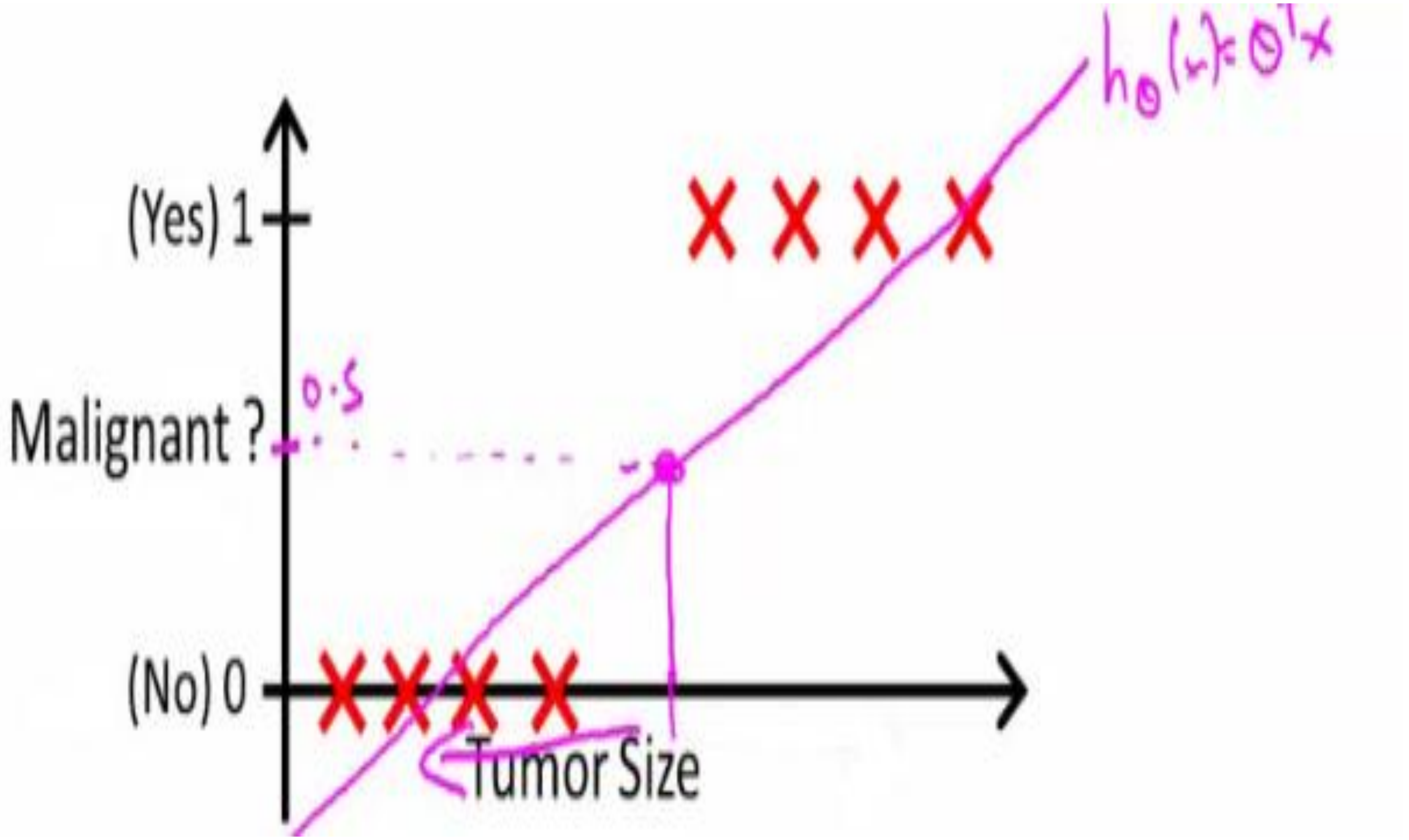
Logistic Regression

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?
  - Tumor 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


$h_\theta(x) = \theta^T x$
(Yes) 1
0.5
Malignant ?
(No) 0
Tumor Size

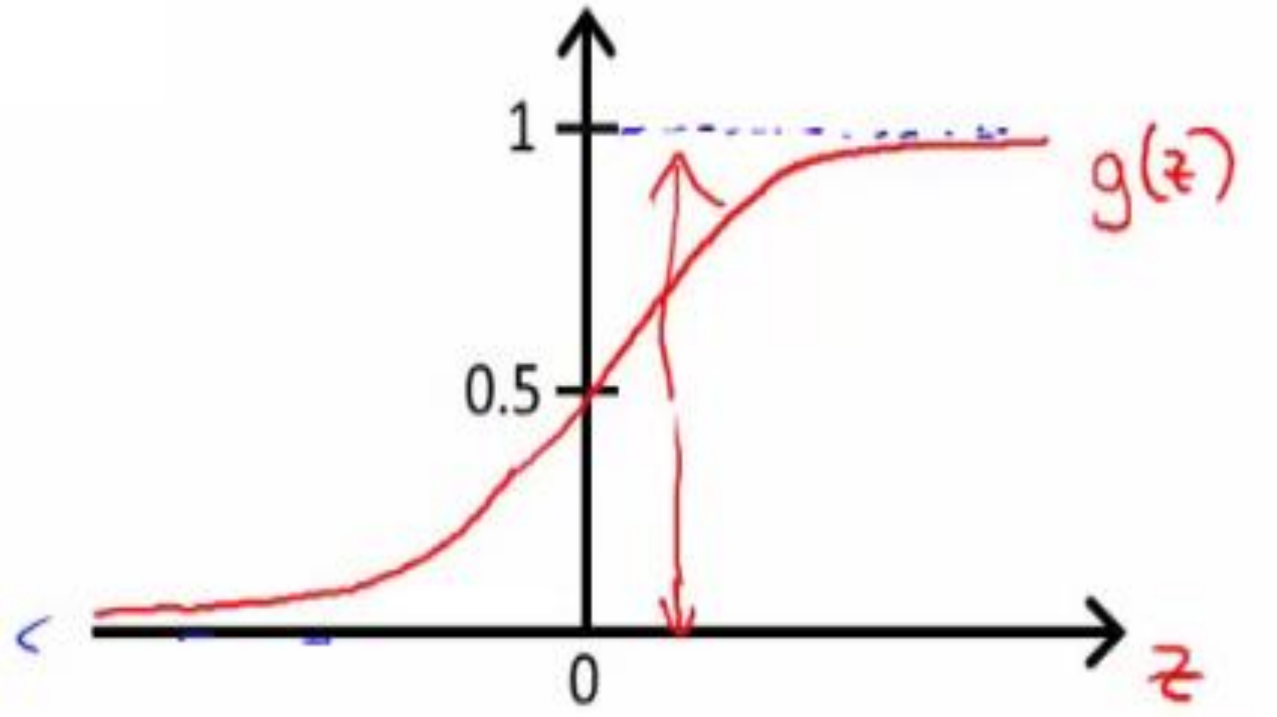
- We can see above this does a reasonable job of stratifying the data points into one of two classes
  - But what if we had a single Yes with a very small tumor
  - This would lead to classifying all the existing yeses as nos
- Another issue with linear regression
  - We know Y is 0 or 1
  - Hypothesis 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

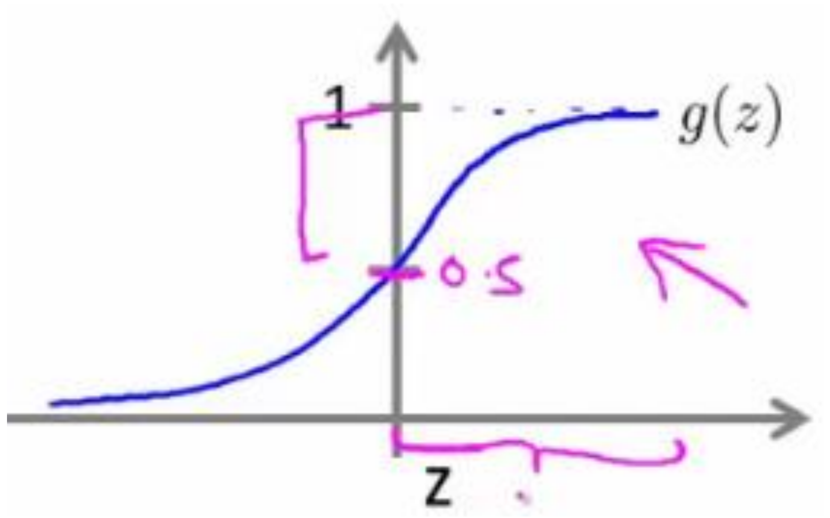
Interpreting hypothesis output

- 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

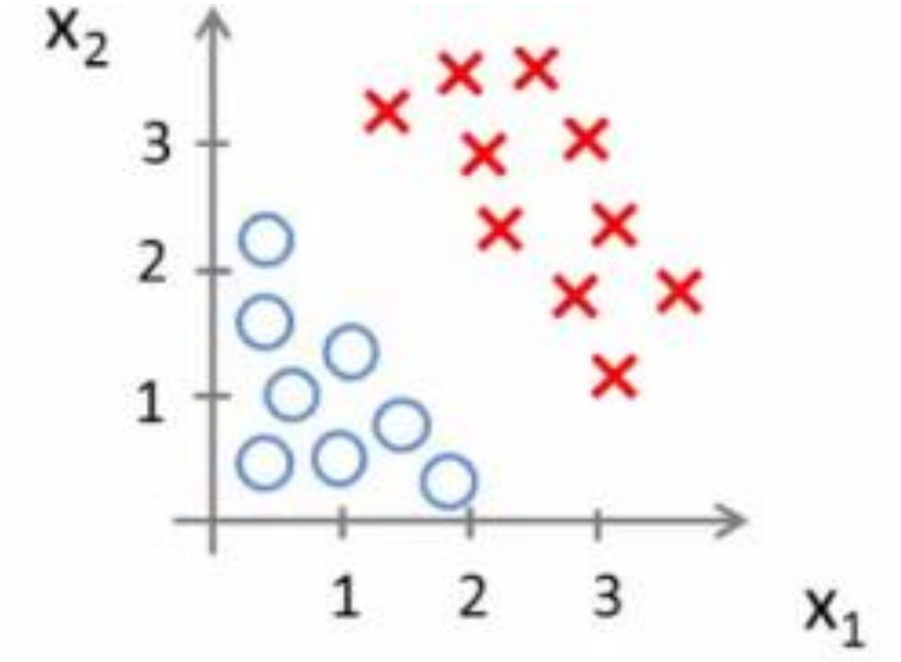


- So if z is positive, g(z) is greater than 0.5
  - $z = (\theta^T x)$
- So when
  - $\theta^T x >= 0$ Then $h_\theta >= 0.5$

- 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

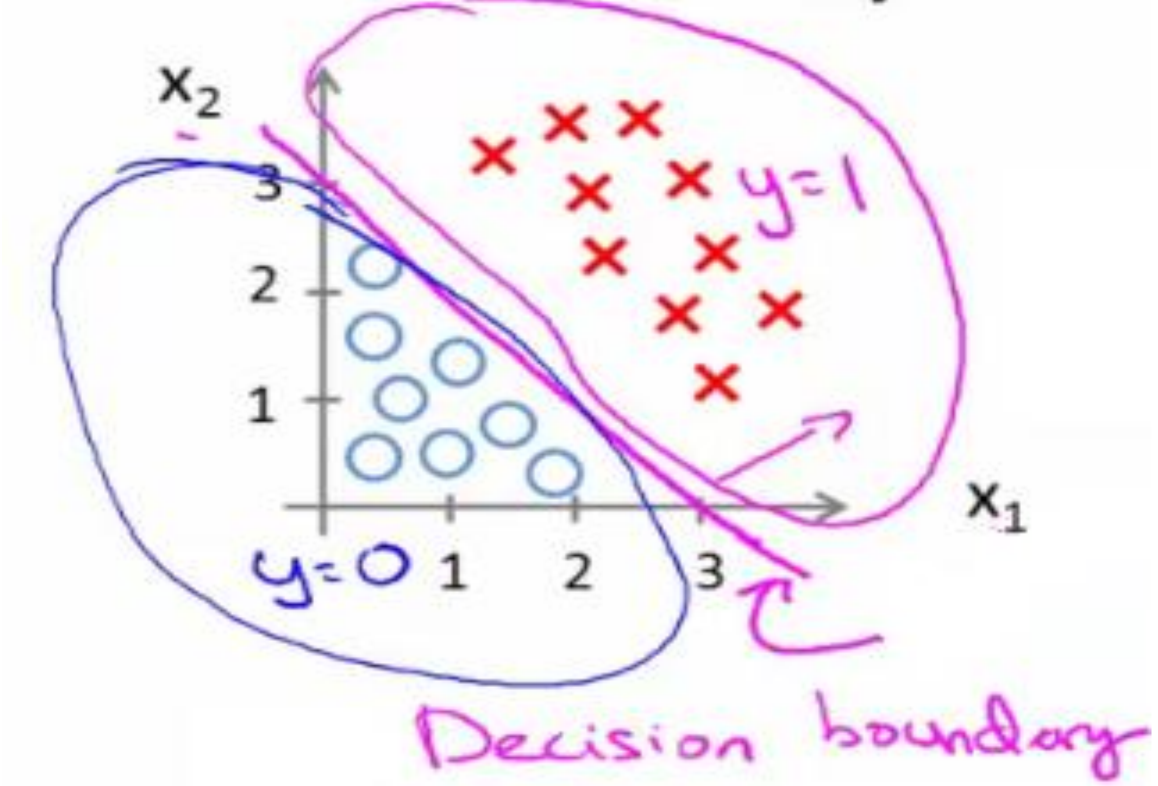
Decision Boundary

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



- So, for example
  - $\theta_0 = -3; \theta_1 = 1; \theta_2 = 1$
- 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**

Decision Boundary



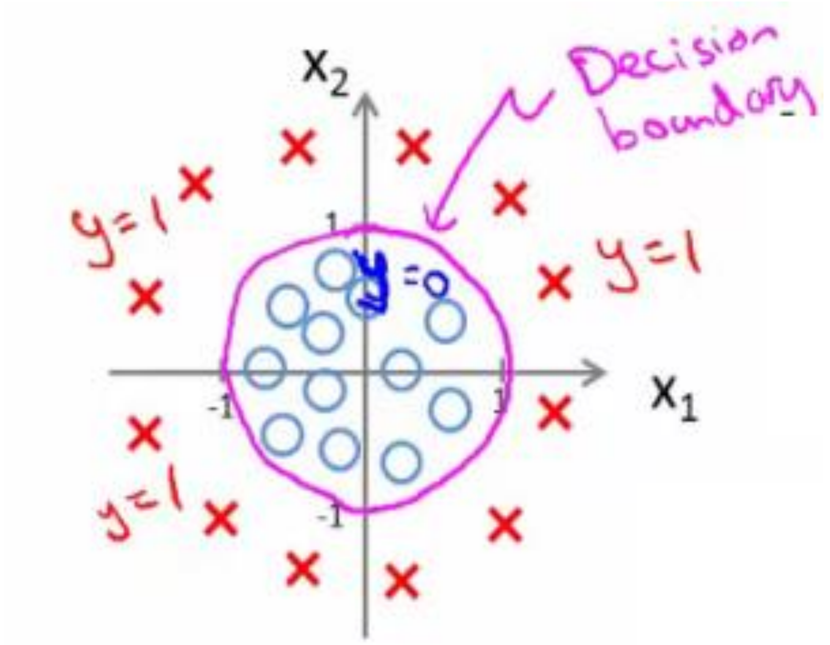
- Means we have these two regions on the graph
  - Blue = false
  - Magenta = true
  - Line = decision boundary
    - Concretely, the straight line is the set of points where $h_\theta(x) = 0.5$ exactly
  - The decision boundary is a property of the hypothesis
    - Means we can create the boundary with 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

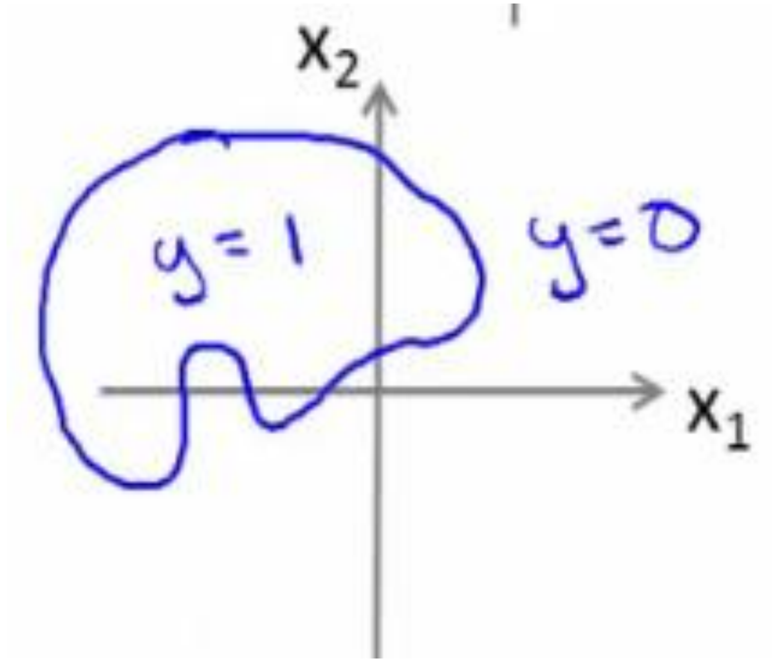
- Get logistic regression to fit a complex non-linear data set
  - Like polynomial regress add higher order terms
  - So say we have:

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


x_2
x_1
$y=1$
$y=0$

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 do 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;
    - $\text{cost}(h_\theta(x^i), y) = 1/2(h_\theta(x^i) - y^i)^2$
    - Which evaluates to the cost for an individual example using the same measure as used in linear regression
  - We can **redefine J(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 - $J(\theta)$ - for determining the parameters
  - Our hypothesis function has a non-linearity (sigmoid function of $h_\theta(x)$)
    - This is a complicated non-linear function

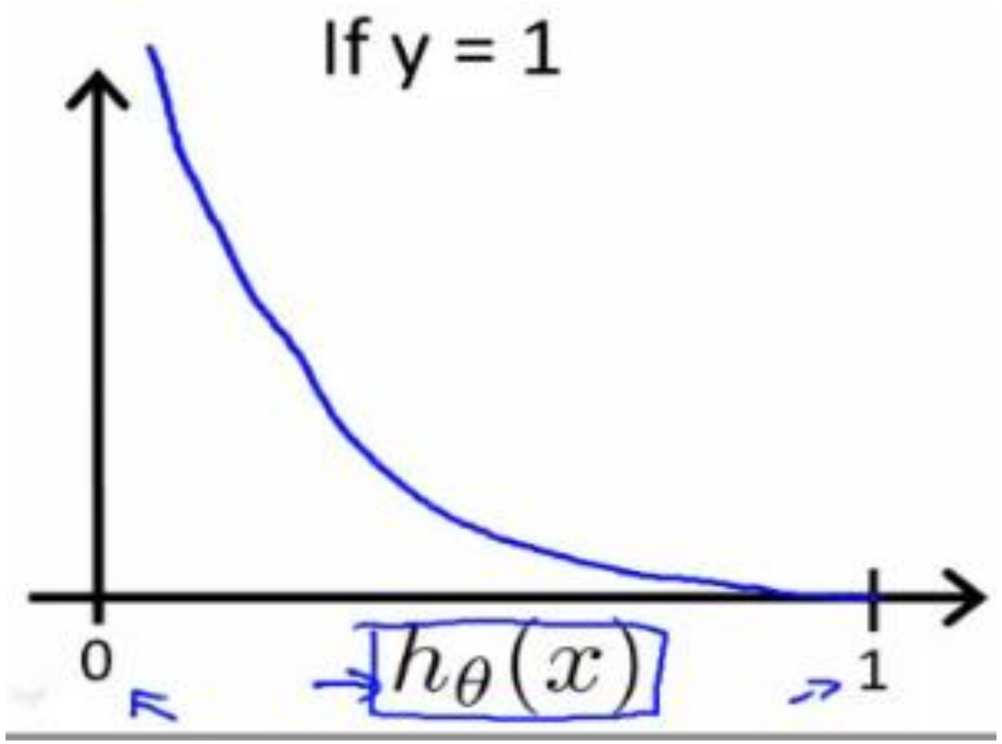
- If you take $h_\theta(x)$ and plug it into the Cost() function, and them plug the Cost() function into J(θ) and plot J(θ) we find many local optimum -> *non convex function*
- Why is this a problem
  - Lots of local minima mean gradient descent may not find the global optimum - may get stuck in a global 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

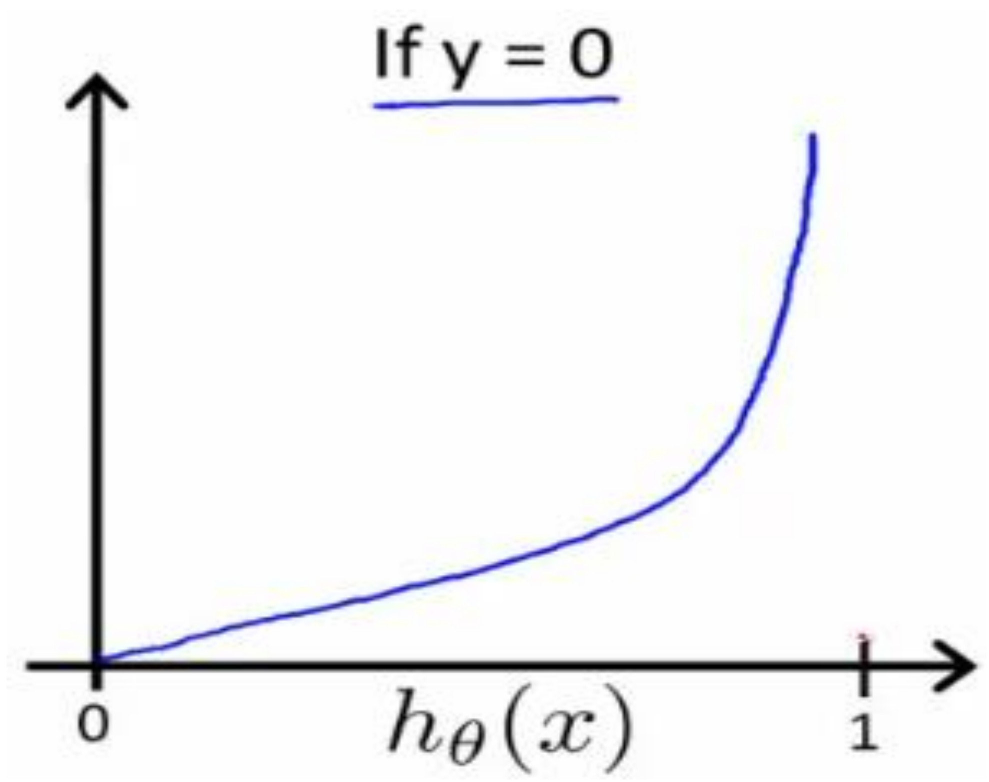
- To get around this we need a different, convex Cost() function which means we can apply gradient descent

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

- **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 $-\log(h_\theta(x))$


If y = 1
0
$h_\theta(x)$
1

- 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

- The logistic regression function:

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

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

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
    - **$\mathrm{cost}(h_{\theta,}(x),y) = -y\log(h_\theta(x)) - (1-y)\log(1- h_\theta(x))$**
      - 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 $y = 0$

- So, in summary, our cost function for the θ 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 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 | x ; θ)
    - 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)

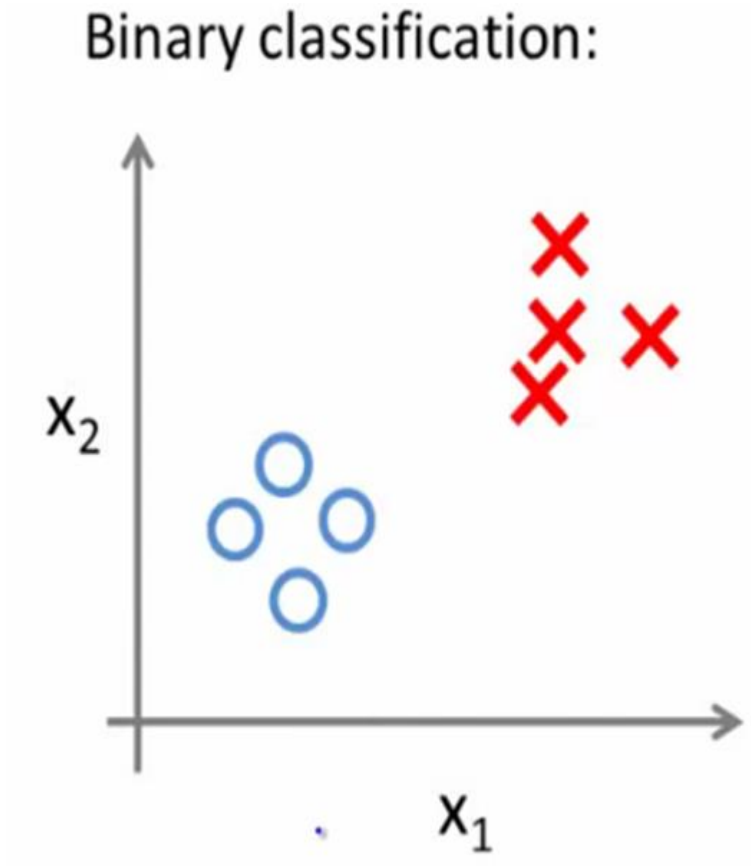
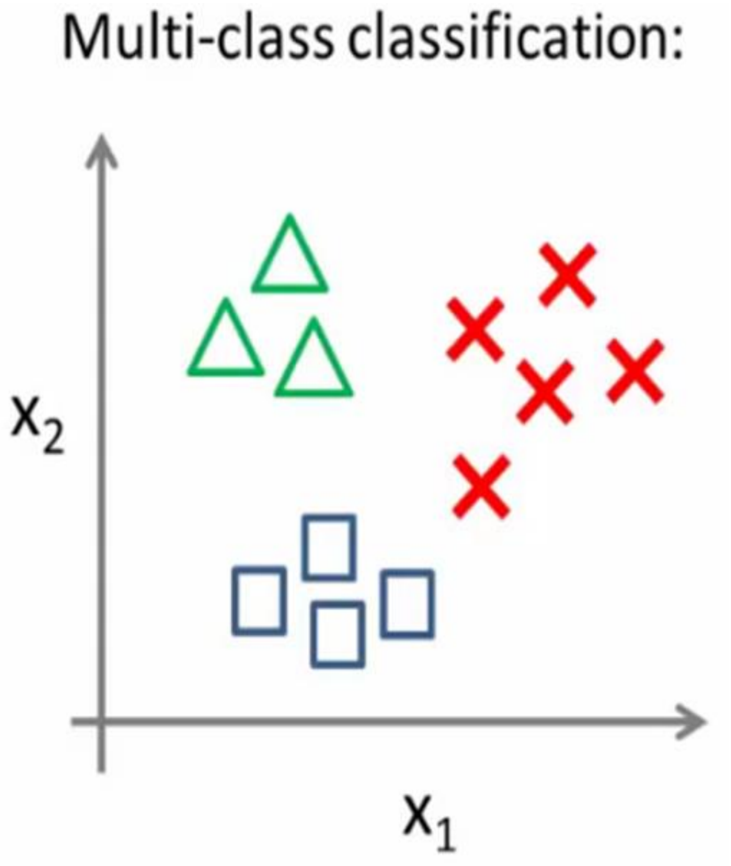
}

- 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
- 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

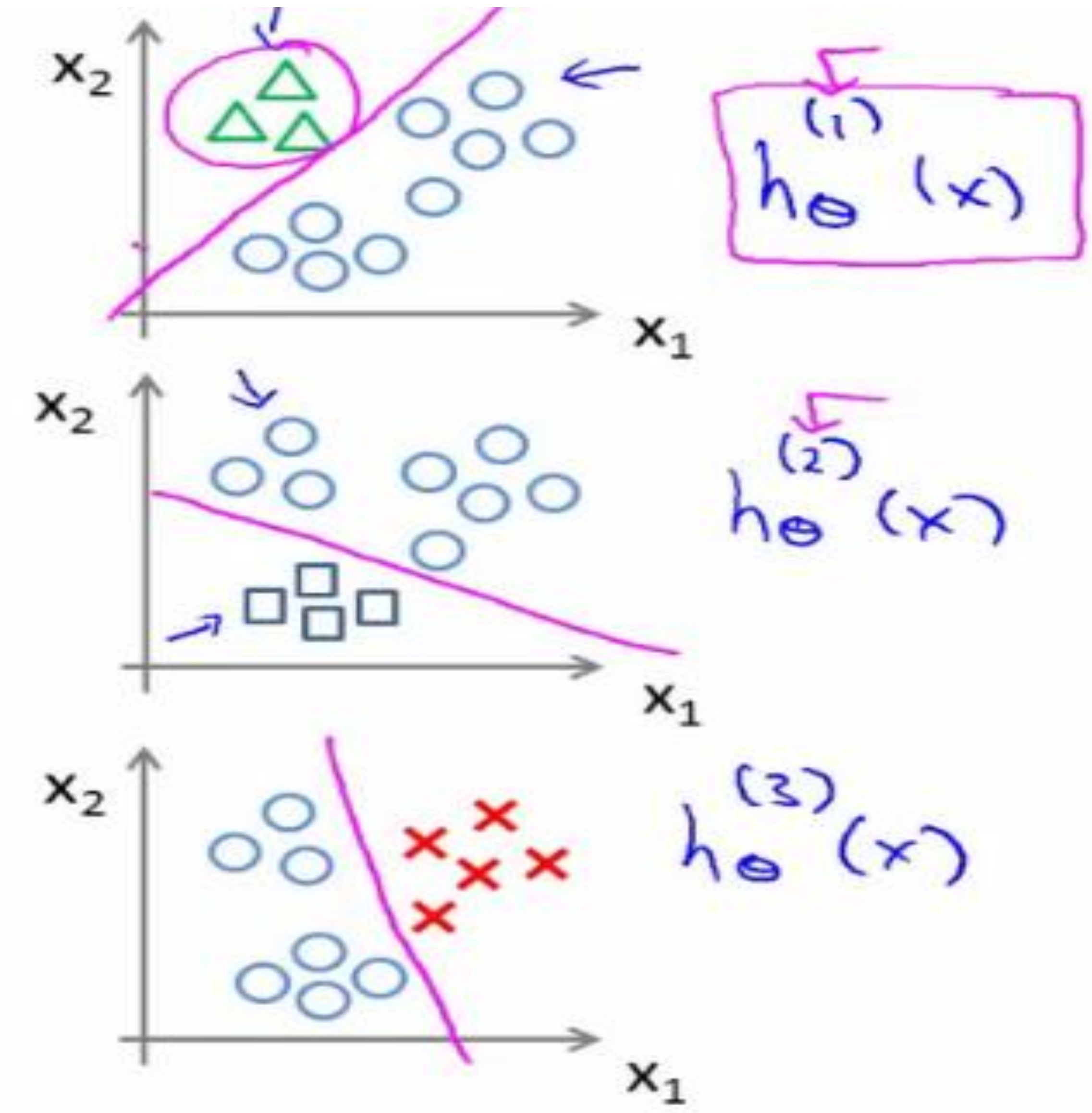
Multiclass classification problems

- 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


Binary classification:
x_2
x_1

Multi-class classification:
x_2
x_1

- 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 trangle (0) $h_\theta^3(x)$
      - $P(y=1 \mid x_3; \theta)$


x₂
x₁
h_θ^(1)(x)
x₂
x₁
h_θ^(2)(x)
x₂
x₁
h_θ^(3)(x)

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