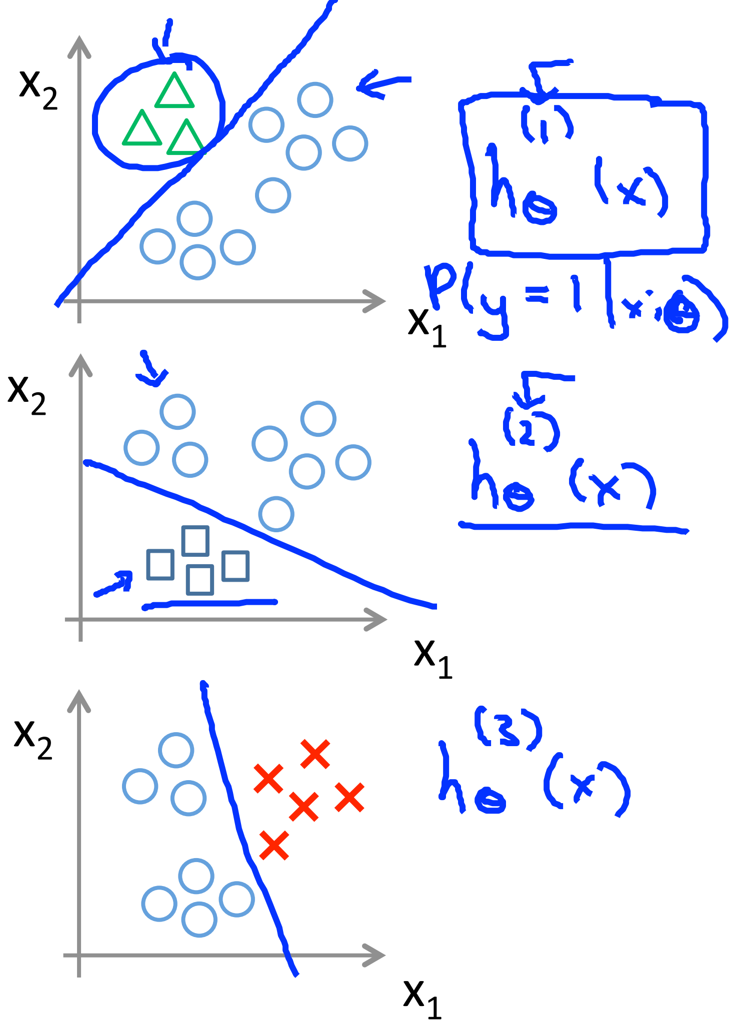


One-vs-all (one-vs-rest):



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

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