# Logistic Regression

THE 2ND BRAIN, THE 3RD EYE

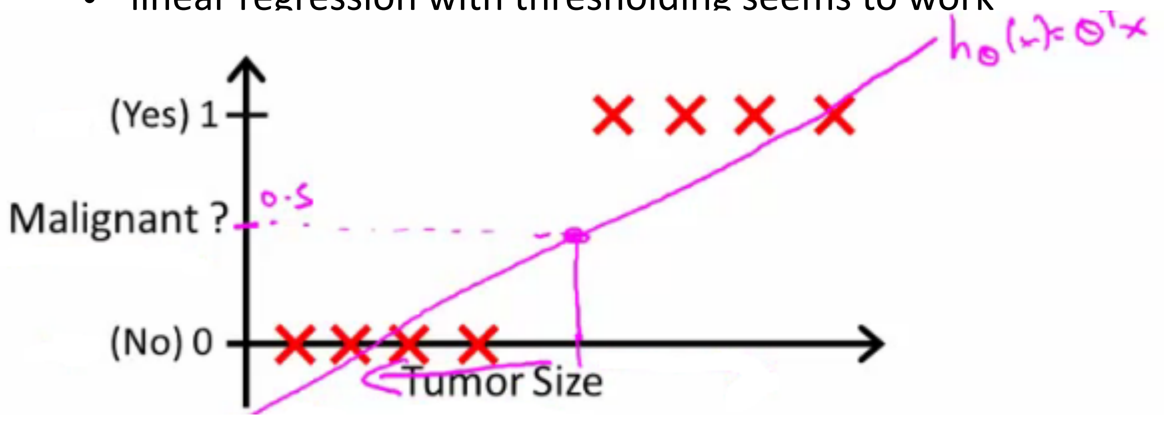
**JP @ 2B3E**

# Classification

- 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)

# Classification

- Start with **binary class problems**
  - multi-class classification:an extension of binary classification
- How do we develop a classification algorithm?
  - Tumour size vs malignancy (0 or 1)
  - *could* use linear regression
    - Then threshold the classifier output
      - i.e. anything over some value is yes, else no
    - our example
      - linear regression with thresholding seems to work



# Classification

- 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
  - existing nos → yeses
- 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 which is always either 0 or 1
  - Logistic regression is a **classification algorithm** - NOT REGRESSION

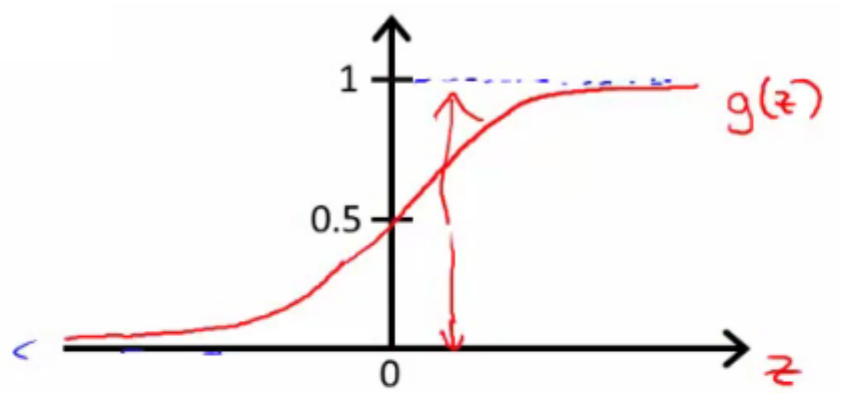
# Hypothesis representation

- What function is used to represent our hypothesis in classification
- We want our classifier to output values between 0 and 1
  - linear regression: $h_\theta(x) = (\theta^T x)$
  - For classification hypothesis: $h_\theta(x) = g((\theta^T x))$
    - 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

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

# Hypothesis representation

- Sigmoid function shape
  - Crosses 0.5 at the origin,
  - then flattens out: Asymptotes at 0 and 1



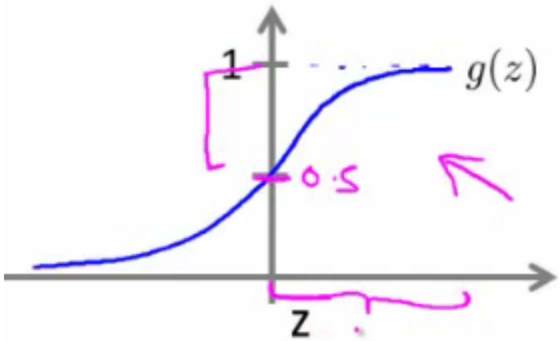

- Given this we need to fit θ to our data

# Interpretation
## 1. Probability

- $h_\theta(x) \simeq$ the estimated probability that y=1 on input x
  - Example
    - If X is a feature vector with $x_0 = 1$ (bias) 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
    - $h_\theta(x) = P(y=1 | x ; \theta)$
    - Meaning: 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
    - $P(y=1 | x ; \theta) + P(y=0 | x ; \theta) = 1$
    - $P(y=0 | x ; \theta) = 1 - P(y=1 | x ; \theta)$

# Interpretation

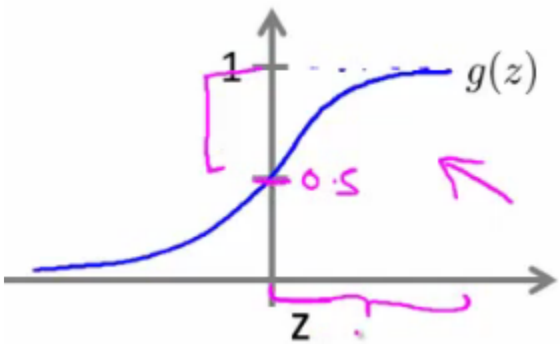
## 2. Decision Boundary




- 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
    - Otherwise, we predict y = 0
  - When is it exactly that $h_\theta(x)$ is greater than 0.5?
    - g(z) is greater than or equal to 0.5
    - when z is greater than or equal to 0

# Interpretation

## 2. Decision Boundary

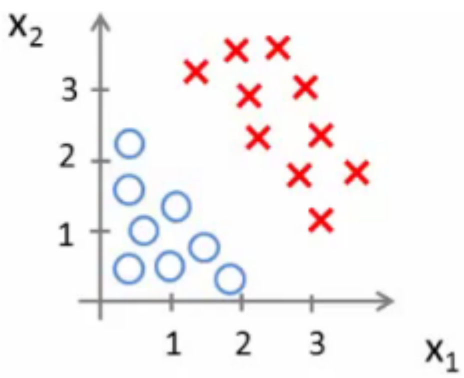



- So if z is positive, g(z) is greater than 0.5
  - $z = (\theta^T x)$
- So when
  - $\theta^T x >= 0$
  - Then $h_\theta >= 0.5$

- 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
  - —> better understand how the hypothesis makes its predictions

# Interpretation

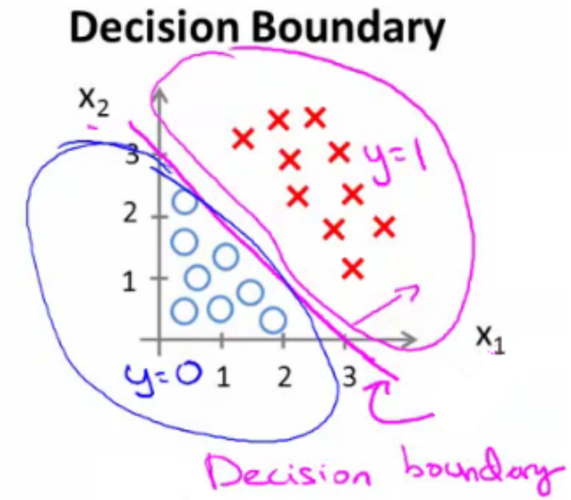
## 2. Decision Boundary




- $h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$
- 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?
  - z here becomes $\theta^T$ 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**

# Interpretation

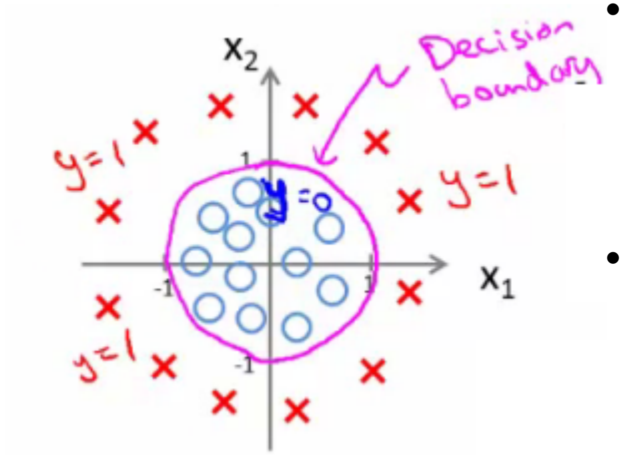
## 2. Decision Boundary




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

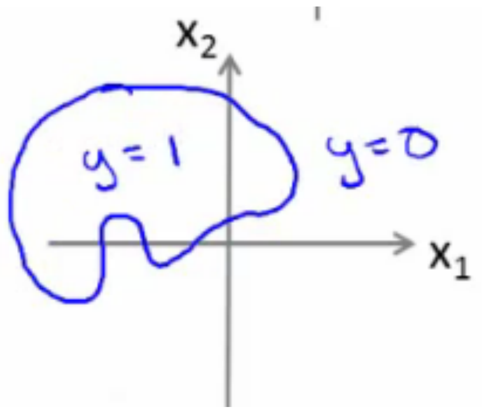
# Non-linear decision boundaries

- Get logistic regression to fit a complex non-linear data set
  - Like polynomial regression, 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 $\theta^T$ 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



# Non-linear decision boundaries

- 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 fit the parameters

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

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

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

# Cost function for logistic regression

- Given
  - 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

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

# Cost function for logistic regression

- Instead of writing the squared error term, we can write
  - If we define "cost()" as;

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

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

# Cost function for logistic regression

- To further simplify it we can get rid of the superscripts

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

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

- 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....

# Cost function for logistic regression

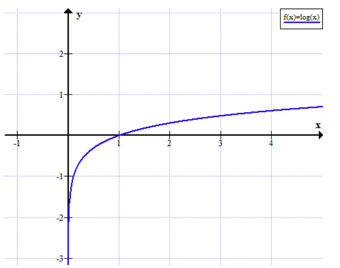
$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m}\frac{1}{2}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

- 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 then 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 local minimum
  - We would like a convex function so if you run gradient descent you converge to a global minimum

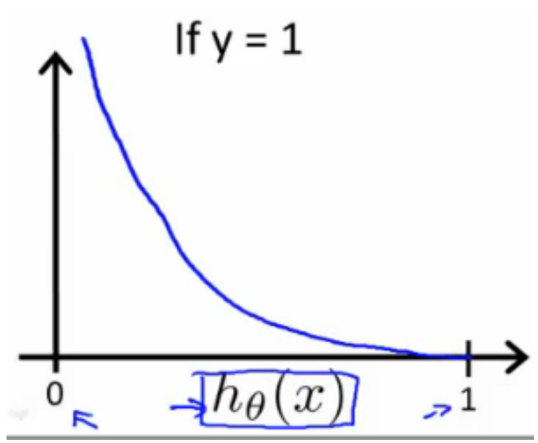
# A convex logistic regression cost function

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

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

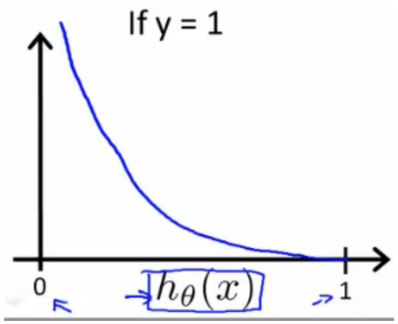


- **This is our logistic regression cost function**
  - This is the penalty the algorithm pays
  - Plot the function
- Plot y = 1
  - So $h_\theta(x)$ evaluates as $-\log(h_\theta(x))$



# A convex logistic regression cost function

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

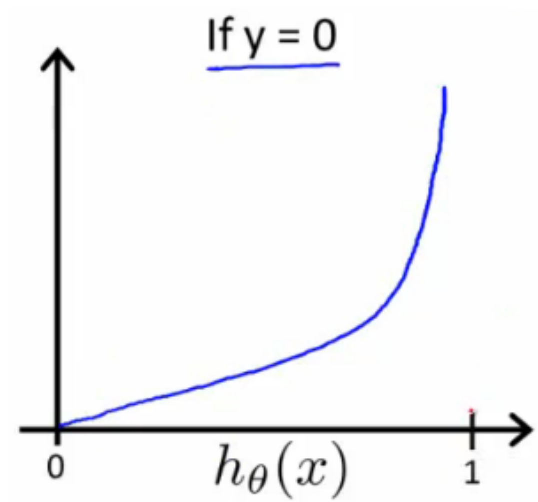



- So when we're right, cost function is 0
  - Else it slowly increases cost function as we become "more" wrong
  - X axis is what we predict
  - Y axis is the cost associated with that prediction
- This cost functions has some interesting properties
  - If y = 1 and $h_\theta(x) = 1$
    - If hypothesis predicts exactly 1 and that's exactly correct then that (cost) 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; θ) = 0) but y = 1 this will penalize the learning algorithm with a massive cost

# A convex logistic regression cost function

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

- 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(θ) 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, we should be able to implement a fully functional logistic regression function
- Logistic regression cost function is as follows

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

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

Note: $y = 0$ or $1$ always

# Simplified cost function and gradient descent

- 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
    - **$\mathrm{cost}(h_{\theta,}(x),y) = -y\log(\ h_\theta(x)\ ) - (1-y)\log(\ 1 - h_\theta(x)\ )$**
      - more compact of the two cases above

# Simplified cost function and gradient descent

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

- **cost($h_{\theta,}$ (x),y) = -ylog( $h_\theta$(x) ) - (1-y)log( 1- $h_\theta$(x) )**

- 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!

# Simplified cost function and gradient descent

- 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

# Simplified cost function and gradient descent

- To fit parameters θ:
  - Find parameters θ which minimize J(θ)
  - Once optimized, we have a set of parameters to use in our model for future predictions
- given a 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 | x ; θ)
    - Probability y = 1, given x, parameterized by θ

# Minimizing 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 $\theta_j$)

}

- If you had *n* features, you would have an n+1 column vector for θ
- This equation is the same as the linear regression(why?) rule
  - Proof descried on the next page
  - The only difference is that our definition for the hypothesis has changed

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

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

$$\underset{\text{chain rule}}{=} \frac{-1}{m} \sum_{i=1}^{m} \left[ y^{(i)} \frac{\frac{\partial}{\partial \theta_j} h\theta\left(x^{(i)}\right)}{h\theta\left(x^{(i)}\right)} + (1 - y^{(i)}) \frac{\frac{\partial}{\partial \theta_j}\left(1 - h\theta\left(x^{(i)}\right)\right)}{1 - h\theta\left(x^{(i)}\right)} \right]$$

$$\underset{h_\theta(x)=\sigma\left(\theta^\top x\right)}{=} \frac{-1}{m} \sum_{i=1}^{m} \left[ y^{(i)} \frac{\frac{\partial}{\partial \theta_j} \sigma\left(\theta^\top x^{(i)}\right)}{h_\theta\left(x^{(i)}\right)} + (1 - y^{(i)}) \frac{\frac{\partial}{\partial \theta_j}\left(1 - \sigma\left(\theta^\top x^{(i)}\right)\right)}{1 - h_\theta\left(x^{(i)}\right)} \right]$$

$$\underset{\sigma'}{=} \frac{-1}{m} \sum_{i=1}^{m} \left[ y^{(i)} \frac{\sigma\left(\theta^\top x^{(i)}\right)\left(1 - \sigma\left(\theta^\top x^{(i)}\right)\right) \frac{\partial}{\partial \theta_j}\left(\theta^\top x^{(i)}\right)}{h\theta\left(x^{(i)}\right)} - (1 - y^{(i)}) \frac{\sigma\left(\theta^\top x^{(i)}\right)\left(1 - \sigma\left(\theta^\top x^{(i)}\right)\right) \frac{\partial}{\partial \theta_j}\left(\theta^\top x^{(i)}\right)}{1 - h\theta\left(x^{(i)}\right)} \right]$$

$$\underset{\sigma\left(\theta^\top x\right)=h_\theta(x)}{=} \frac{-1}{m} \sum_{i=1}^{m} \left[ y^{(i)} \frac{h_\theta\left(x^{(i)}\right)\left(1 - h_\theta\left(x^{(i)}\right)\right) \frac{\partial}{\partial \theta_j}\left(\theta^\top x^{(i)}\right)}{h_\theta\left(x^{(i)}\right)} - (1 - y^{(i)}) \frac{h_\theta\left(x^{(i)}\right)\left(1 - h_\theta\left(x^{(i)}\right)\right) \frac{\partial}{\partial \theta_j}\left(\theta^\top x^{(i)}\right)}{1 - h_\theta\left(x^{(i)}\right)} \right]$$

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

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

$$\underset{\text{cancel}}{=} \frac{-1}{m} \sum_{i=1}^{m} \left[ y^{(i)} - h_\theta\left(x^{(i)}\right) \right] x_j^{(i)}$$

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

# Minimizing the logistic regression cost function

- Monitoring gradient descent to check it's working
  - same as in linear regression
- When implementing logistic regression with gradient descent, we have to update all the θ 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(θ), and we want to minimize it
  - We need to write code which can take θ as input and compute the following
    - 1) J(θ)   2) Partial derivative of 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

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

# Advanced Optimization

- 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

# Advanced Optimization

- 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

# Gradient Descent Example

- Say we have the following example

Example:

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

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

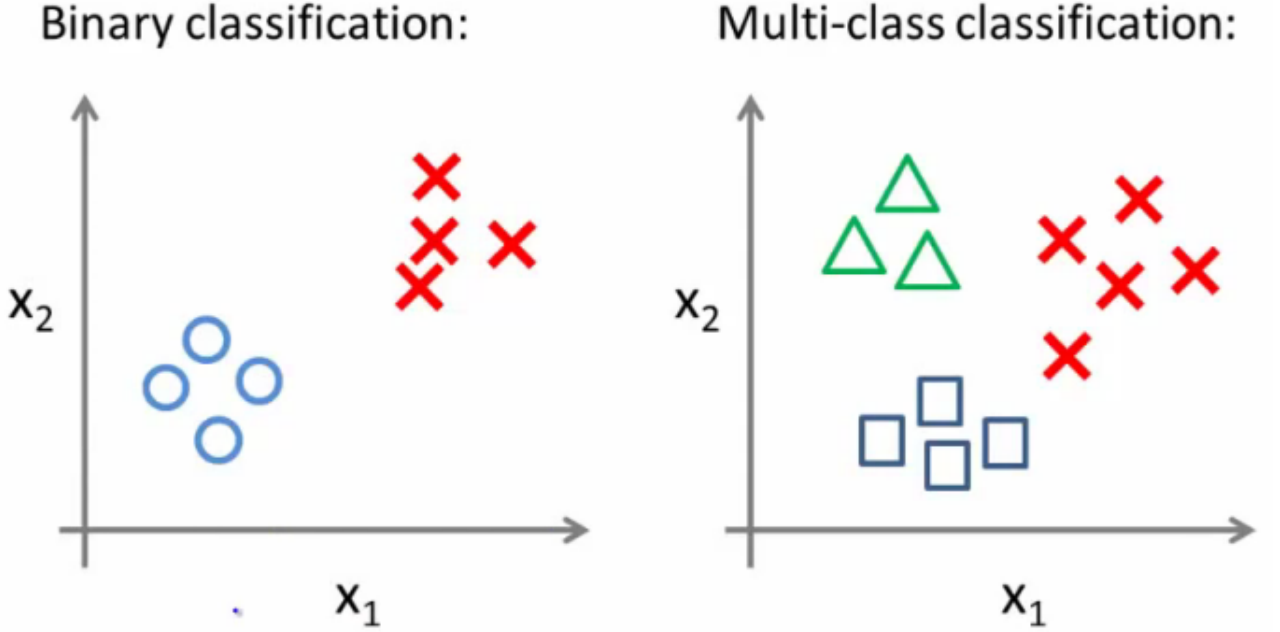
$$\frac{\partial}{\partial \theta_1} J(\theta) = 2(\theta_1 - 5)$$

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

- 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 $2(\theta_i - 5)$

# Multiclass classification problems

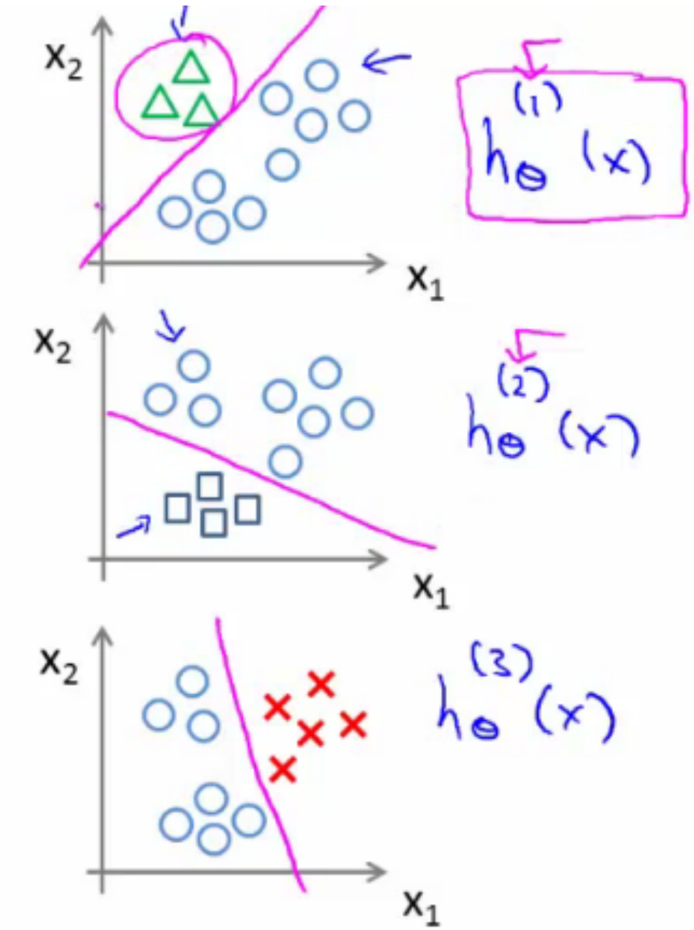
- Getting logistic regression for multiclass classification using **one vs. all**
- Multiclass - more than yes or no (1 or 0)
  - Classification with multiple classes for assignment



# Multiclass classification problems

- Given a dataset with three classes, how do we get a learning algorithm to work?
  - Use one vs. all other classification make binary classification work for multi-class 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) $h_\theta^3(x)$
        - $P(y=1 \mid x_3; \theta)$

# Multiclass classification problems




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