06: Logistic Regression

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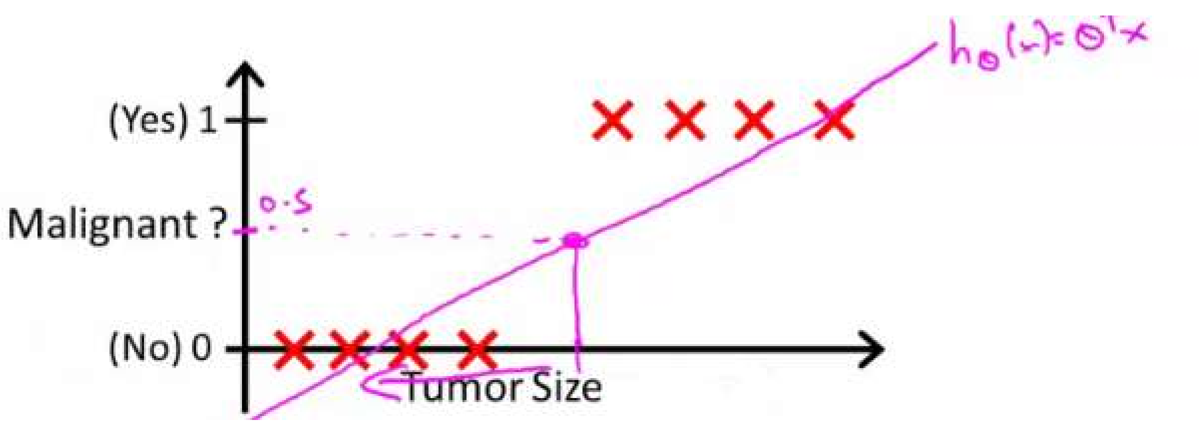
Classification

- 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

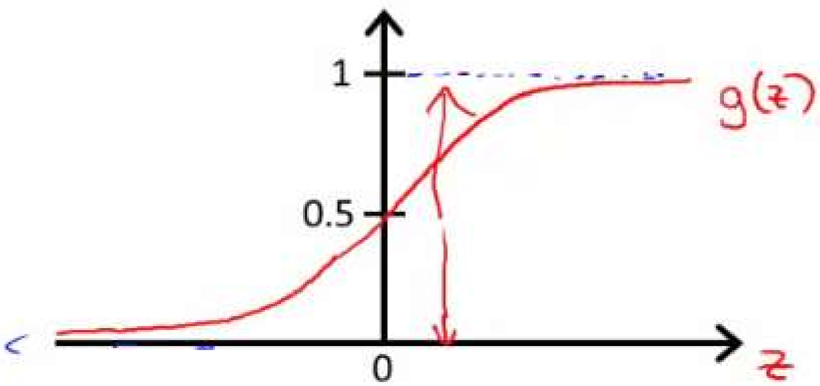
- Logistic regression is a **classification algorithm** - don't be confused

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 θ to our data

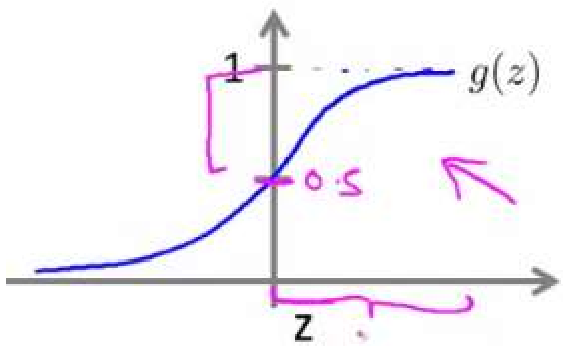
Interpreting hypothesis output

- 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 = 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 θ
- 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

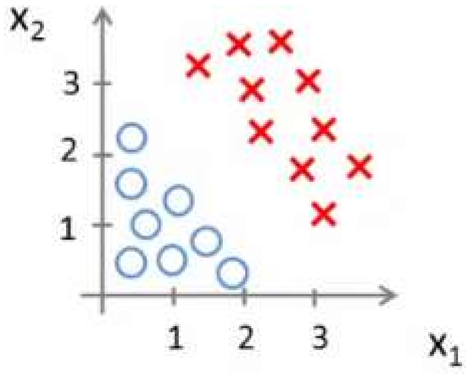
- Gives a better sense of what the hypothesis function is computing
- Better understand of what the hypothesis function looks like
    - One way of using the sigmoid function is;
        - When the probability of y being 1 is greater than 0.5 then we can predict y = 1
        - Else we predict y = 0
    - When is it exactly that $h_\theta(x)$ 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



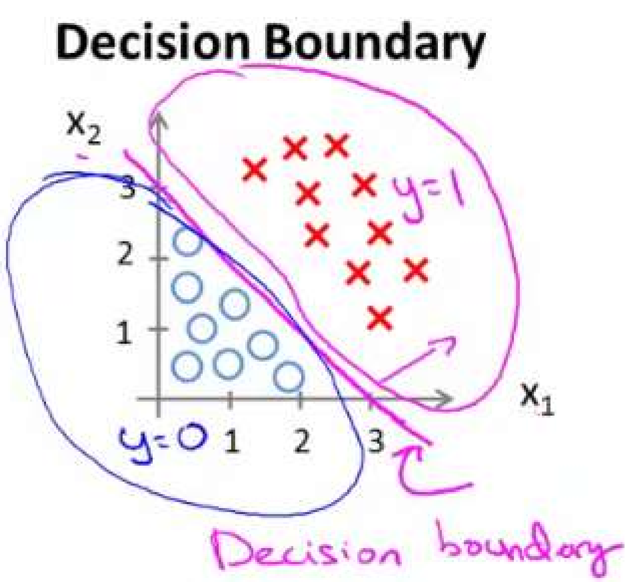
        - So if z is positive, g(z) is greater than 0.5
            - $z = (\theta^T x)$
        - So when
            - $\theta^T x >= 0$
        - Then $h_\theta >= 0.5$
- So what we've shown is that the hypothesis predicts y = 1 when $\theta^T x >= 0$
    - The corollary of that when $\theta^T x <= 0$ then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

Decision boundary

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



- So, for example
  - θ_0 = -3
  - θ_1 = 1
  - θ_2 = 1
- So our parameter vector is a column vector with the above values
  - So, θ^T is a row vector = [-3,1,1]
- What does this mean?
  - The z here becomes θ^T x
  - We predict "y = 1" if
    - $-3x_0 + 1x_1 + 1x_2 >= 0$
    - $-3 + x_1 + x_2 >= 0$
- We can also re-write this as
  - If ($x_1 + x_2 >= 3$) then we predict y = 1
  - If we plot
    - $x_1 + x_2 = 3$ we graphically plot our **decision boundary**



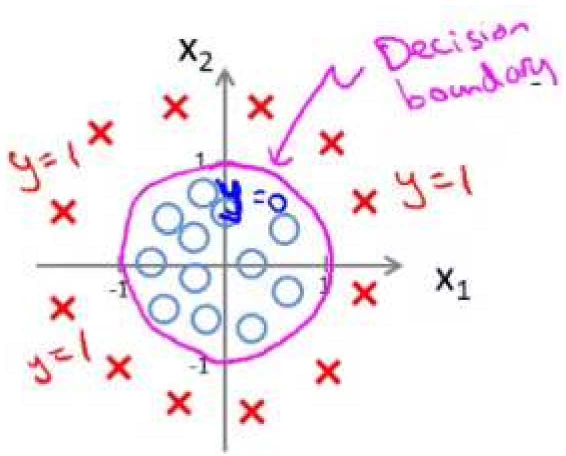
- Means we have these two regions on the graph
  - Blue = false
  - Magenta = true

- 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
    - $5 - x_1 > 0$
    - $5 > x_1$

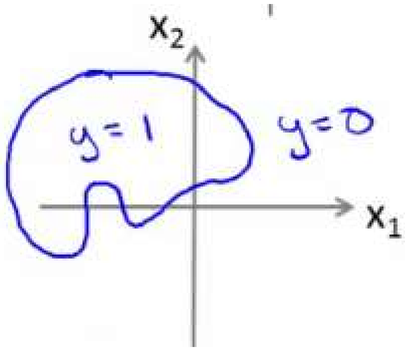
Non-linear decision boundaries

- Get logistic regression to fit a complex non-linear data set
  - Like polynomial regress add higher order terms
  - So say we have
    - $h_\theta(x) = g(\theta_0 + \theta_1x_1 + \theta_3x_1^2 + \theta_4x_2^2)$
    - We take the transpose of the θ vector times the input vector
      - Say θ^T was [-1,0,0,1,1] then we say;
      - Predict that "y = 1" *if*
        - $-1 + x_1^2 + x_2^2 >= 0$

          or
        - $x_1^2 + x_2^2 >= 1$
      - 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 θ 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: $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \cdots, (x^{(m)}, y^{(m)})\}$

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

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

- 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 (θ)
    - Given the training set how to we chose/fit θ?
- Linear regression uses the following function to determine θ

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

- Instead of writing the squared error term, we can write

- If we define "cost()" as;
  - $cost(h_\theta(x^i), y) = 1/2(h_\theta(x^i) - y^i)^2$
  - Which evaluates to the cost for an individual example using the same measure as used in linear regression
- We can **redefine J(θ) as**

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

  - 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

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

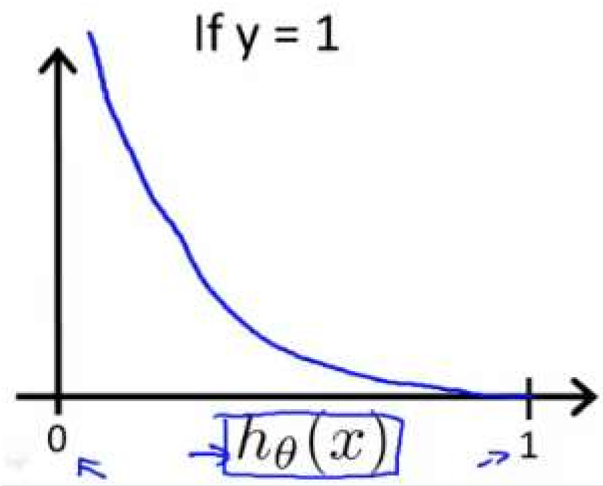
- What does this actually mean?
  - This is the cost you want the learning algorithm to pay if the outcome is $h_\theta(x)$ and the actual outcome is y
  - If we use this function for logistic regression this is a **non-convex function** for parameter optimization
    - Could work....
- What do we mean by non convex?
  - We have some function - J(θ) - 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 Cost() function, and them plug the Cost() function into J(θ) and plot J(θ) 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 global 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

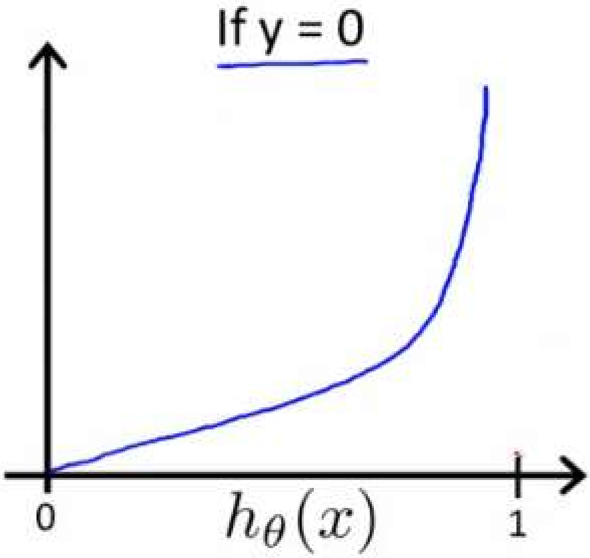
- To get around this we need a different, convex Cost() function which means we can apply gradient descent

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

- **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 thats 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

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

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

Note: $y = 0$ 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
    - **cost(h_θ, (x),y) = -ylog($h_\theta(x)$) - (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 θ parameters can be defined as

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

- 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 θ:
  - Find parameters θ which minimize J(θ)
  - 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 θ 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 θ

How to minimize the logistic regression cost function

- Now we need to figure out how to minimize J(θ)
  - 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 θ_j)

}

- If you had *n* features, you would have an n+1 column vector for θ
- 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 θ values (θ_0 to θ_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(θ), and we want to minimize it
  - We need to write code which can take θ as input and compute the following
    - J(θ)
    - Partial derivative if J(θ) with respect to j (where j=0 to j = n)

$$J(\theta)$$

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

- 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 θ sequentially
- So, we must;
  - Supply code to compute J(θ) 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
    - θ_1 and θ_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 θ_1 and θ_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, gradent] = costFunction(THETA)
```

- Input for the cost function is **THETA**, which is a vector of the θ parameters
- Two return values from **costFunction** are
  - **jval**
    - How we compute the cost function θ (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 θ_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, funtionVal, 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 (**f**ind **min**imum of **unc**onstrained 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

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

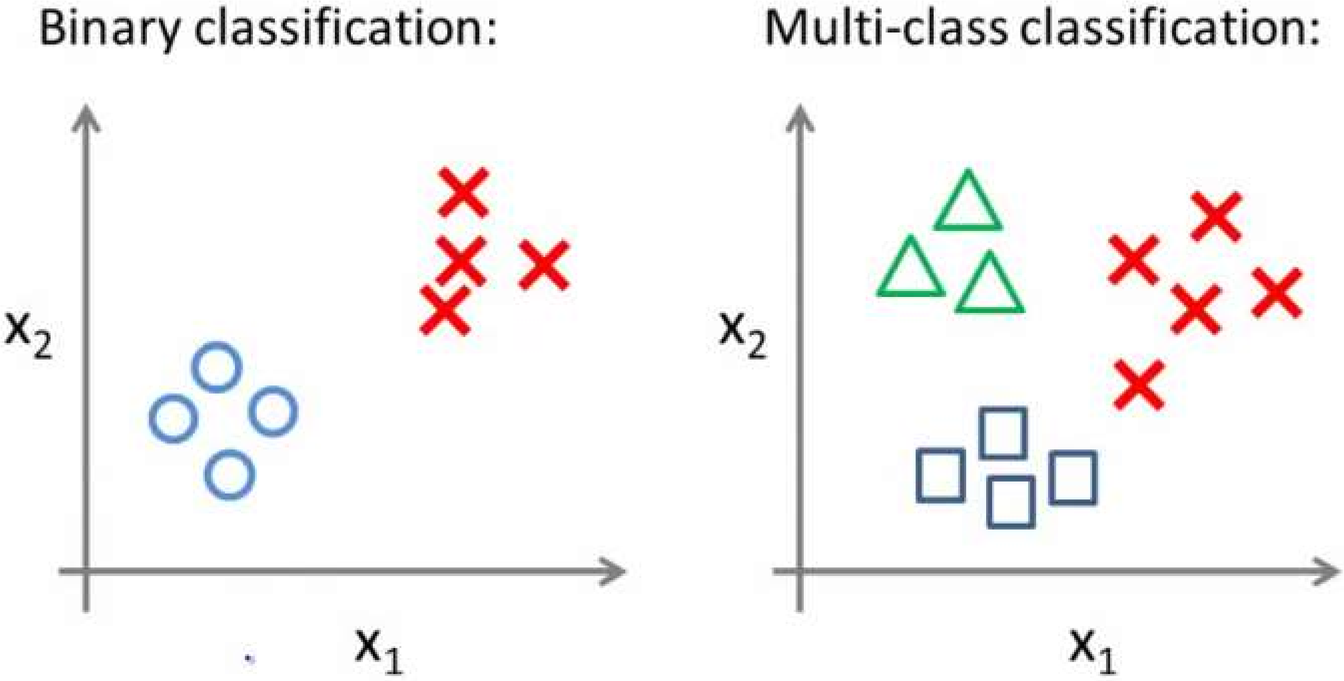
$\vdots$

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

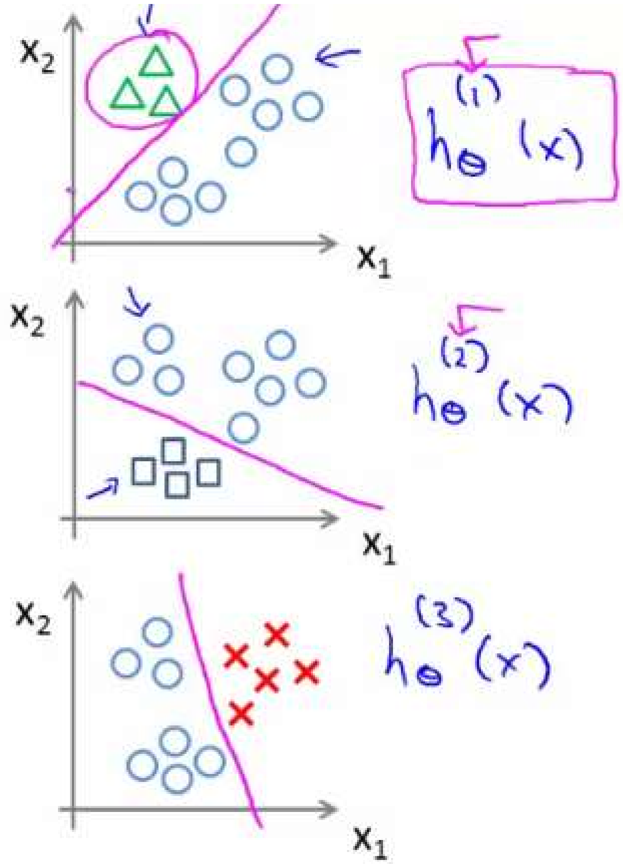
- Here
  - theta is a n+1 dimensional column vector
  - Octave indexes from 1, not 0
- Write a cost function which captures the cost function for logistic regression

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) $h_\theta^1(x)$
        - $P(y=1 \mid x_1; \theta)$
      - Crosses (1) vs triangle and square (0) $h_\theta^2(x)$
        - $P(y=1 \mid x_2; \theta)$
      - Square (1) vs crosses and square (0) $h_\theta^3(x)$
        - $P(y=1 \mid x_3; \theta)$



- **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 $h_\theta^{(i)}(x) = 1$