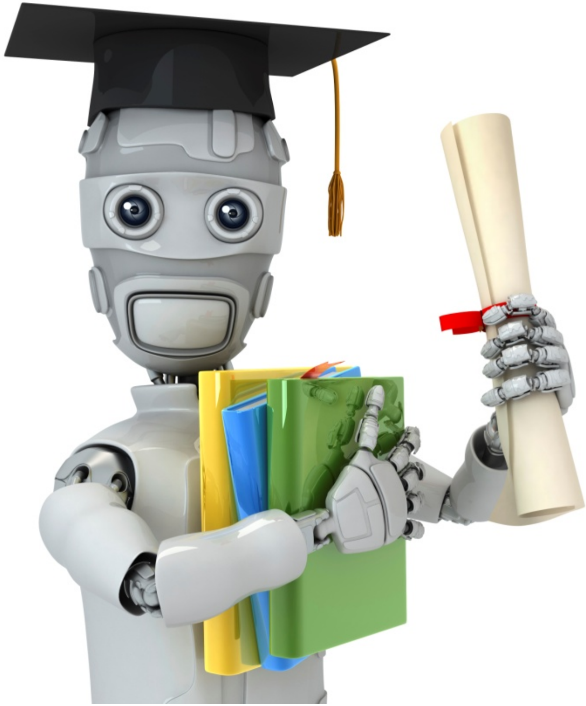


Machine Learning

Logistic Regression

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

Classification

output y is discrete value

Classification examples

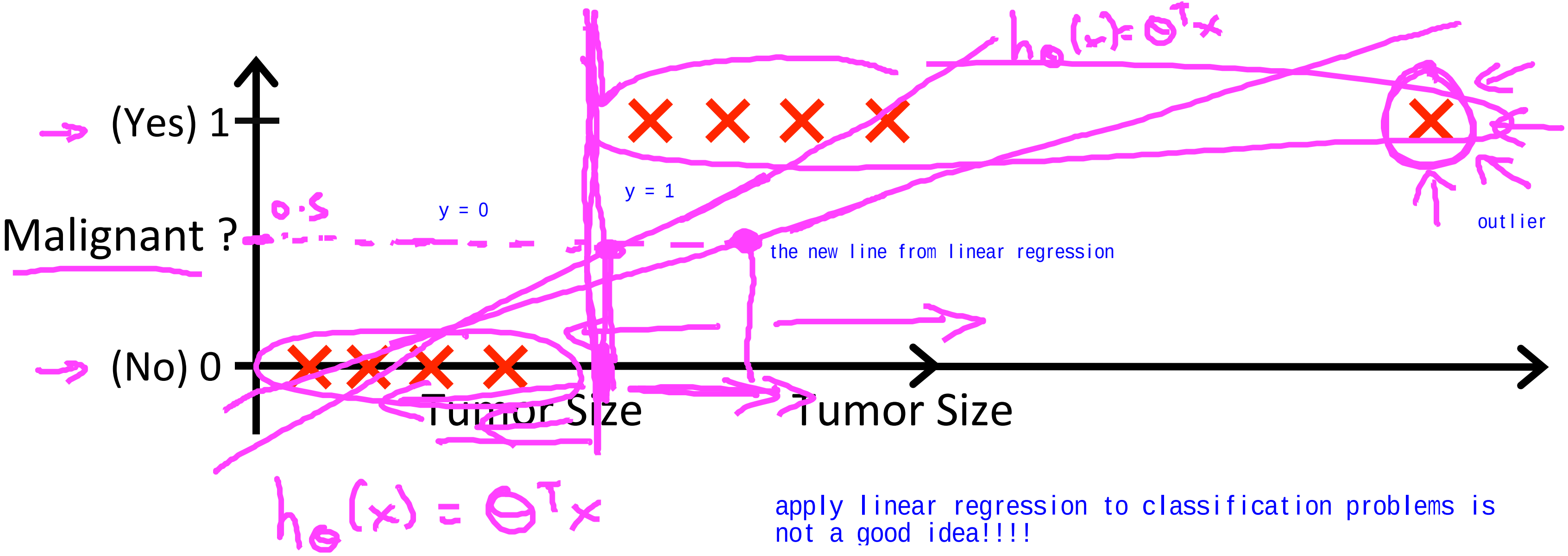
- Email: Spam / Not Spam?
- Online Transactions: Fraudulent (Yes / No)?
- Tumor: Malignant / Benign ?

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

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`



apply linear regression to classification problems is not a good idea!!!!

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"

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

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

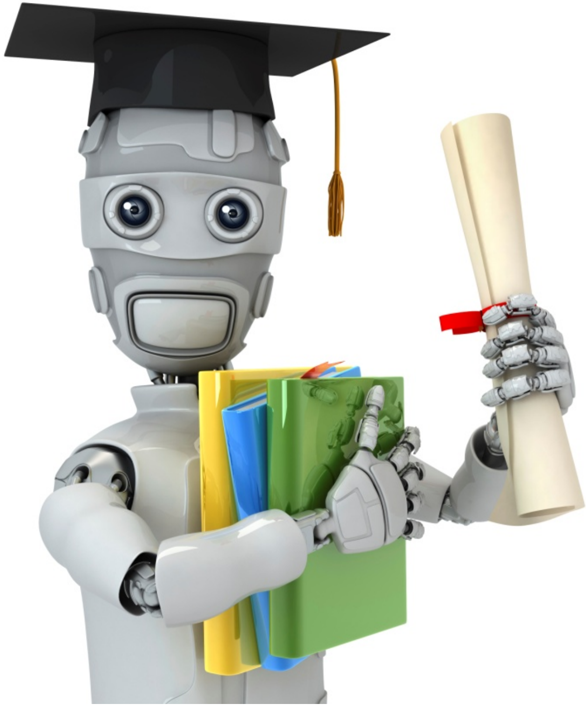
Logistic Regression: $0 \leq h_\theta(x) \leq 1$

Classification

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

Logistic Regression

Hypothesis Representation



Machine Learning

we want our function to satisfy this property

Logistic Regression Model

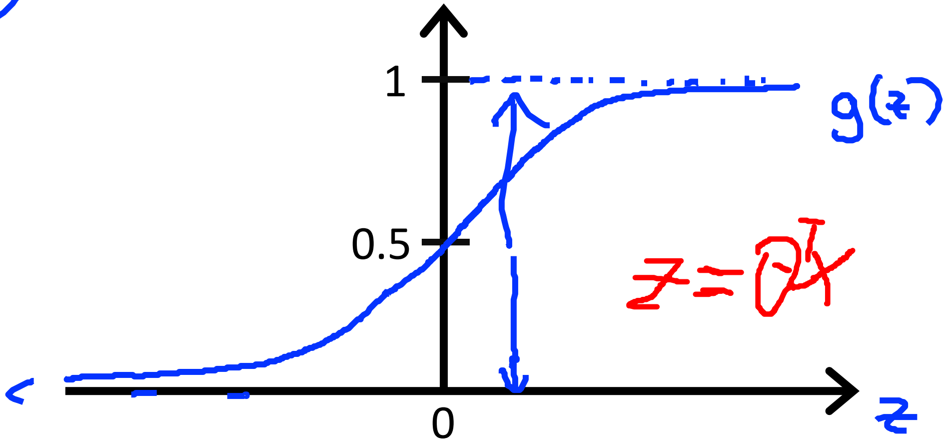
Want $\boxed{0 \le h_\theta(x) \le 1}$

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

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

$\theta^T x$

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



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

$h_\theta(x) = 0.7$ $\quad y=1$

interpretation of the output value

Tell patient that 70% chance of tumor being malignant

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

written formally

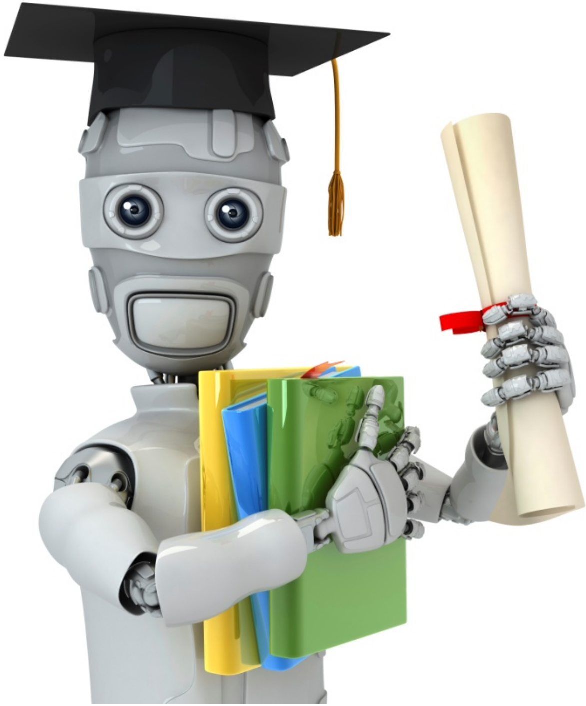
"probability that y = 1, given x, parameterized by θ"

$y = 0$ 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

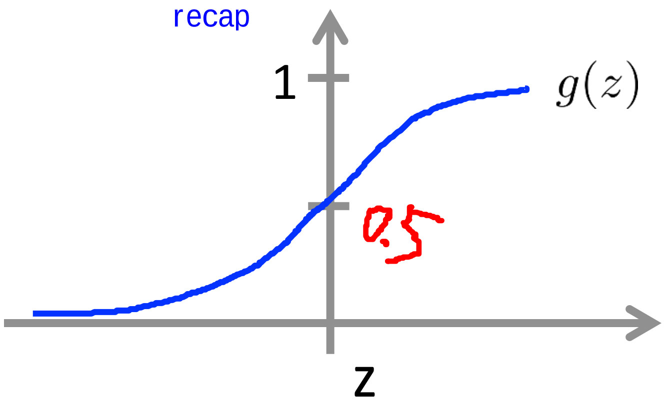
Decision boundary

Machine Learning

Logistic regression

$$h_\theta(x) = g(\theta^T x) = P(y=1 \mid x;\theta)$$

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



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

$= \theta^T x \geq 0$ ✓

$g(z) \geq 0.5$

when $z \geq 0$

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

whenever theta'*x >=0

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

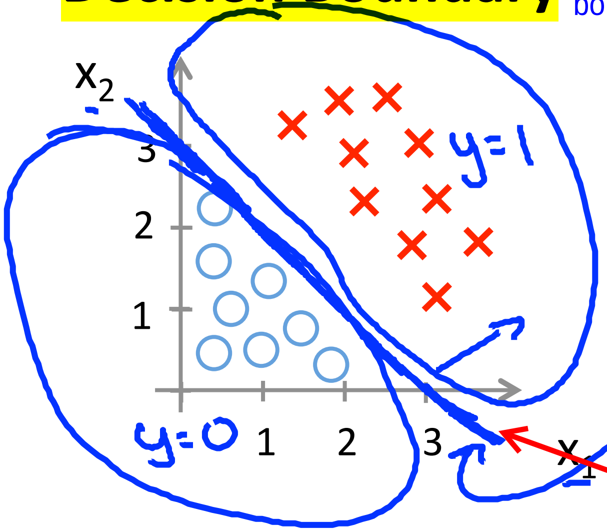
$= \theta^T x < 0$ ✓

$g(z) < 0.5$

when $z < 0$

Decision Boundary

linear decision boundary



suppose we choose this parameter set

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

$$h_\theta(x) = g(\underbrace{\theta_0}_{-3} + \underbrace{\theta_1}_{1} x_1 + \underbrace{\theta_2}_{1} x_2)$$

Decision boundary

This line is called the decision boundary

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

$\rightarrow x_1 + x_2 \geq 3$

x_1, x_2

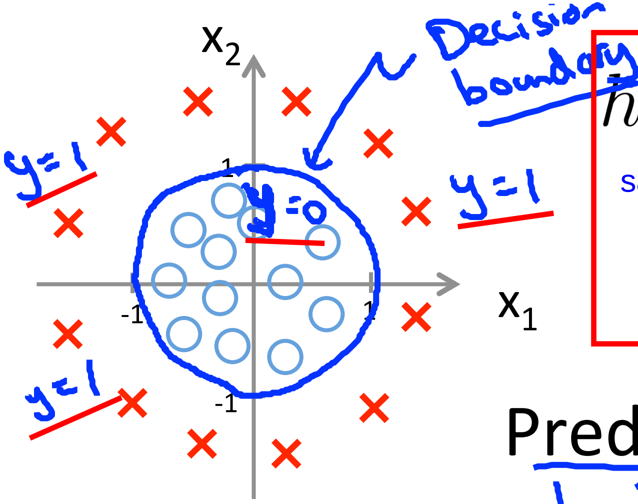
$\rightarrow h_\theta(x) = 0.5$

$\boxed{x_1 + x_2 = 3}$

$x_1 + x_2 < 3$

$\rightarrow y = 0$

Non-linear decision boundaries



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

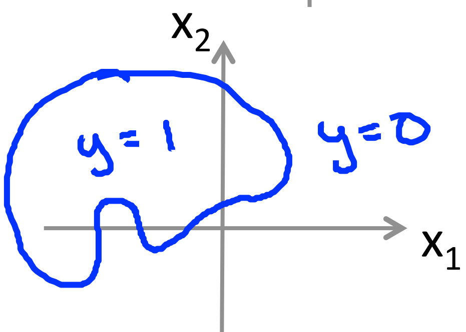
same as the polynomial fit

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

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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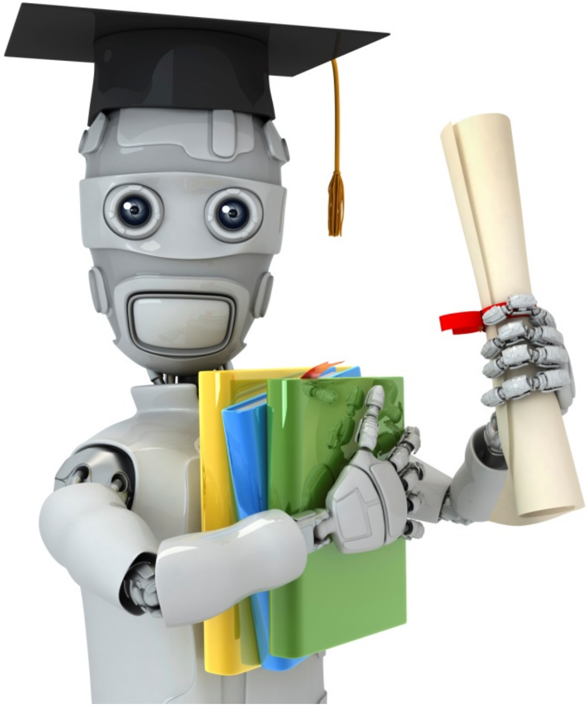


Machine Learning

Logistic Regression

Cost function

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

m examples

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

n features

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

my hypothesis

How to choose parameters θ ?

Cost function

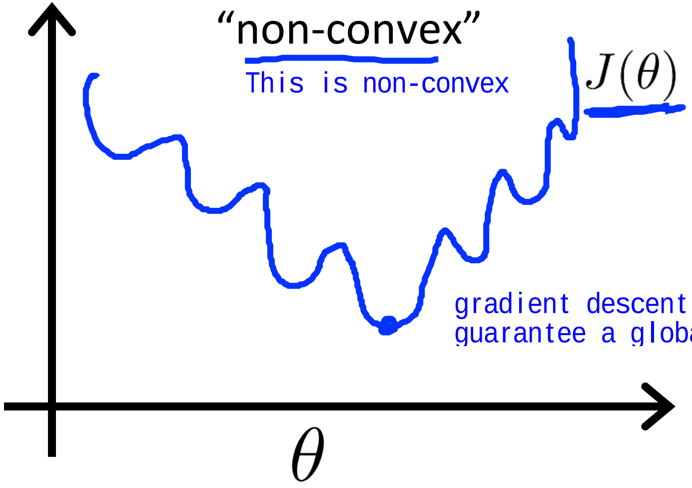
→ ~~Linear~~ regression: $J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \cancel{\frac{1}{2}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2}$

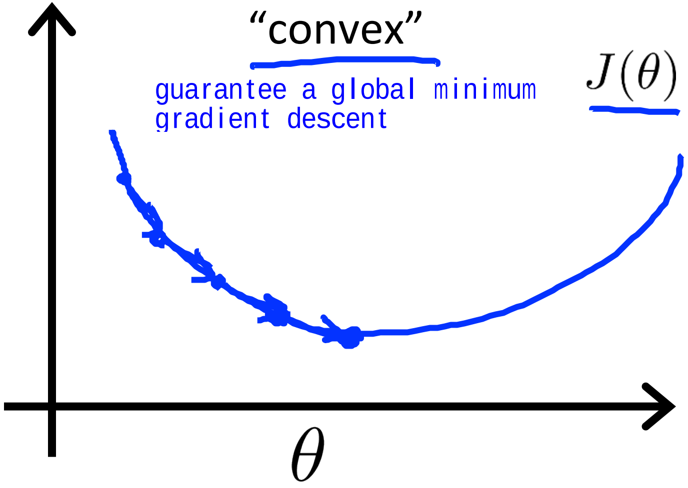
Logistic

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

we want to minimize a cost function

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





Logistic regression cost function

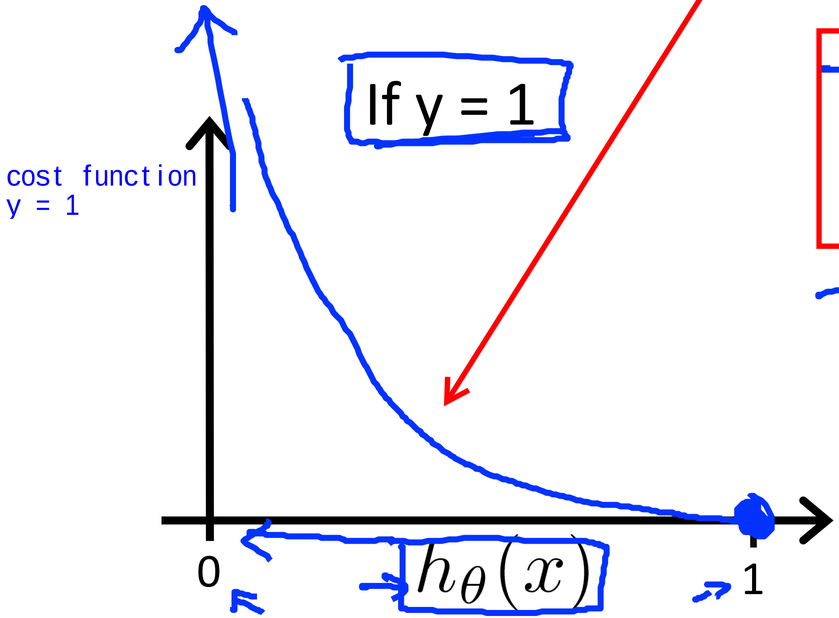
cost function is linear regression for logistic regression is not convex, we have to define a new cost function so that it can be convex!

predicted value

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

actual value

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



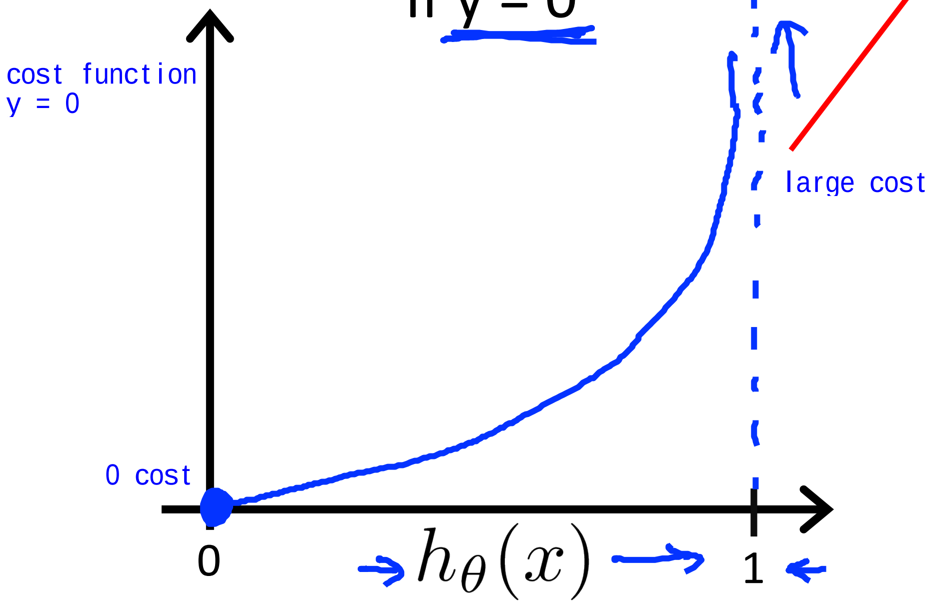
$\mathrm{Cost} = 0$ if $y = 1, h_\theta(x) = 1$
But as $h_\theta(x) \to 0$
$Cost \to \infty$

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.

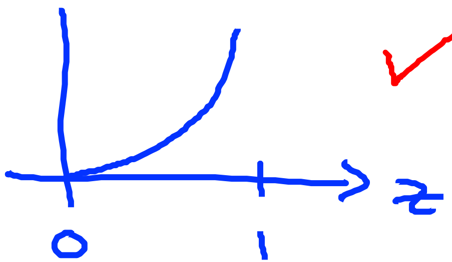
Logistic regression cost function

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

If y = 0



$-\log(1-z)$



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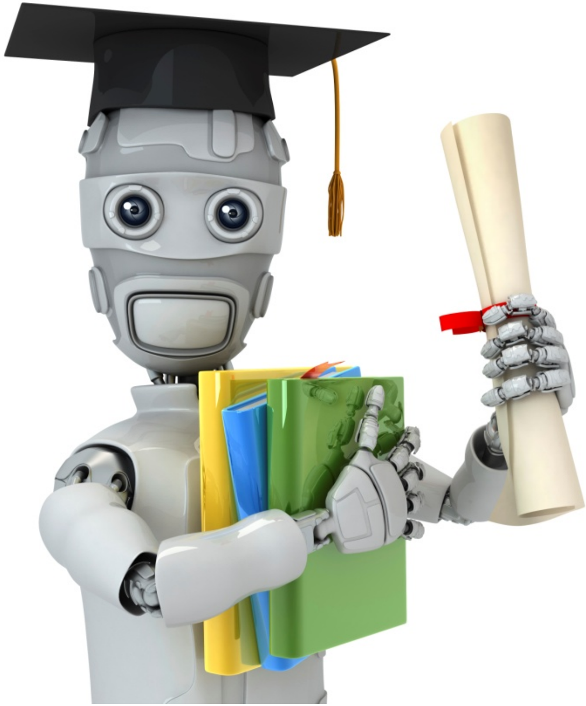

Machine Learning

Logistic Regression

Simplified cost function and gradient descent

Logistic regression cost function

overall 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

combine them into a single equation

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

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

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

here y can either be 1 or 0,
therefore we can write in this way

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Logistic regression cost function

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

then we can rewrite our cost function as follows

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

This is the cost function that everyone uses, and it is convex!!!

To fit parameters θ :

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

objective!

To make a prediction given new x :

Output $\boxed{h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}}$ $\Longrightarrow$ $p(y=1 \mid x;\theta)$

output of hypothesis can be interpreted as the probability of y=1

Gradient Descent

We use gradient descent to minimize the cost function

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

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

Repeat $\{$

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

same as usual!

(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

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

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

Repeat {

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

(simultaneously update all θ_j)

}

$$\Theta = \begin{bmatrix} \Theta_0 \\ \Theta_1 \\ \Theta_2 \\ \vdots \\ \Theta_n \end{bmatrix}$$

for i = 0 to n

we would like to use vector notation to improve the efficiency!

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

linear regression

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

logistic regression

Algorithm looks identical to linear regression!

feature scaling can also help your gradient descent algorithm to run faster!

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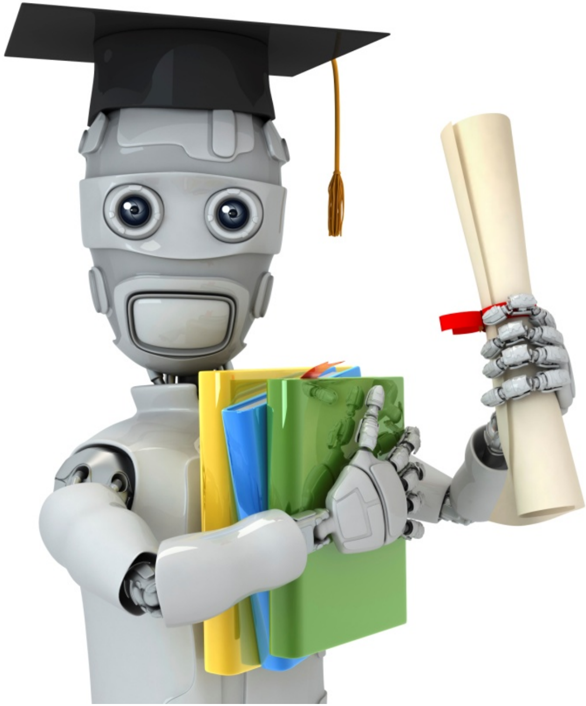

Machine Learning

Logistic Regression

Advanced optimization

Optimization algorithm

gradient descent review

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 $j = 0, 1, \ldots, n$)

supply code here!

Gradient descent:

Repeat $\{$

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

$\}$

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

more sophisticated algorithms beyond the scope of this course!

It is possible to implement (use software) them without understand them thoroughly!

Advantages: of those algorithms!

- No need to manually pick α
- Often faster than gradient descent. details are beyond the scope of this course!

Disadvantages:

- More complex

example of how to use these algorithms

Example:

$\min_\theta J(\theta)$

$$\theta = \begin{bmatrix}\theta_1 \\ \theta_2\end{bmatrix}$$

exact solution!

$\theta_1 = 5, \theta_2 = 5.$

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

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

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

compute cost function

gradient, 2x1 vector

```
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);
```

means you are going to provide the gradient

max iterations

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

@ is a pointer of our defined function

we can then can this function!

unc = unconstrained

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

we have to have at least 2 variables!

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Apply in logistic regression

Note: These algorithms are faster than gradient descent but they are hard to debug. When you have a large ML problem, you should use these advanced optimization algorithms!

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

our function has to return the cost function and the gradients

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

This is the template

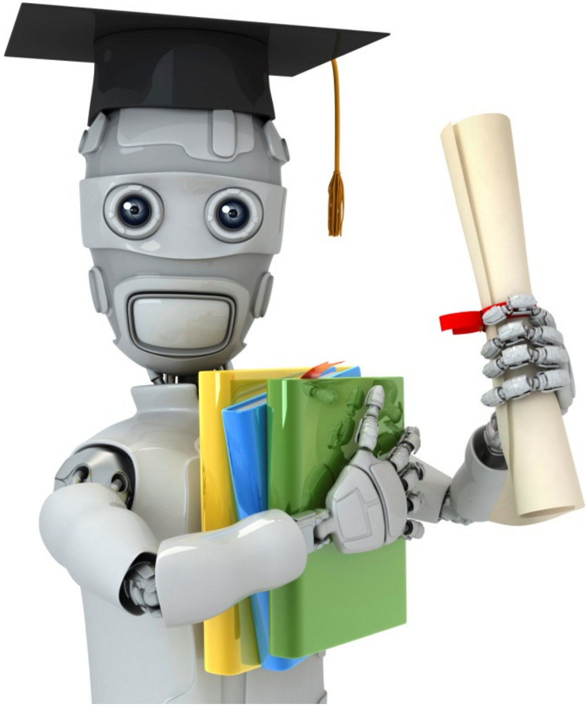
jVal = [code to compute $J(\theta)$];

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



Logistic Regression

Multi-class classification: One-vs-all

Machine Learning

Multiclass classification not just 0,1, but with multiple cases

Examples!

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

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

Medical diagrams: Not ill, Cold, Flu

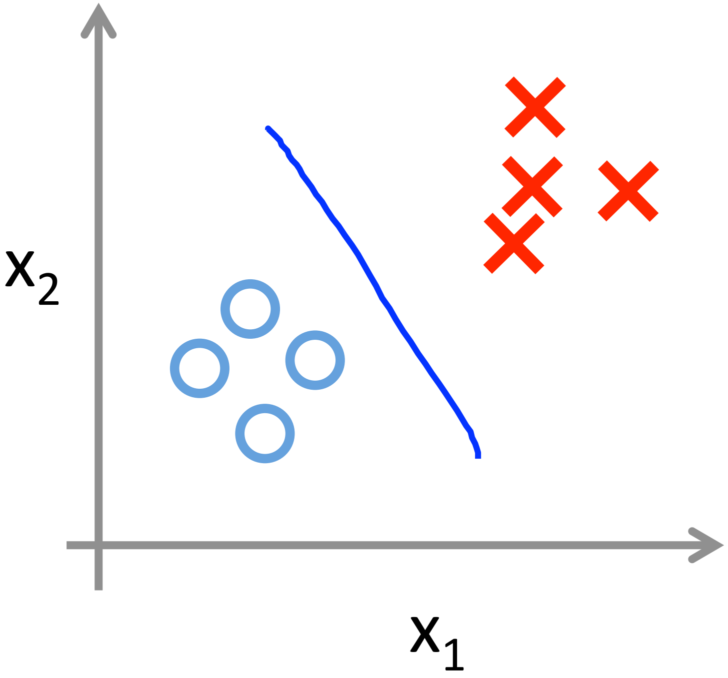
$y=1$ 2 3

Weather: Sunny, Cloudy, Rain, Snow

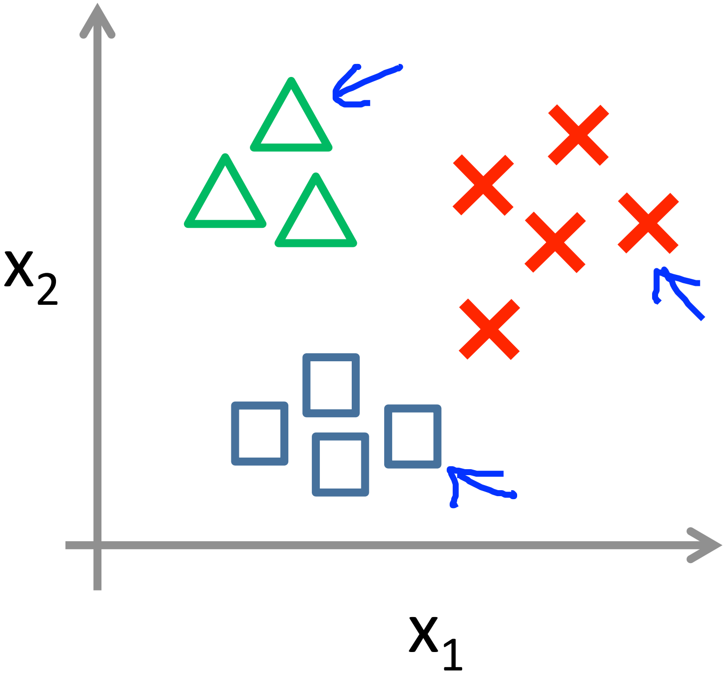
$y=1$ 2 3 4

0 1 2 3

Binary classification:



Multi-class classification:



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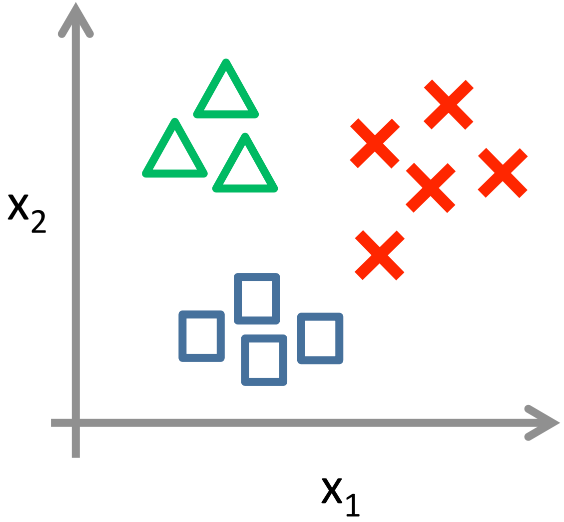
the main idea is to turn the multi case to binary case

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

we create as a new sort of fake training set where classes two and three get assigned to the negative class



we do the same thing for class 2

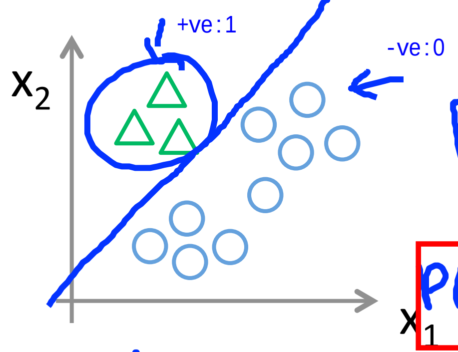
and so on so forth

Class 1: △

Class 2: □

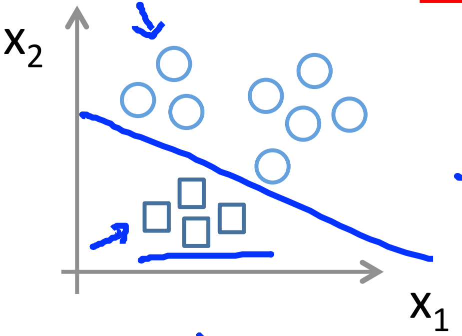
Class 3: ✕

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

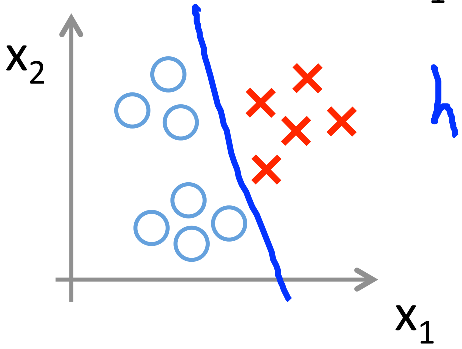


$h_\theta^{(1)}(x)$

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



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



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

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One-vs-all

To summarize

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

To make a prediction

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

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

test h(x) for all classes and choose whichever the h gives us the largest value