Week 3

Classification & Representation

Terminology - for binary classification

1) $y \in (0, 1)$

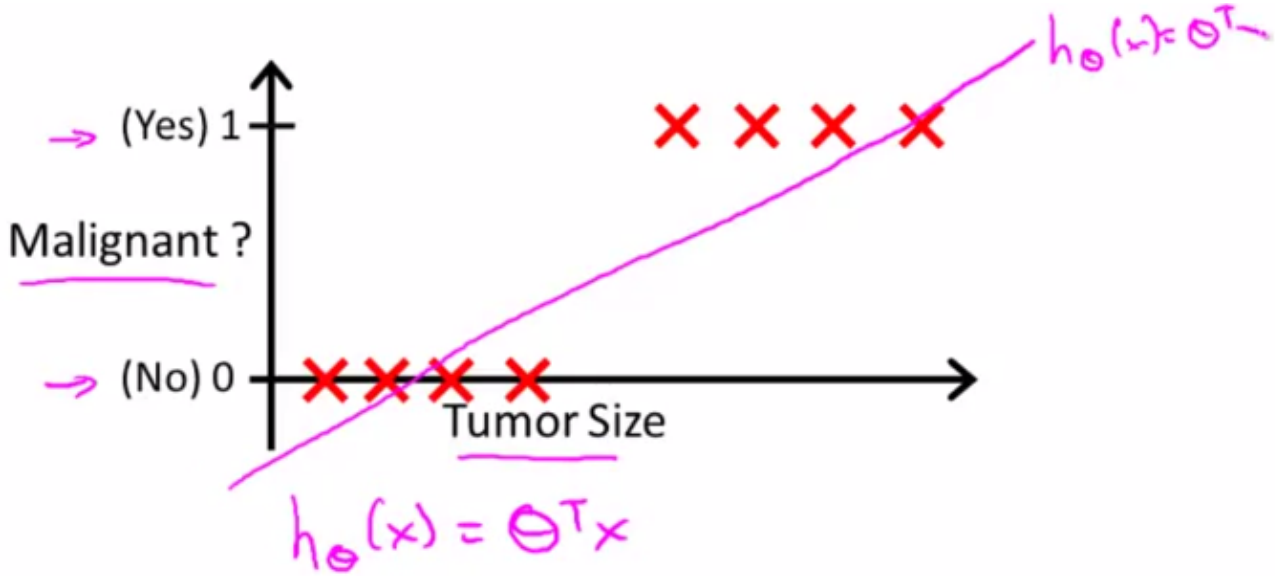
- 0 - *Negative Class*
  - also denoted −
- 1 - Positive Class
  - also denoted +

2) $y^{(i)}$ - label i

3) $x^{(i)}$ - feature i

Example - Context

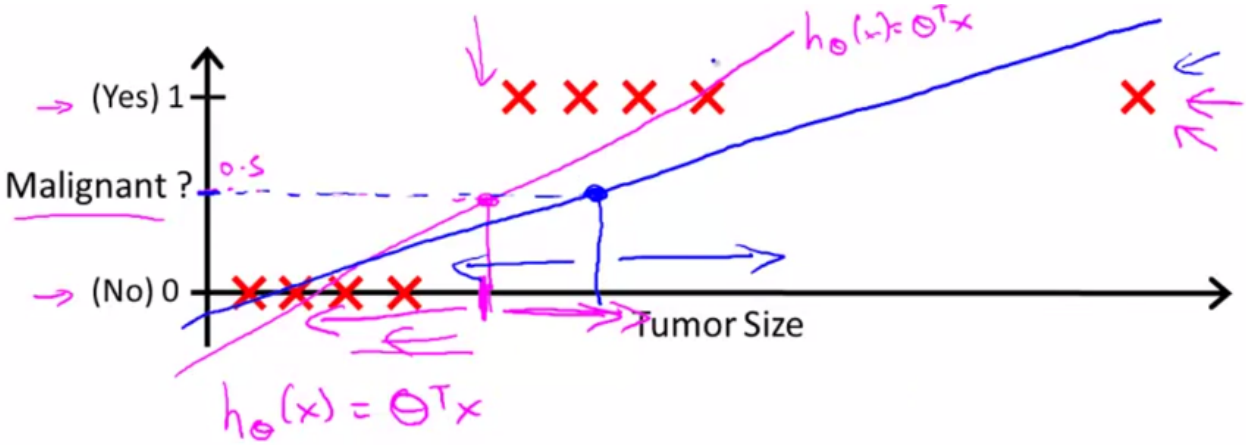
Using Linear Regression for classification problems



In order to make prediction, we can then ***Threshold*** the values at 0.5 for the regression line.

- if $h_\theta(x) \geq 0.5 \rightarrow y = 1$
- if $h_\theta(x) \leq 0.5 \rightarrow y = 0$

NOTE What if we have an outlier?



Notice how our threshold of 0.5 moves as a result of the outlier. i.e. Applying linear regression to classification isnt a good idea as it can quickly become skewed

The hypothesis $h_\theta(x)$ can be also be > 1 or < 0 even if the labels are only meant to be y = 1,0

Logistic Regression Model

Hypothesis Function

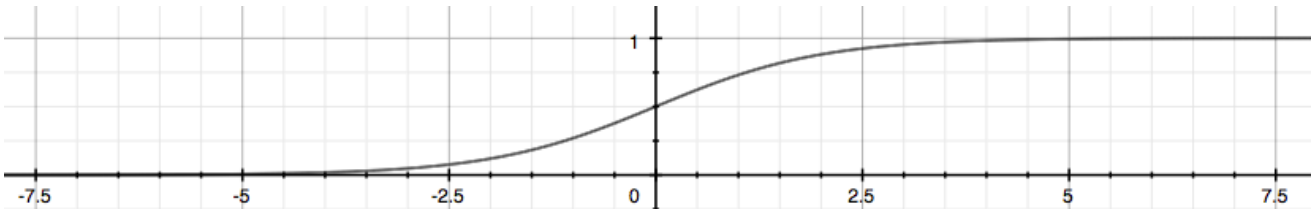
We want $0 \leq h_\theta(x) \leq 1$

Recall that $h_\theta(x) = \theta^T x$, we want it to map with respect to the bounds specified so we apply a sigmoid function g onto it

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

Where $g(z)$ is the ***Sigmoid Function*** (also called the *logistic function*)

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



Equation - Logistic Regression Hypothesis

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

Interpretation

The function g(z), shown here, maps any real number to the (0, 1) interval, making it useful for transforming an arbitrary-valued function into a function better suited for classification. Try playing with interactive plot of sigmoid function : (https://www.desmos.com/calculator/bgontvxotm).

We start with our old hypothesis (linear regression), except that we want to restrict the range to 0 and 1. This is accomplished by plugging $\theta^T x$ into the Logistic Function.

h_θ will give us the **probability** that our output is 1. For example, $h_\theta(x) = 0.7$ gives us the probability of 70% that our output is 1. i.e $h_\theta(x) =$ estimated probability that $y = 1$ on input x

$$h_\theta(x) = P(y = 1 | x; \theta) = 1 - P(y = 0 | x; \theta)$$
$$P(y = 0 | x; \theta) + P(y = 1 | x; \theta) = 1$$

Our probability that our prediction is 0 is just the complement of our probability that it is 1 (e.g. if probability that it is 1 is 70%, then the probability that it is 0 is 30%).

Expression Example:

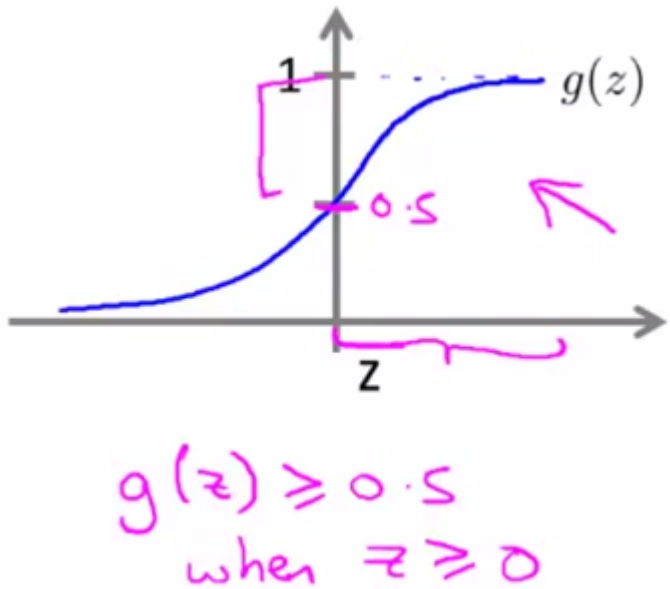
> Probability that $y = 1$, given x, parametrized by θ
>
> $h_\theta(x) = P(y = 1 | x; \theta)$

i.e.

- Inverse, probability of $y = 0$ occurring
  - $h_\theta(x) - 1 = P(y = 0|x; \theta)$
- The summation is equal to 1
  - $P(y = 1|x; \theta) + P(y = 0|x; \theta) = 1$

Decision Boundary

When is $y = 1$ w.r.t $\theta^T x$?



Hence, we get $y = 1$ when:

$$h_\theta(x) = g(\theta^T x) \geq 0.5$$
$$\textbf{when } \theta^T x \geq 0$$

Conversely, $y = 0$ when:

$$h_\theta(x) = g(z) < 0.5$$
$$\textbf{when } z = \theta^T x < 0$$

Remember:

$$z = 0, e^0 = 1 \Rightarrow g(z) = 1/2$$
$$z \to \infty, e^{-\infty} \to 0 \Rightarrow g(z) = 1$$
$$z \to -\infty, e^{\infty} \to \infty \Rightarrow g(z) = 0$$

So if our input to g is $\theta^T X$, then that means:

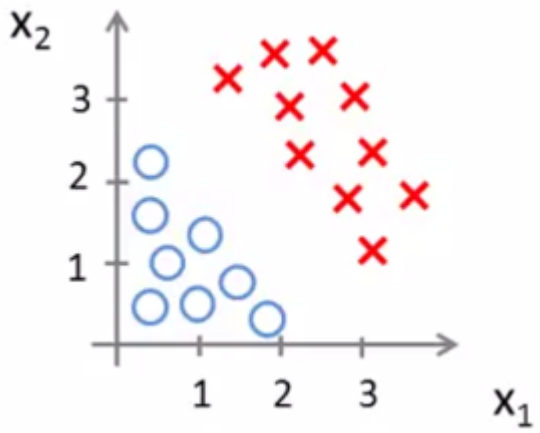
From these statements we can now say:

$$\theta^T x \geq 0 \Rightarrow y = 1$$
$$\theta^T x < 0 \Rightarrow y = 0$$

The **decision boundary** is the line that separates the area where y = 0 and where y = 1. It is created by our hypothesis function.

Example: linear boundary

Say we have the following data:



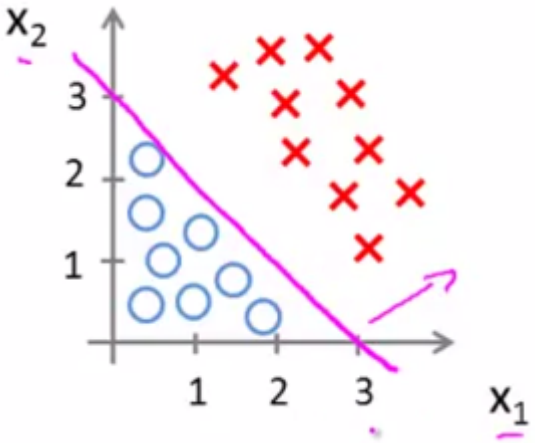
Where the hypothesis has been determined to be:

$$h_\theta(x) = g(-3 + 1 * x_1 + 1 * x_2)$$

Then $y = 1$ if:

$$-3 + x_1 + x_2 \geq 0$$
$$x_1 + x_2 \geq 3$$

Plotting this inequality: Everything to the right of the pink line is then determined to be the "red x" region

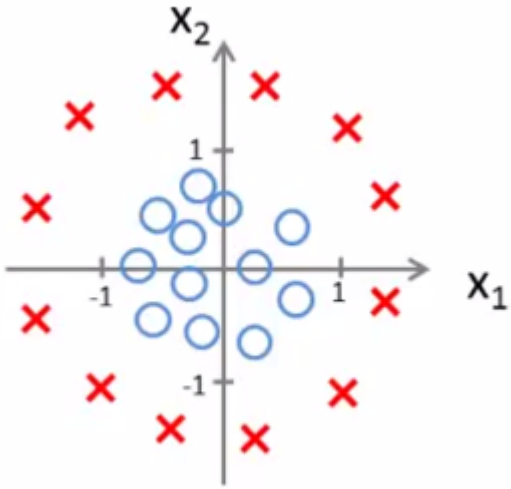


Term: Decision Boundary

> - The pink line in the above diagram
> - The function that separates the classification regions
>   - In the above example: $x_1 + x_2 = 3$
> - NOTE the decision boundary is a property of the hypothesis function and its parameters and not a property of the data set

Example: Non-Linear decision boundaries

Say we have the following data:



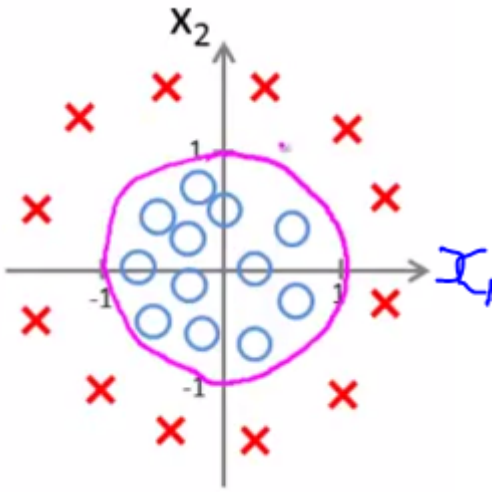
Where the hypothesis has been determined to be:

$$h_\theta(x) = g(-1 + x_1^2 + x_2^2)$$

Then $y = 1$ if:

$$-1 + x_1^2 + x_2^2 \geq 0$$
$$x_1^2 + x_2^2 \geq 1$$

Plotting this inequality: Everything outside the pink circle is $y = 1$



with the decision boundary defined by $x_1^2 + x_2^2 = 1$

Cost Function

How do we choose our parameters θ?

System Set up

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

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

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

Context:

We cannot use the same cost function that we use for linear regression because the Logistic Function will cause the output to be wavy, causing many local optima. In other words, it will not be a convex function.

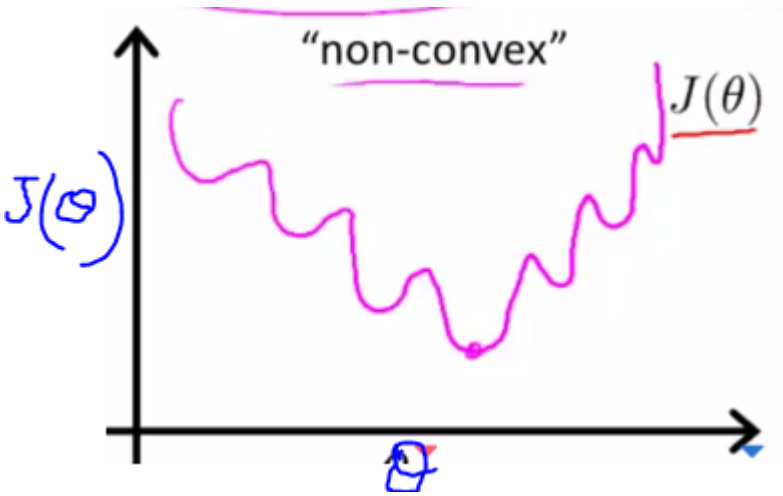
Recall that the *cost function* for linear regression is:

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

But recall that the hypothesis for logistic regression is: (non-linear)

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

This non-linearity will produce a "non-convec" cost function when put into the cost function $J(\theta)$



The problem with this is that we will struggle to find the global optimal solution to the cost function. Hence we define a cost function that will give us a convex function which is easier to optimize.

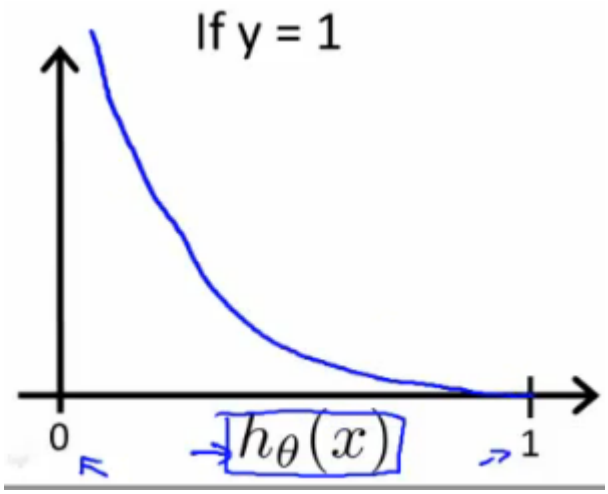
Function: Logistic Regression cost Function

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

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

Intuition: $y = 1$

Plot of $-log(h_\theta(x))$ as $J(\theta)$ vs $h_\theta(x)$:



Observe that:

$$\lim_{h_\theta(x) \to 1} Cost = 0$$

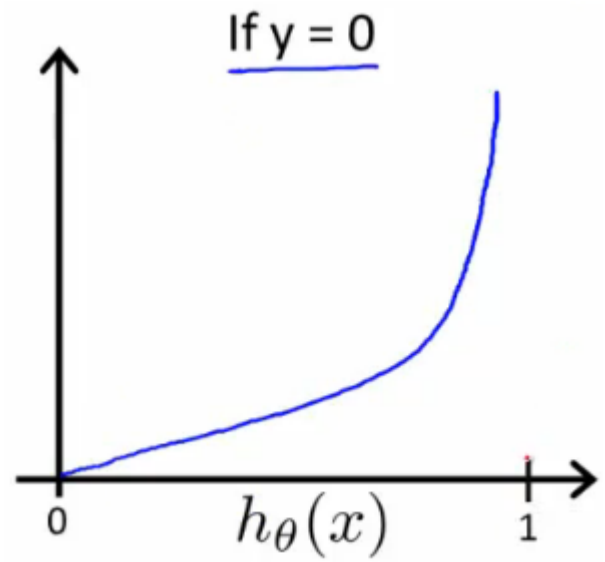
$$\lim_{h_\theta(x) \to 0} Cost = \infty$$

i.e The closer the hypothesis function h predicts 0 when it should be 1 the greater the cost value J will be (rapid growth towards infinity closer to 0 we get)

Intuition: $y = 0$

Similar to the previous example we have the following but the inverse

Plot of $-log(1 - h_\theta(x))$ as $J(\theta)$ vs $h_\theta(x)$:



Simplified Cost Function

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

We can simplify the function above into:

$$Cost(h_\theta(x), y) = -y \log(h_\theta(x)) - (1 - y) \log(1 - h_\theta(x))$$

Function: Logistic Regression cost Function

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

NOTE

- The above cost function is convex
- This cost function can be derived from the principle of *maximum likelihood estimation*

Fitting Parameters - Gradient Descent

Algorithm Gradient Descent

Minimizing $J(\theta)$

$$\begin{aligned} &Repeat\ \{ \\ &\theta_j := \theta_j - \frac{\alpha}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} \\ &\} \end{aligned}$$

Vectorized Implementation

Vectorized - Cost Function

$$h = g(X\theta)$$
$$g(z) = \frac{1}{1 + e^{-z}}$$
$$J(\theta) = \frac{1}{m} \cdot \left(-y^T \log(h) - (1 - y)^T \log(1 - h)\right)$$

Vectorized - Updating of Gradient Descent

$$\theta := \theta - \alpha \frac{1}{m} \sum_{i=1}^{m} [(h_\theta(x^{(i)}) - y^{(i)}) \cdot x^{(i)}]$$

OR

$$\theta := \theta - \frac{\alpha}{m} X^T (g(X\theta) - \vec{y})$$

Advanced Optimization

Example of more advanced optimization algorithms

- Conjugate gradient
- BFGS
- L-BFGS

Advantages	Disadvantages
No need to manually pick α	More Complex
Often faster then gradient descent	

Example

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

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

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

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

```
function [jVal, gradient] = costFunction(theta)
  jVal = (theta(1)-5)^5 + (theta(2)-5)^2

  gradient = zeros(2,1);
  gradient(1) = 2*(theta(1)-5);
  gradient(2) = 2*(theta(2)-5);
end
```

```
options = optimset('GradObj', 'on', 'MaxIter', 100);
initialTheta = zeros(2,1);
[optTheta, functionVal, exitFlag] = fminunc(@costFunction, initialTheta, options);
% @costFunction : a pointer to the function
```

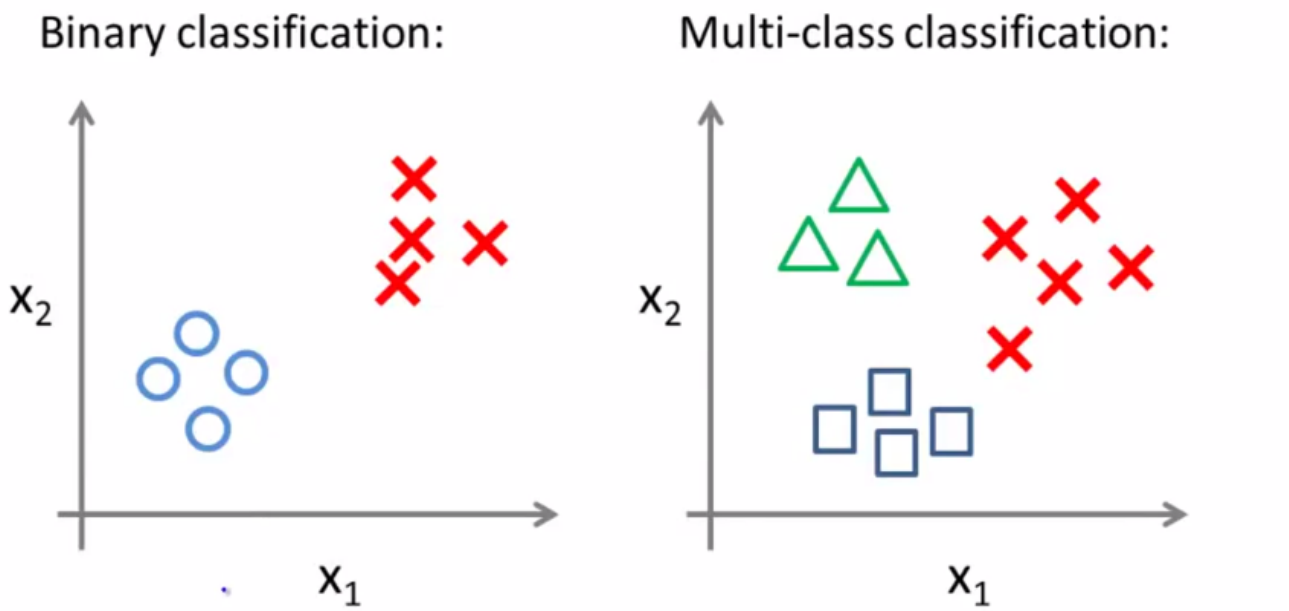
NOTE `initialTheta` $\in R^d$ where $d \geq 2$

Use with logistic regression

```
function [jVal, gradient] = costFunction(theta)
  jVal = [...code to compute J(theta)...];
  gradient = [...code to compute derivative(s) of J(theta)...];
end
```

Multiclass Classification

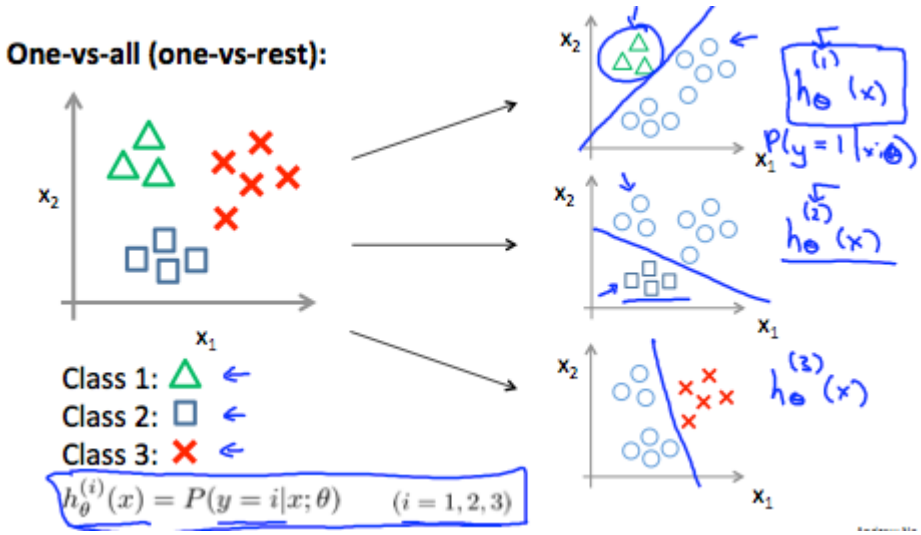
Given a data set with 3 classes, left graph



Classification: One-VS-All

Using *one-vs-all* classification we can separate the 3 different classes.

The idea is that we will change this problem into 3 different binary classification problems.



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

Where:

- $i = 1$ triangles
- $i = 2$ squares
- $i = 3$ circles

Summary

Train a logistic regression classifier $h_\theta^{(i)}$ 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:

$$
\begin{aligned}
&y \in \{0, 1 \dots n\} \\
&h_\theta^{(0)}(x) = P(y = 0|x;\theta) \\
&h_\theta^{(1)}(x) = P(y = 1|x;\theta) \\
&\cdots \\
&h_\theta^{(n)}(x) = P(y = n|x;\theta) \\
&\text{prediction} = \max_i(h_\theta^{(i)}(x))
\end{aligned}
$$

Dealing with Over-fitting -> Regularization

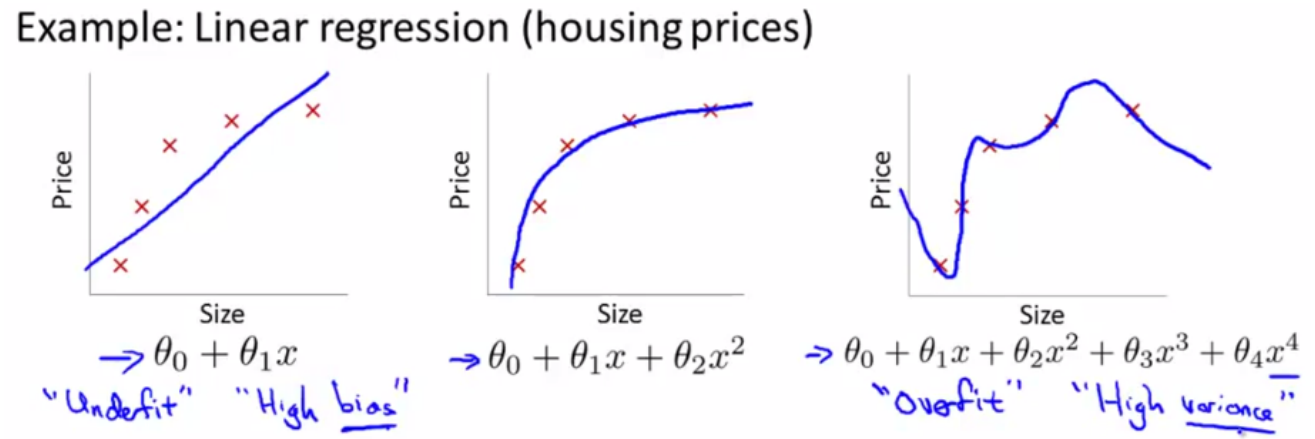
Definition: Over-Fitting

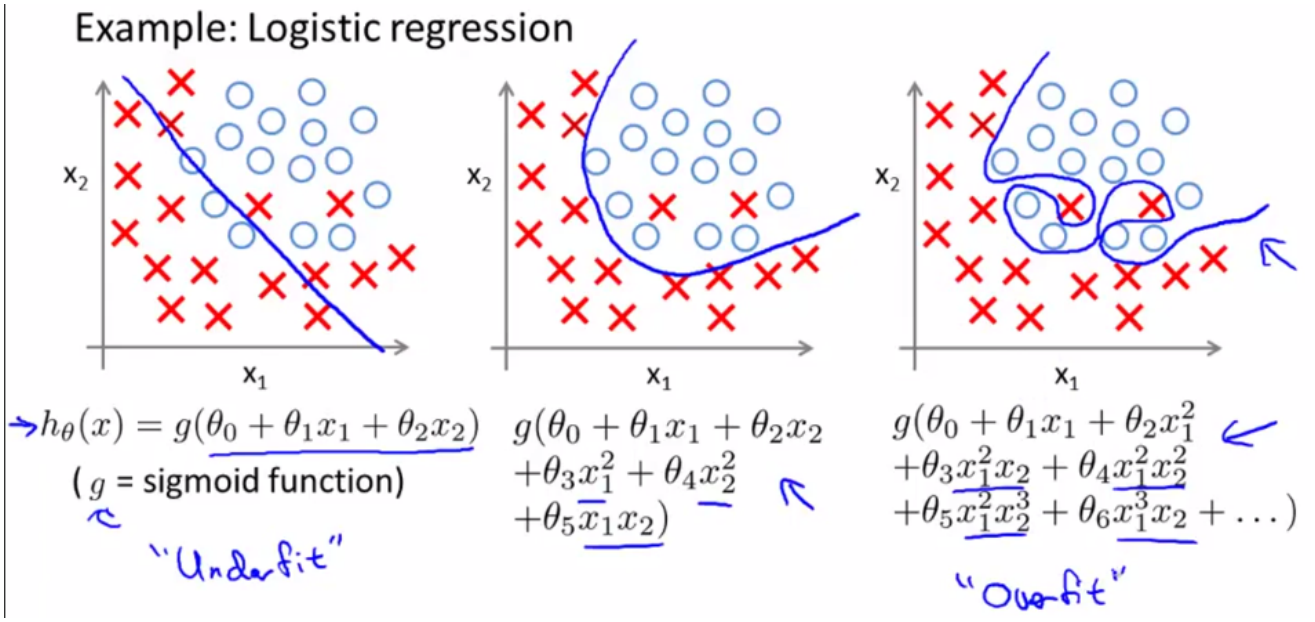
> If we have to many features (and not enough data), the learning hypothesis may fit the training set very well $J(\theta) \approx 0$ but fail to generalize to new examples
>
> i.e. It makes accurate prediction for examples in the training set, but it does not generalize well to make accurate predictions on new, preciously unseen examples

Definition: Underfitting / high bias

> When the form of our hypothesis function h maps poorly to the trend of the data. It is usually caused by a function that is too simple or uses too few features.

Example Visual Illustration

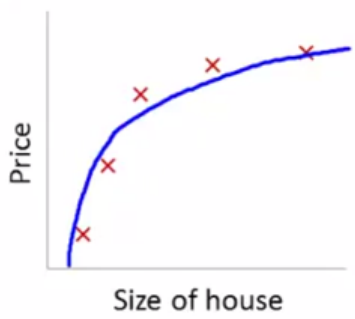




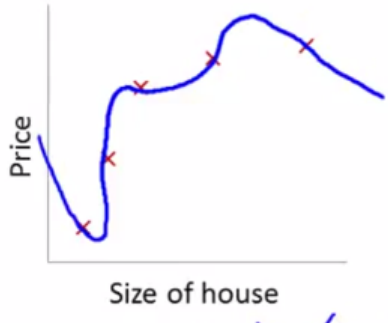
Addressing Overfitting

- Reduce number of features
  - Manually select which features to keep
  - Model selection algorithm (later in course)
- ***Regularization***
  - Keep all the features, reduce magnitude/values of paramaters θ_j
  - Works well when we have a lot of features, each of which contributes a bit to predicting y

Intuition behind Regularization



$\theta_0 + \theta_1 x + \theta_2 x^2$



$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

Suppose we penalize and make θ_3, θ_4 really small.

$$\min_\theta \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 + 1000\,\theta_3^2 + 1000\,\theta_4^2$$

Then $\theta_3 \approx 0$ and $\theta_4 \approx 0$ -> then we get a function that resembles $\theta_0 + \theta_1 x + \theta_2 x^2$

Core Idea

> Small values for parameters $\theta_0, \theta_1, \ldots \theta_n$
>
> - Simpler hypothesis
> - Less prone to overfitting

Solution - Cost Function for Regularization

Cost Function: Regularize all parameters

$$J(\theta) = \min_\theta \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n} \theta_j^2$$

Notation

- λ : regularization parameter

NOTE

- that θ_0 isn't regularized, by convention
- The second summation term keeps the parameters small.
- The λ term controls the trade of between (the two summation terms) training the data well and keeping the parameters small.
  - It determines how much the costs of our theta parameters are inflated.
  - The larger it is, the more the parameters will made small -> smooth out the function too much and cause under-fitting

Using the above cost function with the extra summation, we can smooth the output of our hypothesis function to reduce overfitting. If lambda is chosen to be too large, it may smooth out the function too much and cause underfitting.

Regularized *Linear Regression*

We can apply regularization to both linear regression and logistic regression. We will approach linear regression first.

Algorithm:

$$\begin{aligned}&\textbf{Repeat } \{\\ &\quad \theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)} \\ &\quad \theta_j := \theta_j - \alpha \left[\left(\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} \right) + \frac{\lambda}{m} \theta_j \right] \qquad j \in \{1, 2 \ldots n\} \\ &\}\end{aligned}$$

- The first equation is as such because regularization isnt applied to $j = 0$
- The second equation is obtained from $\partial J / \partial \theta_j$

The last equation is equivalent to:

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

Note The term $(1 - \alpha \frac{\lambda}{m})$ usually between $\in (0, 1)$ acts as a shrinking term once multiplied onto parameter θ i.e its exactly the same as gradient descent but whe re the parameter θ is shrunk my some small amount

Regularized *Normal Equation*

Formula:

$$\theta = \left(X^T X + \lambda \cdot L \right)^{-1} X^T y$$

$$\text{where } L = \begin{bmatrix} 0 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix}$$

$$\text{where } L \in R^{(n+1) \times (n+1)}$$

Non-Inevitability

Recall that the *Normal Equation* is of the form $\theta = (X^T X)^{-1} X^T y$ Suppose $m \leq n$ then $X^T X$ is non-invertible/singular

Solution: ***Regularized form helps with this!***

As long as $\lambda > 0$, then the term $X^T X + \lambda \cdot L$ is *invertible*

$$\theta = \left(X^T X + \lambda \cdot L \right)^{-1} X^T y$$

Regularized Logistic Regression

We can regularize logistic regression in a similar way that we regularize linear regression.

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}[y^{(i)}\ \log(h_\theta(x^{(i)})) + (1-y^{(i)})\ \log(1-h_\theta(x^{(i)}))] + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

Note Well: The second sum, $\sum_j^n = \theta_j^2$ **means to explicitly exclude** the bias term, θ_0. I.e. the θ vector is indexed from 0 to n (holding n+1 values, θ_0 through θ_n), and this sum explicitly skips θ_0, by running from 1 to n, skipping 0.

Algorithm

Just like with linear regression, we will want to **separately** update θ_0 and the rest of the parameters because we do not want to regularize θ_0.

$$\begin{aligned}
&\textbf{Repeat } \{ \\
&\quad \theta_0 := \theta_0 - \alpha\ \frac{1}{m}\ \sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_0^{(i)} \\
&\quad \theta_j := \theta_j - \alpha\ \left[\left(\frac{1}{m}\ \sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}\right) + \frac{\lambda}{m}\theta_j\right] \qquad\qquad j \in \{1,2...n\} \\
&\}
\end{aligned}$$

This is identical to the gradient descent function presented for linear regression.

Advanced Optimization

Same as last section but with modified cost function J

```
function [jVal, gradient] = costFunction(theta)
    jVal = [code to compute J]
    gradient(1) = [code to compute partial J wrt \theta_0]
    etc...
    gradient(n+1)  = [code to compute partial J wrt \theta_n]
```