Logistic Regression

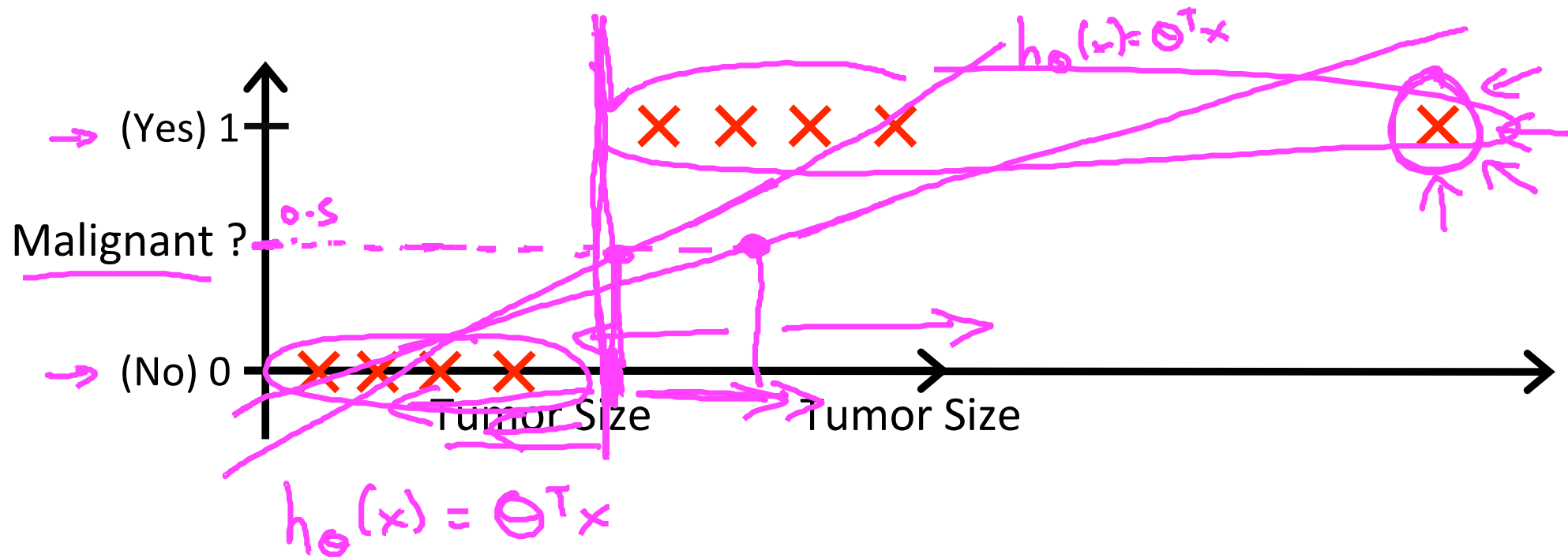## Classification

Machine Learning

Classification

→ Email: Spam / Not Spam?

→ Online Transactions: Fraudulent (Yes / No)?

→ Tumor: Malignant / Benign ?

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

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

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

$$\rightarrow y \in \{0, 1, 2, 3\}$$

Threshold classifier output $h_\theta(x)$ at 0.5:
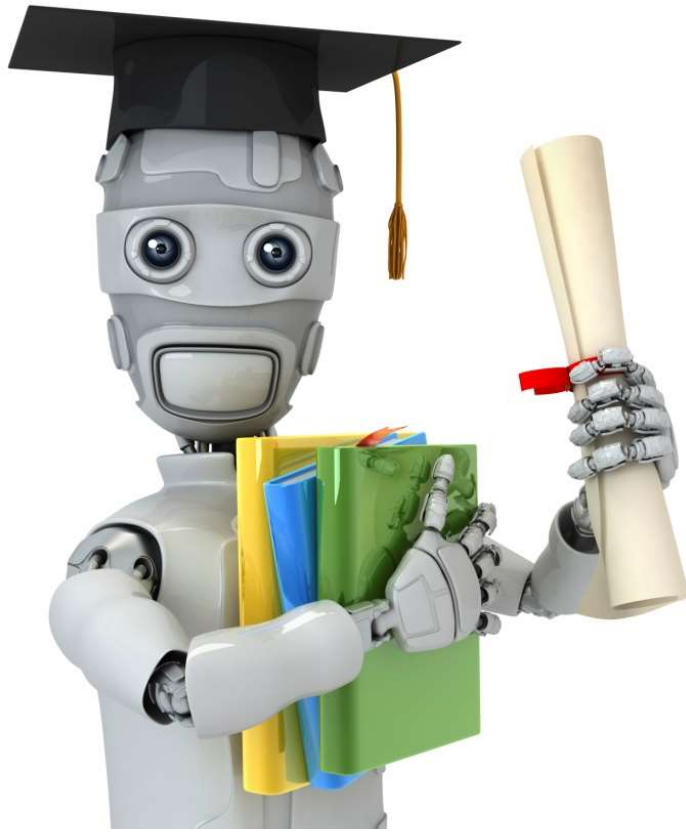
If $h_\theta(x) \geq 0.5$, predict "y = 1"

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

Andrew Ng

Classification: $y = 0$ or 1

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

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

Classification

Logistic Regression

Hypothesis Representation

Machine Learning

Logistic Regression Model

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

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

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

$\theta^T x$

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

Sigmoid function
Logistic function

1

0.5

0

$g(z)$

z
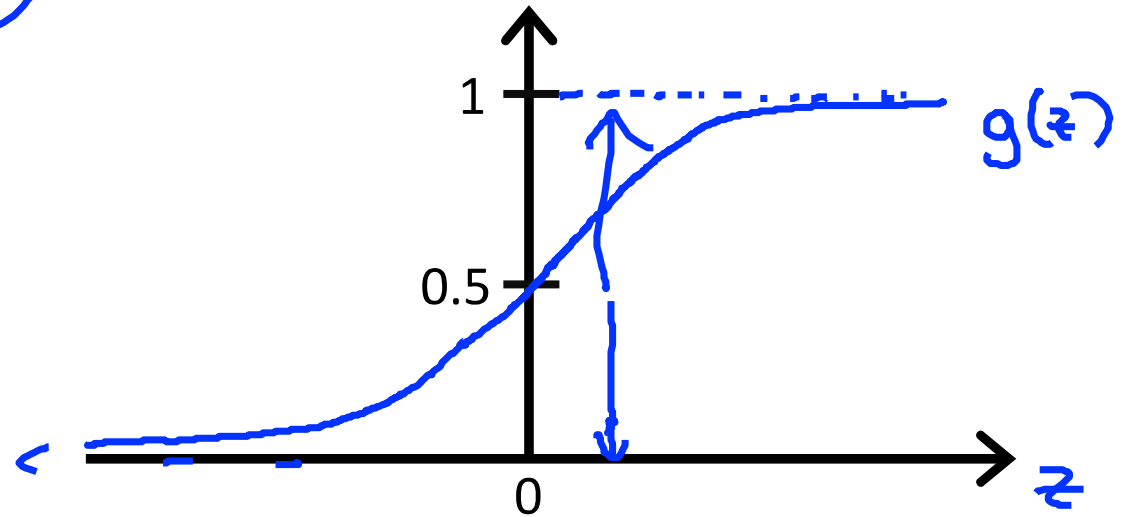
Parameter θ.

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

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

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

$y = 0$ or 1

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

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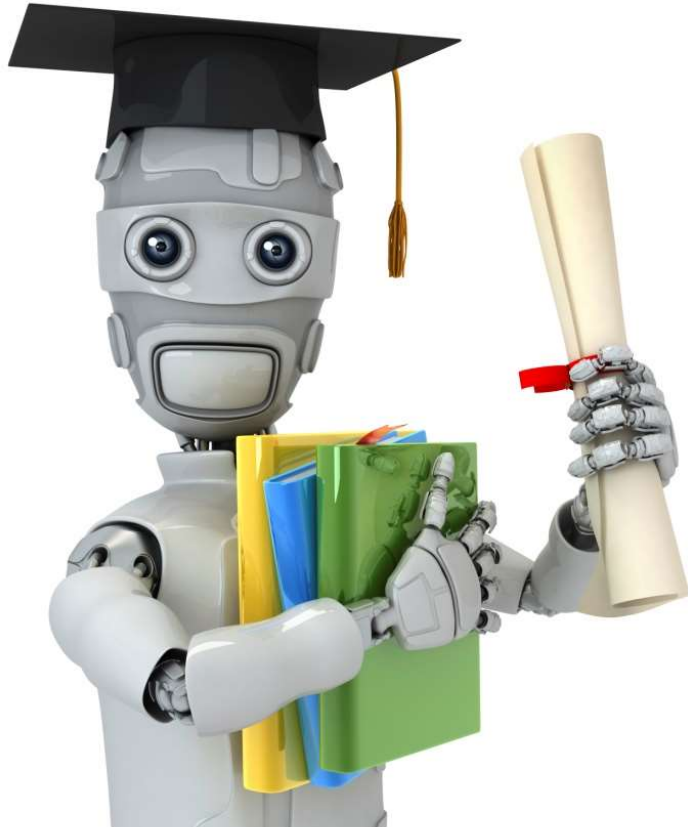
Logistic Regression

Decision boundary

Machine Learning
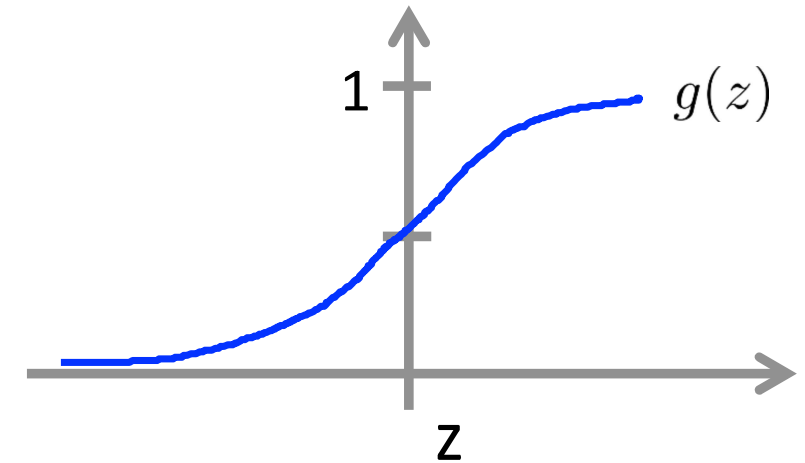
Logistic regression

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

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

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

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

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

$$\theta^T x < 0$$

1 ── $g(z)$

z

$g(z) \geq 0.5$
when $z \geq 0$

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

$g(z) < 0.5$
when $z < 0$

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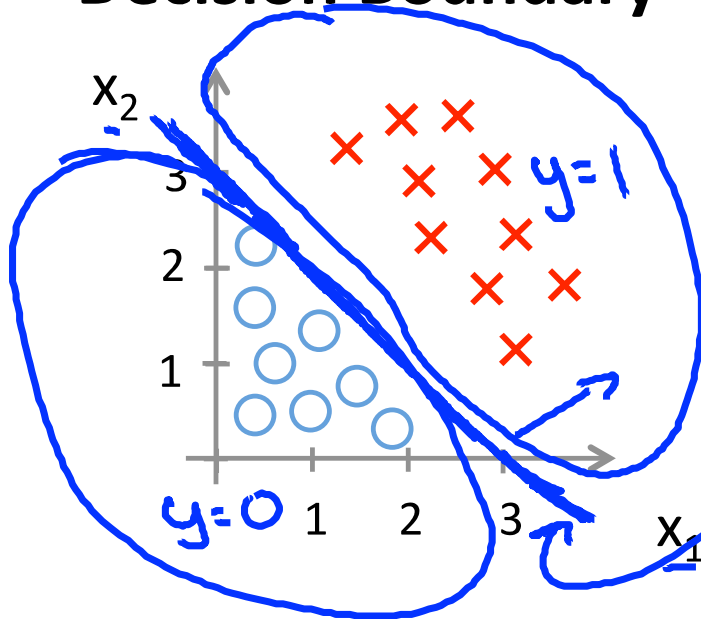
$$\theta = \begin{bmatrix} -3 \\ 1 \\ 1 \end{bmatrix}$$

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

$$-3 \qquad 1 \qquad 1$$

Decision boundary

Predict "$y = 1$" if $\quad -3 + x_1 + x_2 \geq 0$

$\theta^T x$

$\rightarrow x_1 + x_2 \geq 3$
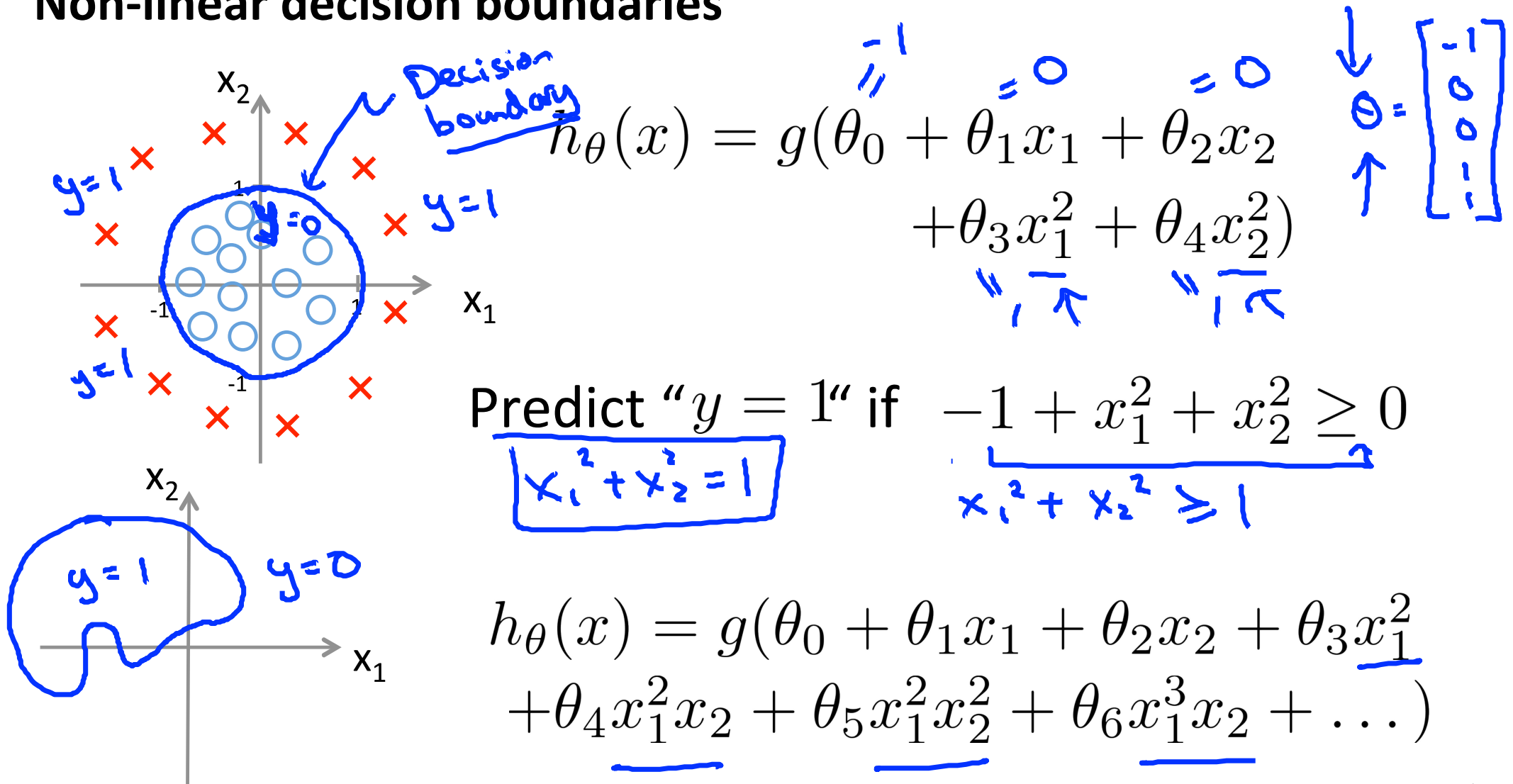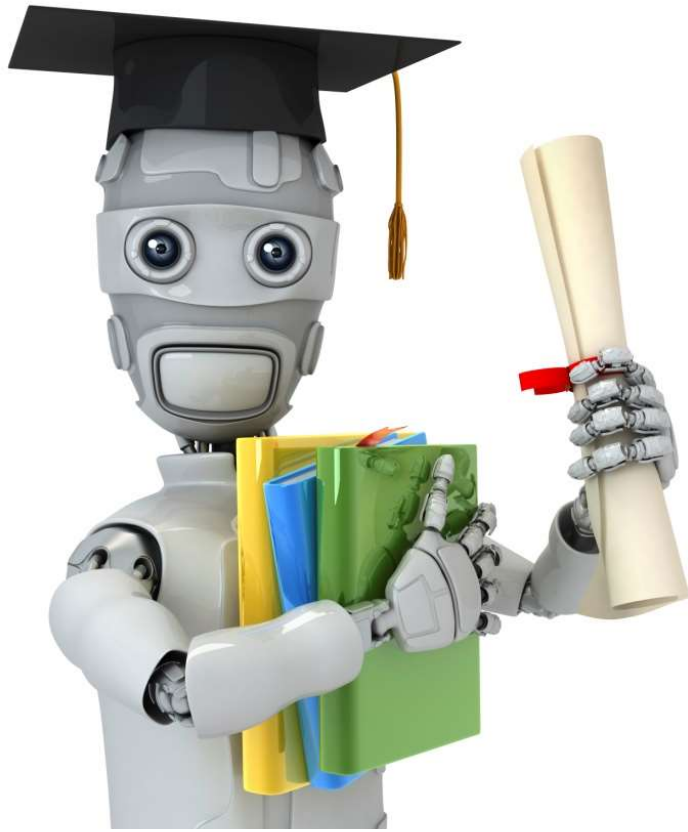
x_1, x_2

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

$x_1 + x_2 = 3$

$x_1 + x_2 < 3$

$y = 0$

Non-linear decision boundaries

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

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

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

$$x_1^2 + x_2^2 = 1$$

$$x_1^2 + x_2^2 \geq 1$$

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

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Logistic Regression

Cost function

Machine Learning

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

m examples

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

$$h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}$$
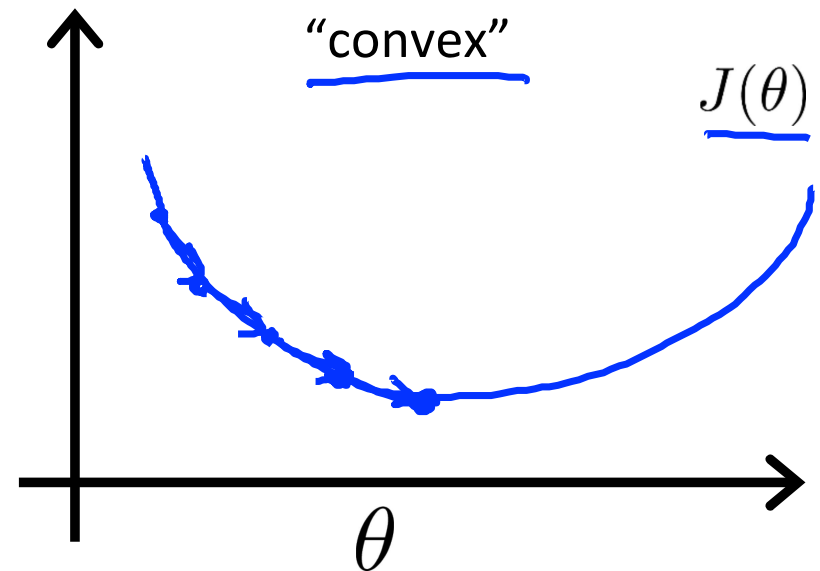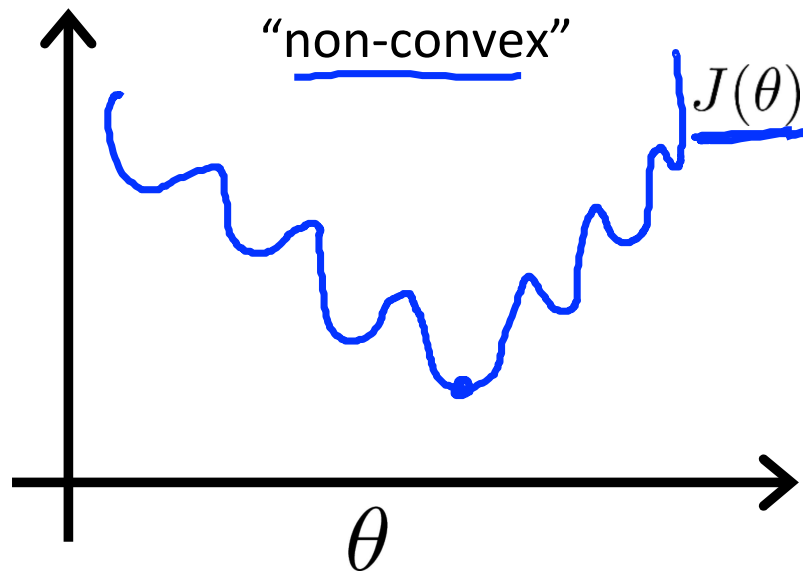
How to choose parameters θ ?

Cost function

→ Linear regression: $J(\theta) = \dfrac{1}{m} \sum\limits_{i=1}^{m} \underline{\dfrac{1}{2}} \cancel{\left(h_\theta(x^{(i)}) - y^{(i)} \right)^2}$

Logistic

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

$\mathrm{Cost}\left(h_\theta(x^{(i)}), y^{(i)} \right) = \dfrac{1}{2}\left(h_\theta(x^{(i)}) - y^{(i)} \right)^2$

$\dfrac{1}{1 + e^{-\theta^T x}}$

"non-convex"

$J(\theta)$

θ

"convex"

$J(\theta)$

θ

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Logistic regression cost function

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

If y = 1

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

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

$Cost \to \infty$

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.

$h_\theta(x)$

0   1

Logistic regression cost function

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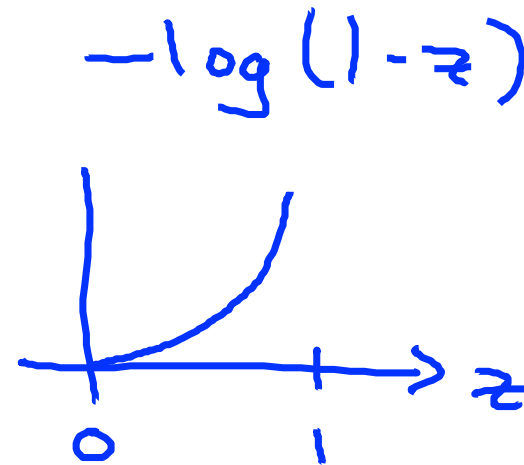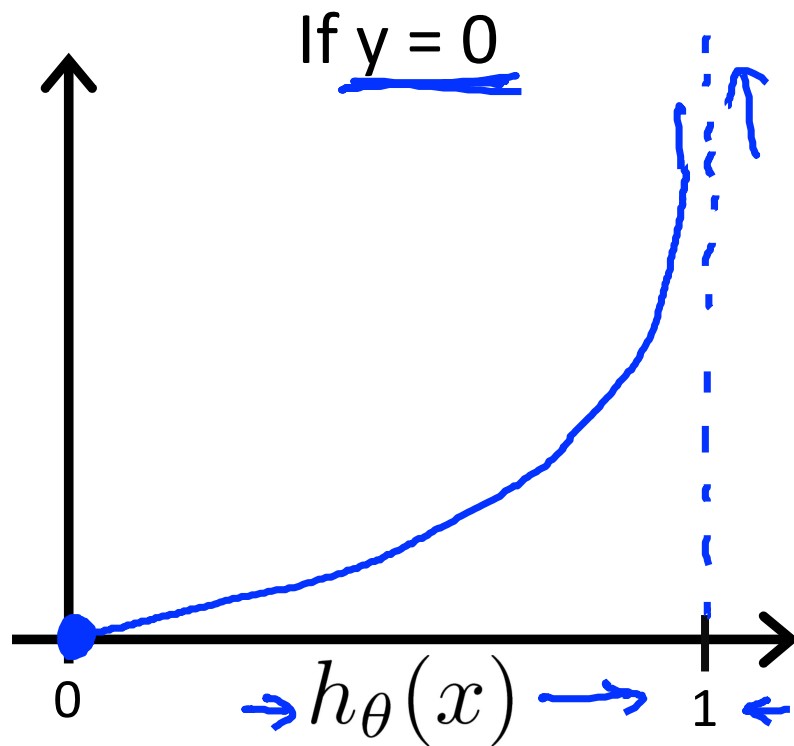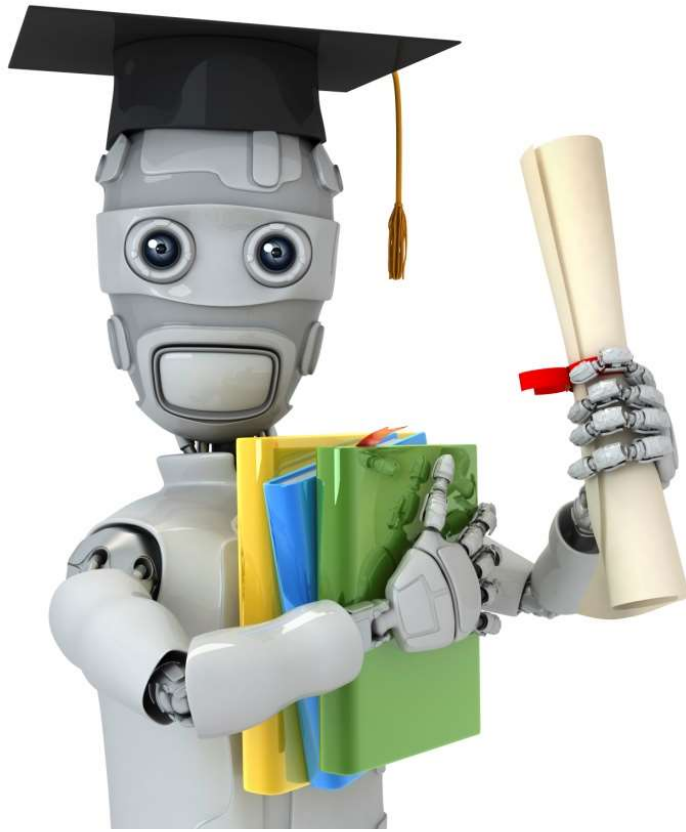
If y = 0

$-\log(1-z)$

Logistic Regression

Simplified cost function and gradient descent

Machine Learning

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: $y = 0$ or 1 always

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

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

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

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

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

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

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

Repeat {

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

}

(simultaneously update all θ_j)

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

Gradient Descent

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

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

Repeat {
$$\theta_j := \theta_j - \alpha \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$$
}
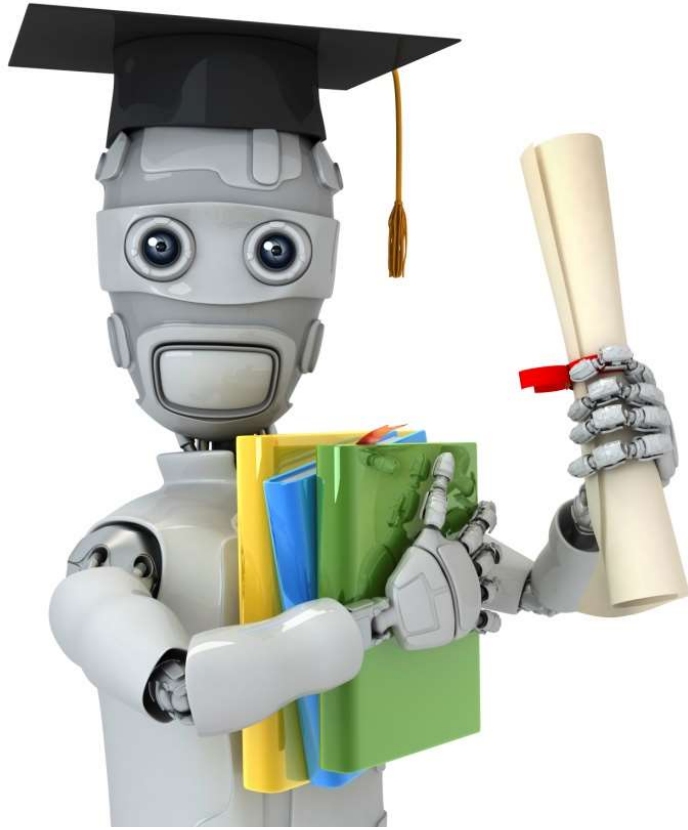
(simultaneously update all θ_j)

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

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

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

Algorithm looks identical to linear regression!

Logistic
Regression

Advanced
optimization

Machine Learning

Optimization algorithm

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

Given θ, we have code that can compute

- $J(\theta)$

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

Gradient descent:

Repeat $\{$

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

$\}$

Optimization algorithm

Given θ, we have code that can compute

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

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

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

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

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

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

```
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);
```

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

$$\texttt{theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix} \begin{matrix} \texttt{theta(1)} \leftarrow \\ \\ \texttt{theta(2)} \\ \\ \texttt{theta(n+1)} \end{matrix}$$
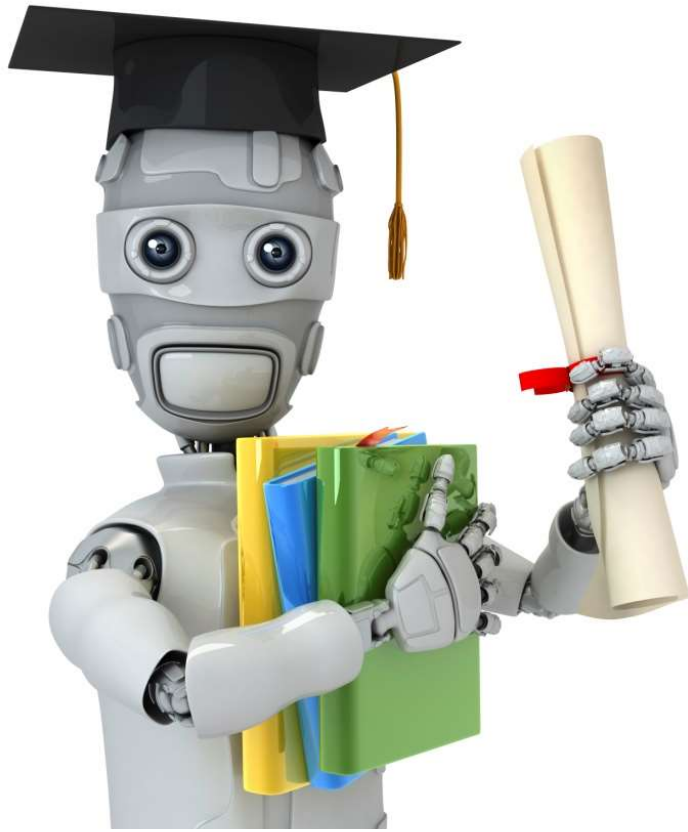
function [**jVal**, **gradient**] **= costFunction(theta)**

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 $\frac{\partial}{\partial \theta_n} J(\theta)$] ;

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Logistic Regression

Multi-class classification: One-vs-all

Machine Learning

Multiclass classification

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

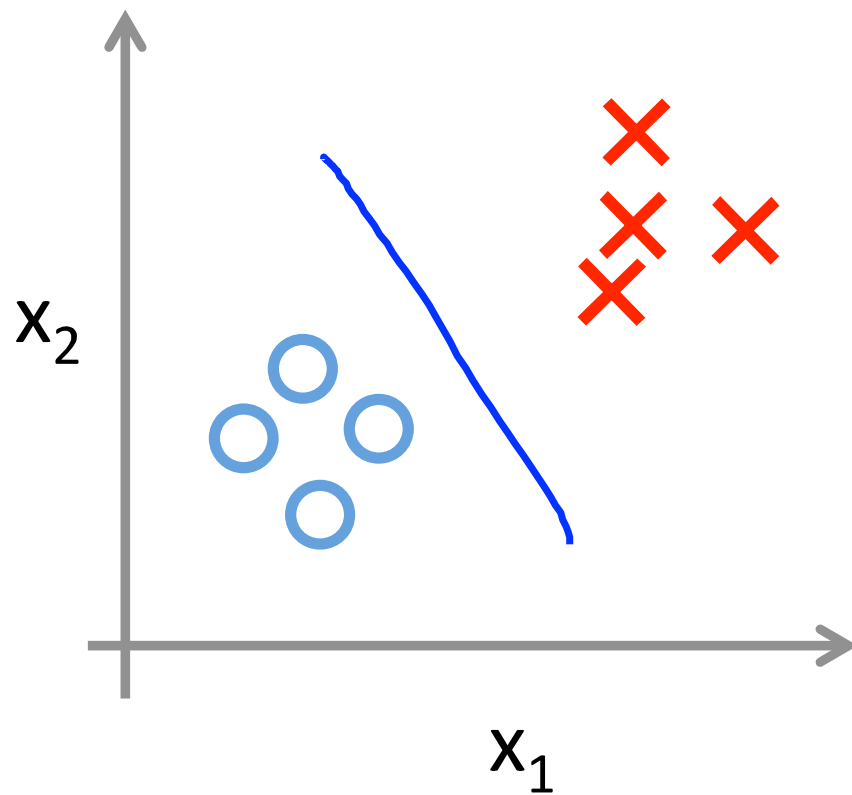$y=1$　　$y=2$　　$y=3$　　$y=4$

Medical diagrams: Not ill, Cold, Flu
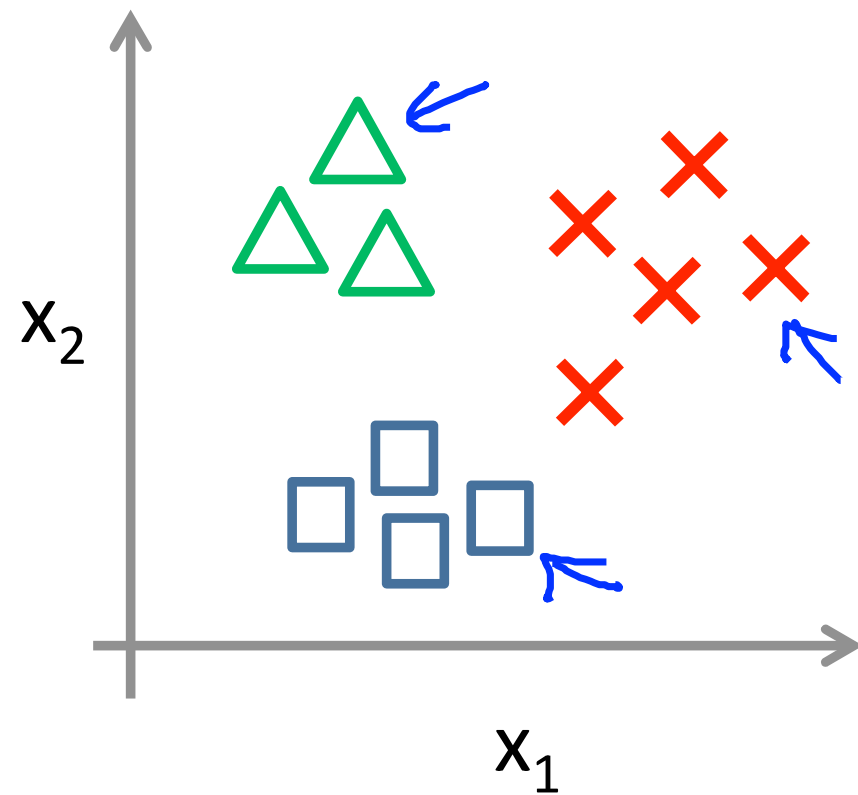
$y=1$　　2　　3
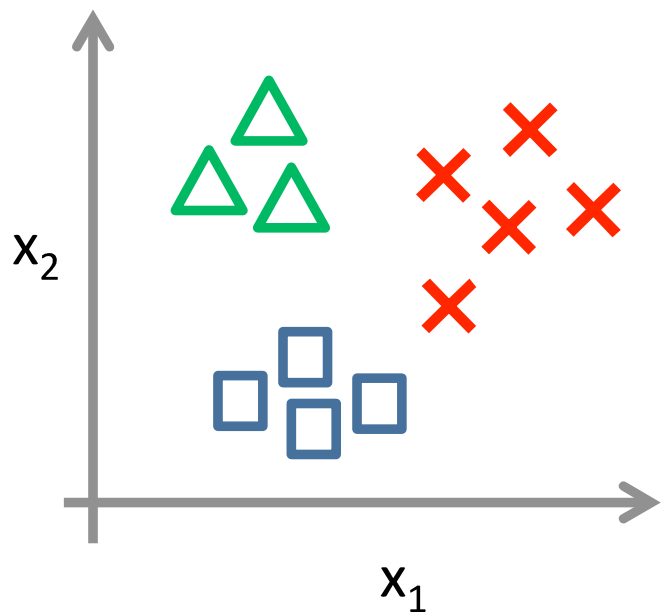
Weather: Sunny, Cloudy, Rain, Snow

$y=1$　　2　　3　　4 ⟵

0　　1　　2　　3

Binary classification:

Multi-class classification:

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

Class 1: △ ←

Class 2: □ ←

Class 3: ✖ ←

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

$h_\theta^{(1)}(x)$

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

$h_\theta^{(2)}(x)$

$h_\theta^{(3)}(x)$

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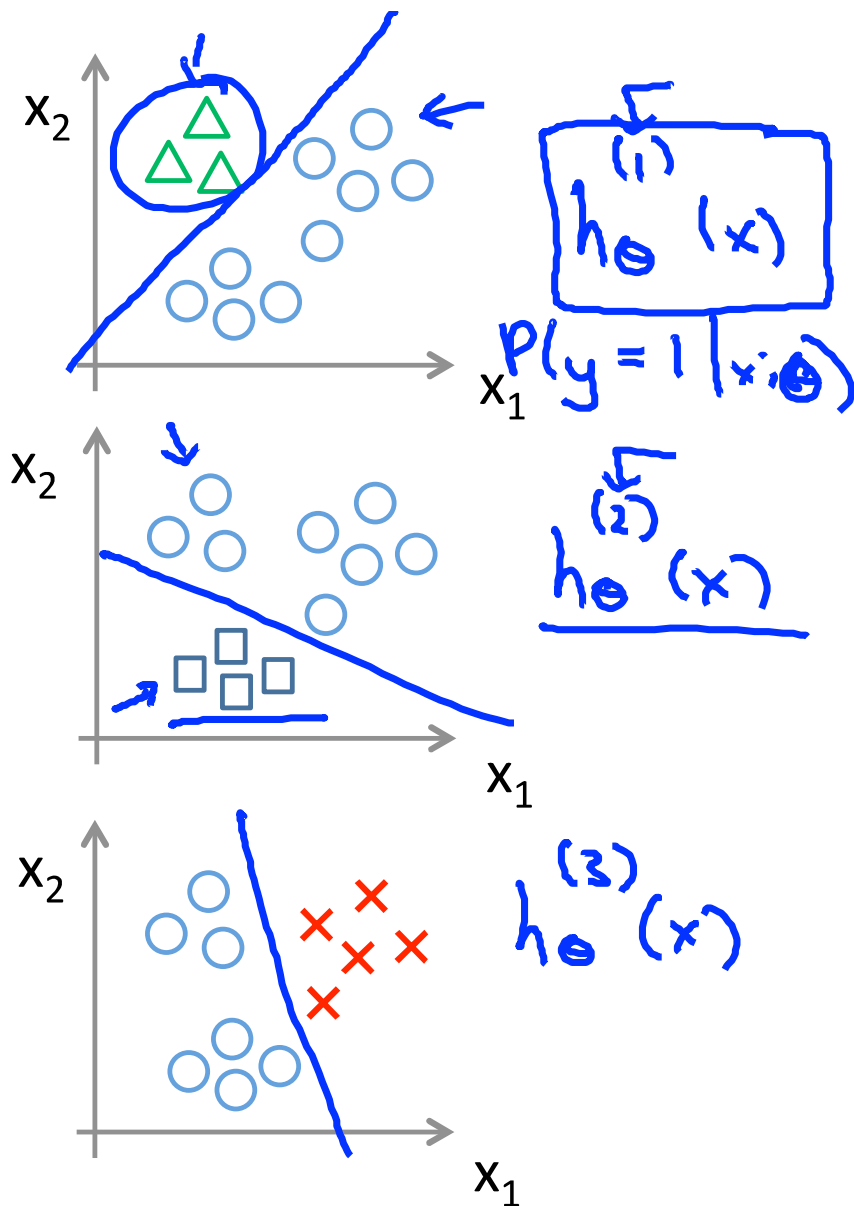
One-vs-all

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

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