

# 06: Logistic Regression

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## Classification

- Where  $y$  is a discrete value
  - Develop the logistic regression algorithm to determine what class a new input should fall into
- Classification problems
  - Email -> spam/not spam?
  - Online transactions -> fraudulent?
  - Tumor -> Malignant/benign
- Variable in these problems is  $Y$ 
  - $Y$  is either 0 or 1
    - 0 = negative class (absence of something)
    - 1 = positive class (presence of something)
- Start with **binary class problems**
  - Later look at multiclass classification problem, although this is just an extension of binary classification
- How do we develop a classification algorithm?
  - Tumour size vs malignancy (0 or 1)
  - We *could* use linear regression
    - Then threshold the classifier output (i.e. anything over some value is yes, else no)
    - In our example below linear regression with thresholding seems to work



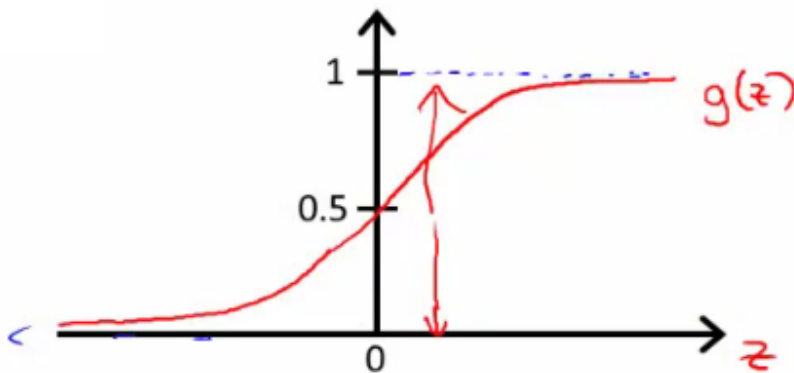
- We can see above this does a reasonable job of stratifying the data points into one of two classes
  - But what if we had a single Yes with a very small tumour
  - This would lead to classifying all the existing yeses as nos
- Another issues with linear regression
  - We know  $Y$  is 0 or 1
  - Hypothesis can give values large than 1 or less than 0
- So, logistic regression generates a value where is always either 0 or 1
  - Logistic regression is a **classification algorithm** - don't be confused

## Hypothesis representation

- What function is used to represent our hypothesis in classification
- We want our classifier to output values between 0 and 1
  - When using linear regression we did  $h_{\theta}(x) = (\theta^T x)$
  - For classification hypothesis representation we do  $h_{\theta}(x) = g(\theta^T x)$ 
    - Where we define  $g(z)$ 
      - $z$  is a real number
    - $g(z) = 1/(1 + e^{-z})$ 
      - This is the **sigmoid function**, or the **logistic function**
    - If we combine these equations we can write out the hypothesis as

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

- What does the sigmoid function look like
- Crosses 0.5 at the origin, then flattens out]
  - Asymptotes at 0 and 1



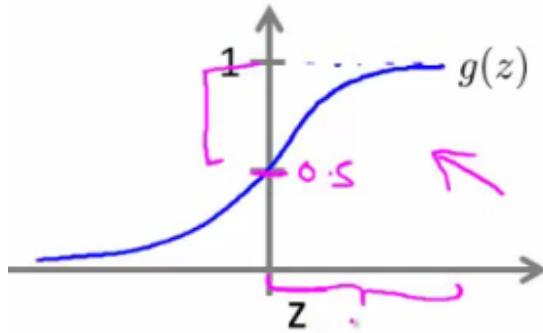
- Given this we need to fit  $\theta$  to our data

## Interpreting hypothesis output

- When our hypothesis ( $h_{\theta}(x)$ ) outputs a number, we treat that value as the estimated probability that  $y=1$  on input  $x$ 
  - Example
    - If  $X$  is a feature vector with  $x_0 = 1$  (as always) and  $x_1 = \text{tumourSize}$
    - $h_{\theta}(x) = 0.7$ 
      - Tells a patient they have a 70% chance of a tumor being malignant
  - We can write this using the following notation
    - $h_{\theta}(x) = P(y=1|x; \theta)$
  - What does this mean?
    - Probability that  $y=1$ , given  $x$ , parameterized by  $\theta$
- Since this is a binary classification task we know  $y = 0$  or  $1$ 
  - So the following must be true
    - $P(y=1|x; \theta) + P(y=0|x; \theta) = 1$
    - $P(y=0|x; \theta) = 1 - P(y=1|x; \theta)$

## Decision boundary

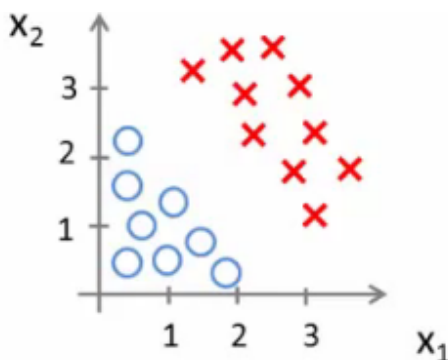
- Gives a better sense of what the hypothesis function is computing
- Better understand of what the hypothesis function looks like
  - One way of using the sigmoid function is;
    - When the probability of  $y$  being 1 is greater than 0.5 then we can predict  $y = 1$
    - Else we predict  $y = 0$
  - When is it exactly that  $h_0(x)$  is greater than 0.5?
    - Look at sigmoid function
      - $g(z)$  is greater than or equal to 0.5 when  $z$  is greater than or equal to 0



- So if  $z$  is positive,  $g(z)$  is greater than 0.5
  - $z = (\theta^T x)$
- So when
  - $\theta^T x \geq 0$
  - Then  $h_0 \geq 0.5$
- So what we've shown is that the hypothesis predicts  $y = 1$  when  $\theta^T x \geq 0$ 
  - The corollary of that when  $\theta^T x \leq 0$  then the hypothesis predicts  $y = 0$
  - Let's use this to better understand how the hypothesis makes its predictions

## Decision boundary

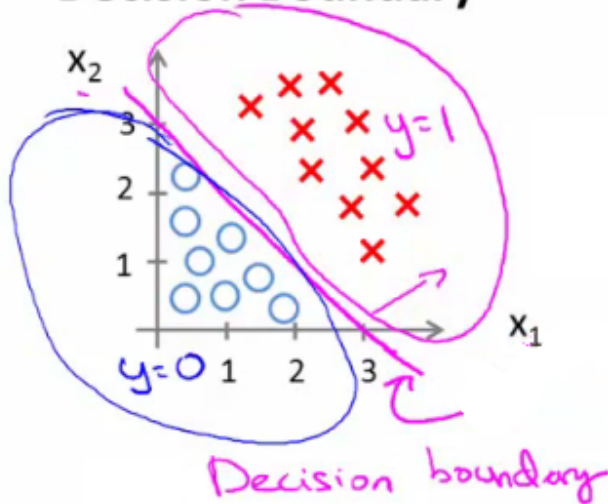
- $h_0(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$



- So, for example
  - $\theta_0 = -3$
  - $\theta_1 = 1$
  - $\theta_2 = 1$
- So our parameter vector is a column vector with the above values
  - So,  $\theta^T$  is a row vector =  $[-3, 1, 1]$

- What does this mean?
  - The  $z$  here becomes  $\theta^T x$
  - We predict " $y = 1$ " if
    - $-3x_0 + 1x_1 + 1x_2 \geq 0$
    - $-3 + x_1 + x_2 \geq 0$
- We can also re-write this as
  - If  $(x_1 + x_2 \geq 3)$  then we predict  $y = 1$
  - If we plot
    - $x_1 + x_2 = 3$  we graphically plot our **decision boundary**

## Decision Boundary

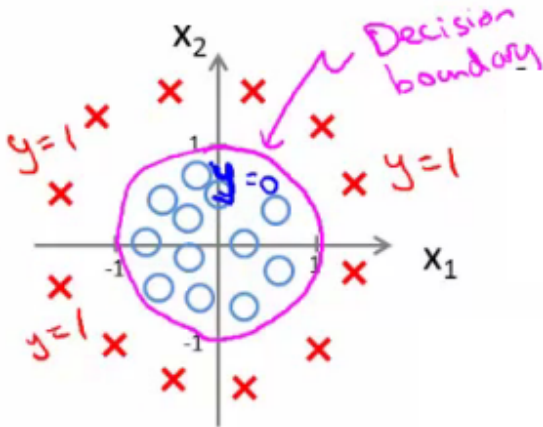


- Means we have these two regions on the graph
  - Blue = false
  - Magenta = true
  - Line = decision boundary
    - Concretely, the straight line is the set of points where  $h_{\theta}(x) = 0.5$  exactly
  - The decision boundary is a property of the hypothesis
    - Means we can create the boundary with the hypothesis and parameters without any data
      - Later, we use the data to determine the parameter values
    - i.e.  $y = 1$  if
      - $5 - x_1 > 0$
      - $5 > x_1$

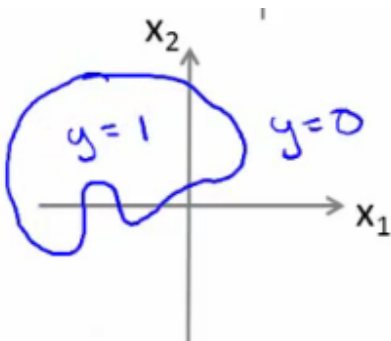
## Non-linear decision boundaries

- Get logistic regression to fit a complex non-linear data set
  - Like polynomial regress add higher order terms
  - So say we have
    - $h_{\theta}(x) = g(\theta_0 + \theta_1 x_1 + \theta_3 x_1^2 + \theta_4 x_2^2)$
    - We take the transpose of the  $\theta$  vector times the input vector
      - Say  $\theta^T$  was  $[-1, 0, 0, 1, 1]$  then we say;
      - Predict that " $y = 1$ " if

- $-1 + x_1^2 + x_2^2 \geq 0$
- or
- $x_1^2 + x_2^2 \geq 1$
- If we plot  $x_1^2 + x_2^2 = 1$ 
  - This gives us a circle with a radius of 1 around 0



- Mean we can build more complex decision boundaries by fitting complex parameters to this (relatively) simple hypothesis
- More complex decision boundaries?
  - By using higher order polynomial terms, we can get even more complex decision boundaries



## Cost function for logistic regression

- Fit  $\theta$  parameters
- Define the optimization object for the cost function we use the fit the parameters
  - Training set of  $m$  training examples
    - Each example has is  $n+1$  length column vector

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

m examples  $x \in \begin{bmatrix} x_0 \\ x_1 \\ \dots \\ x_n \end{bmatrix} \quad x_0 = 1, y \in \{0, 1\}$

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

- This is the situation
  - Set of m training examples
  - Each example is a feature vector which is n+1 dimensional
  - $x_0 = 1$
  - $y \in \{0, 1\}$
  - Hypothesis is based on parameters ( $\theta$ )
    - Given the training set how to we chose/fit  $\theta$ ?
- Linear regression uses the following function to determine  $\theta$

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

- Instead of writing the squared error term, we can write
  - If we define "cost()" as;
    - $\text{cost}(h_{\theta}(x^i), y) = 1/2(h_{\theta}(x^i) - y^i)^2$
    - Which evaluates to the cost for an individual example using the same measure as used in linear regression
  - We can **redefine J( $\theta$ ) as**

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

- Which, appropriately, is the sum of all the individual costs over the training data (i.e. the same as linear regression)
- To further simplify it we can get rid of the superscripts
  - So

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

- What does this actually mean?
  - This is the cost you want the learning algorithm to pay if the outcome is  $h_{\theta}(x)$  and the actual outcome is  $y$

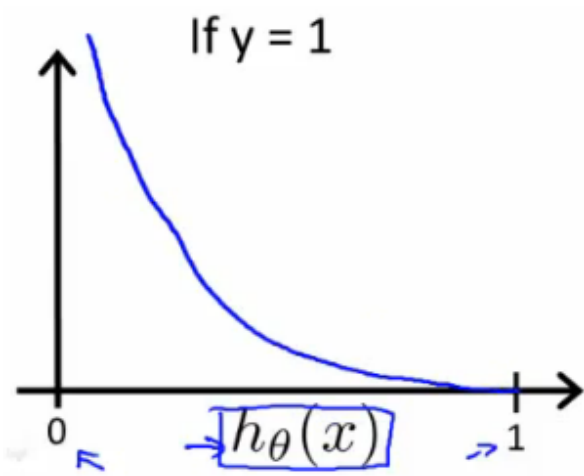
- If we use this function for logistic regression this is a **non-convex function** for parameter optimization
  - Could work....
- What do we mean by non convex?
  - We have some function -  $J(\theta)$  - for determining the parameters
  - Our hypothesis function has a non-linearity (sigmoid function of  $h_\theta(x)$ )
    - This is a complicated non-linear function
  - If you take  $h_\theta(x)$  and plug it into the  $\text{Cost}()$  function, and then plug the  $\text{Cost}()$  function into  $J(\theta)$  and plot  $J(\theta)$  we find many local optimum -> *non convex function*
  - Why is this a problem
    - Lots of local minima mean gradient descent may not find the global optimum - may get stuck in a local minimum
  - We would like a convex function so if you run gradient descent you converge to a global minimum

### A convex logistic regression cost function

- To get around this we need a different, convex  $\text{Cost}()$  function which means we can apply gradient descent

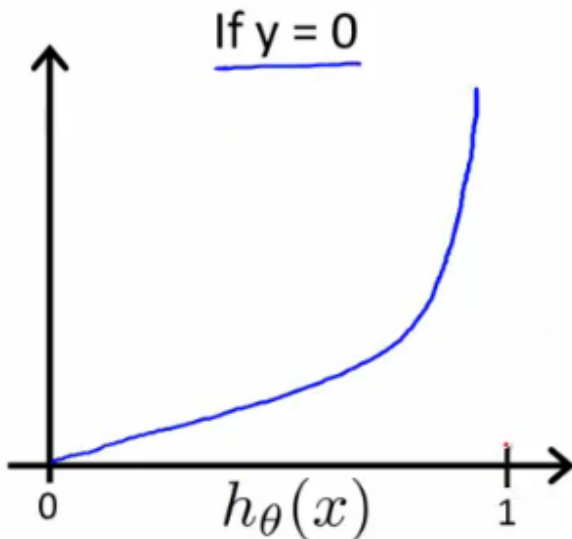
$$\text{Cost}(h_\theta(x), y) = \begin{cases} -\log(h_\theta(x)) & \text{if } y = 1 \\ -\log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$

- **This is our logistic regression cost function**
  - This is the penalty the algorithm pays
  - Plot the function
- Plot  $y = 1$ 
  - So  $h_\theta(x)$  evaluates as  $-\log(h_\theta(x))$



- So when we're right, cost function is 0
  - Else it slowly increases cost function as we become "more" wrong
  - X axis is what we predict
  - Y axis is the cost associated with that prediction
- This cost functions has some interesting properties

- If  $y = 1$  and  $h_{\theta}(x) = 1$ 
  - If hypothesis predicts exactly 1 and that's exactly correct then that corresponds to 0 (exactly, not nearly 0)
- As  $h_{\theta}(x)$  goes to 0
  - Cost goes to infinity
  - This captures the intuition that if  $h_{\theta}(x) = 0$  (predict  $P(y=1|x; \theta) = 0$ ) but  $y = 1$  this will penalize the learning algorithm with a massive cost
- What about if  $y = 0$
- then cost is evaluated as  $-\log(1 - h_{\theta}(x))$ 
  - Just get inverse of the other function



- Now it goes to plus infinity as  $h_{\theta}(x)$  goes to 1
- With our particular cost functions  $J(\theta)$  is going to be convex and avoid local minimum

## Simplified cost function and gradient descent

- Define a simpler way to write the cost function and apply gradient descent to the logistic regression
  - By the end should be able to implement a fully functional logistic regression function
- Logistic regression cost function is as follows

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

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

Note:  $y = 0$  or 1 always

- This is the cost for a single example



- For binary classification problems  $y$  is always 0 or 1
  - Because of this, we can have a simpler way to write the cost function
    - Rather than writing cost function on two lines/two cases
    - Can compress them into one equation - more efficient
- Can write cost function is
  - **$\text{cost}(h_{\theta}(x), y) = -y \log(h_{\theta}(x)) - (1-y) \log(1 - h_{\theta}(x))$** 
    - This equation is a more compact of the two cases above
- We know that there are only two possible cases
  - $y = 1$ 
    - Then our equation simplifies to
      - $-\log(h_{\theta}(x)) - (0) \log(1 - h_{\theta}(x))$
      - $-\log(h_{\theta}(x))$
      - Which is what we had before when  $y = 1$
  - $y = 0$ 
    - Then our equation simplifies to
      - $-(0) \log(h_{\theta}(x)) - (1) \log(1 - h_{\theta}(x))$
      - $= -\log(1 - h_{\theta}(x))$
      - Which is what we had before when  $y = 0$
  - Clever!
- So, in summary, our cost function for the  $\theta$  parameters can be defined as

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

- Why do we chose this function when other cost functions exist?
  - This cost function can be derived from statistics using the principle of **maximum likelihood estimation**
    - Note this does mean there's an underlying Gaussian assumption relating to the distribution of features
  - Also has the nice property that it's convex
- To fit parameters  $\theta$ :
  - Find parameters  $\theta$  which minimize  $J(\theta)$
  - This means we have a set of parameters to use in our model for future predictions
- Then, if we're given some new example with set of features  $x$ , we can take the  $\theta$  which we generated, and output our prediction using

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

- This result is
  - $p(y=1 \mid x; \theta)$ 
    - Probability  $y = 1$ , given  $x$ , parameterized by  $\theta$

## How to minimize the logistic regression cost function

- Now we need to figure out how to minimize  $J(\theta)$ 
  - Use gradient descent as before
  - Repeatedly update each parameter using a learning rate

Repeat {

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

} (simultaneously update all  $\theta_j$ )

- If you had  $n$  features, you would have an  $n+1$  column vector for  $\theta$
- This equation is the same as the linear regression rule
  - The only difference is that our definition for the hypothesis has changed
- Previously, we spoke about how to monitor gradient descent to check it's working
  - Can do the same thing here for logistic regression
- When implementing logistic regression with gradient descent, we have to update all the  $\theta$  values ( $\theta_0$  to  $\theta_n$ ) simultaneously
  - Could use a for loop
  - Better would be a vectorized implementation
- Feature scaling for gradient descent for logistic regression also applies here

## Advanced optimization

- Previously we looked at gradient descent for minimizing the cost function
- Here look at advanced concepts for minimizing the cost function for logistic regression
  - Good for large machine learning problems (e.g. huge feature set)
- *What is gradient descent actually doing?*
  - We have some cost function  $J(\theta)$ , and we want to minimize it
  - We need to write code which can take  $\theta$  as input and compute the following
    - $J(\theta)$
    - Partial derivative of  $J(\theta)$  with respect to  $j$  (where  $j=0$  to  $j=n$ )

$$J(\theta)$$

$$\frac{\partial}{\partial \theta_j} J(\theta) \quad (\text{for } j = 0, 1, \dots, n)$$

- Given code that can do these two things
  - Gradient descent repeatedly does the following update

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

- So update each  $j$  in  $\theta$  sequentially
- So, we must;
  - Supply code to compute  $J(\theta)$  and the derivatives
  - Then plug these values into gradient descent
- Alternatively, instead of gradient descent to minimize the cost function we could use
  - **Conjugate gradient**
  - **BFGS** (Broyden-Fletcher-Goldfarb-Shanno)

- **L-BFGS** (Limited memory - BFGS)
- These are more optimized algorithms which take that same input and minimize the cost function
- These are *very* complicated algorithms
- Some properties
  - **Advantages**
    - No need to manually pick alpha (learning rate)
      - Have a clever inner loop (line search algorithm) which tries a bunch of alpha values and picks a good one
    - Often faster than gradient descent
      - Do more than just pick a good learning rate
    - Can be used successfully without understanding their complexity
  - **Disadvantages**
    - Could make debugging more difficult
    - Should not be implemented themselves
    - Different libraries may use different implementations - may hit performance

## Using advanced cost minimization algorithms

- How to use algorithms
  - Say we have the following example

Example:

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

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

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

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

- Example above
  - $\theta_1$  and  $\theta_2$  (two parameters)
  - Cost function here is  $J(\theta) = (\theta_1 - 5)^2 + (\theta_2 - 5)^2$
  - The derivatives of the  $J(\theta)$  with respect to either  $\theta_1$  and  $\theta_2$  turns out to be the  $2(\theta_i - 5)$
- First we need to define our cost function, which should have the following signature

```
function [jval, gradient] = costFunction(THETA)
```

- Input for the cost function is **THETA**, which is a vector of the  $\theta$  parameters
- Two return values from **costFunction** are
  - **jval**
    - How we compute the cost function  $\theta$  (the underived cost function)
      - In this case =  $(\theta_1 - 5)^2 + (\theta_2 - 5)^2$
  - **gradient**

- 2 by 1 vector
- 2 elements are the two partial derivative terms
- i.e. this is an n-dimensional vector
  - Each indexed value gives the partial derivatives for the partial derivative of  $J(\theta)$  with respect to  $\theta_i$
  - Where  $i$  is the index position in the **gradient** vector
- With the cost function implemented, we can call the advanced algorithm using

```
options= optimset('GradObj', 'on', 'MaxIter', '100'); % define the
options data structure
initialTheta= zeros(2,1); # set the initial dimensions for theta %
initialize the theta values
[optTheta, functionVal, exitFlag]= fminunc(@costFunction,
initialTheta, options); % run the algorithm
```

- Here
  - **options** is a data structure giving options for the algorithm
  - **fminunc**
    - function minimize the cost function (**find minimum of unconstrained multivariable function**)
  - **@costFunction** is a pointer to the costFunction function to be used
- For the octave implementation
  - **initialTheta** must be a matrix of at least two dimensions
- How do we apply this to logistic regression?
  - Here we have a vector

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

```
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  $\frac{\partial}{\partial \theta_1} J(\theta)$ ];

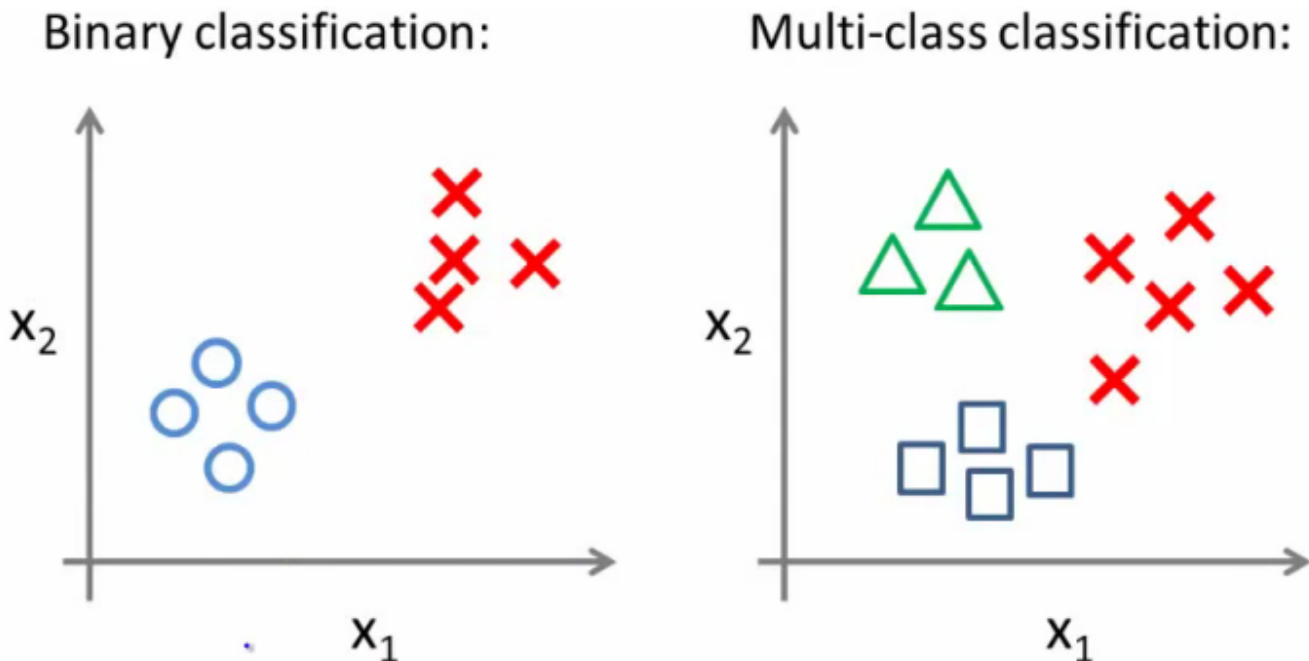
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gradient(n+1) = [code to compute  $\frac{\partial}{\partial \theta_n} J(\theta)$ ];
```

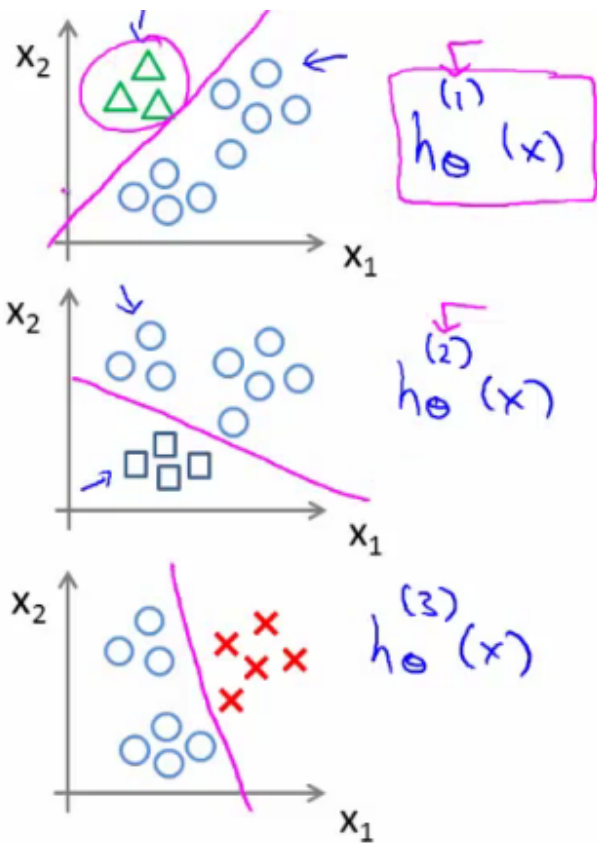
- Here
  - theta is a n+1 dimensional column vector
  - Octave indexes from 1, not 0
- Write a cost function which captures the cost function for logistic regression

# Multiclass classification problems

- Getting logistic regression for multiclass classification using **one vs. all**
- Multiclass - more than yes or no (1 or 0)
  - Classification with multiple classes for assignment



- Given a dataset with three classes, how do we get a learning algorithm to work?
  - Use one vs. all classification make binary classification work for multiclass classification
- **One vs. all classification**
  - Split the training set into three separate binary classification problems
    - i.e. create a new fake training set
      - Triangle (1) vs crosses and squares (0)  $h_{\theta}^1(x)$ 
        - $P(y=1 | x_1; \theta)$
      - Crosses (1) vs triangle and square (0)  $h_{\theta}^2(x)$ 
        - $P(y=1 | x_2; \theta)$
      - Square (1) vs crosses and square (0)  $h_{\theta}^3(x)$ 
        - $P(y=1 | x_3; \theta)$



- **Overall**

- 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 the probability that  $h_{\theta}^{(i)}(x) = 1$