Coursera Machine Learning

Tuesday, 14 June 2022 1:03 pm

What is Machine Learning?

Two definitions of Machine Learning are offered. Arthur Samuel described it as: "the field of study that gives computers the ability to learn without being explicitly programmed." This is an older, informal definition.

Tom Mitchell provides a more modern definition: "A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E."

Example: playing checkers.

E = the experience of playing many games of checkers

T = the task of playing checkers.

P = the probability that the program will win the next game.

In general, any machine learning problem can be assigned to one of two broad classifications:

- Supervised learning
- Unsupervised learning.

Supervised Learning

In supervised learning, we are given a data set and already know what our correct output should look like, having the idea that there is a relationship between the input and the output.

Supervised learning problems are categorized into "regression" and "classification" problems. In a regression problem, we are trying to predict results within a continuous output, meaning that we are trying to map input variables to some continuous function. In a classification problem, we are instead trying to predict results in a discrete output. In other words, we are trying to map input variables into discrete categories.

Example 1:

Given data about the size of houses on the real estate market, try to predict their price. Price as a function of size is a continuous output, so this is a regression problem.We could turn this example into a classification problem by instead making our output about whether the house "sells for more or less than the asking price." Here we are classifying the houses based on price into two discrete categories

Example 2:

(a) Regression - Given a picture of a person, we have to predict their age on the basis of the given picture

(b) Classification - Given a patient with a tumor, we have to predict whether the tumor is malignant or benign

Unsupervised Learning

Unsupervised learning allows us to approach problems with little or no idea what our results should look like. We can derive structure from data where we don't necessarily know the effect of the variables.

We can derive this structure by clustering the data based on relationships among the variables in the data.

With unsupervised learning there is no feedback based on the prediction results.

Example:

Clustering: Take a collection of 1,000,000 different genes, and find a way to automatically group these genes into groups that are somehow similar or related by different variables, such as lifespan, location, roles, and so on.

Non-clustering: The "Cocktail Party Algorithm", allows you to find structure in a chaotic environment. (i.e. identifying individual voices and music from a mesh of sounds at a cocktail party).

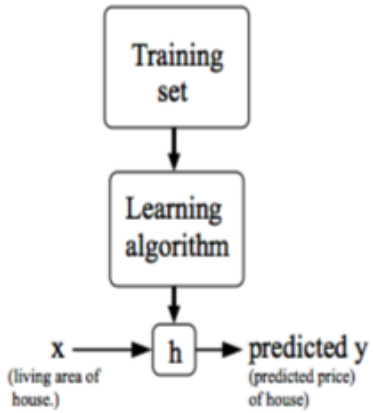
Linear Regression with One Variable

Linear regression predicts a real-valued output based on an input value. We discuss the application of linear regression to housing price prediction, present the notion of a cost function, and introduce the gradient descent method for learning.

Model Representation

To establish notation for future use, we'll use $x^{(i)}$ to denote the "input" variables (living area in this example), also called input features, and $y^{(i)}$ to denote the "output" or target variable that we are trying to predict (price). A pair $(x^{(i)}, y^{(i)})$ is called a training example, and the dataset that we'll be using to learn—a list of m training examples $(x^{(i)}, y^{(i)}); i = 1, ..., m$—is called a training set. Note that the superscript "(i)" in the notation is simply an index into the training set, and has nothing to do with exponentiation. We will also use X to denote the space of input values, and Y to denote the space of output values. In this example, X = Y = $\mathbb{R}$.

To describe the supervised learning problem slightly more formally, our goal is, given a training set, to learn a function h : X → Y so that h(x) is a "good" predictor for the corresponding value of y. For historical reasons, this function h is called a hypothesis. Seen pictorially, the process is therefore like this:



When the target variable that we're trying to predict is continuous, such as in our housing example, we call the learning problem a regression problem. When y can take on only a small number of discrete values (such as if, given the living area, we wanted to predict if a dwelling is a house or an apartment, say), we call it a classification problem.

Training set of housing prices (Portland, OR)

Size in feet² (x)	Price ($) in 1000's (y)
2104	460
1416	232
1534	315
852	178
...	...

m = 47

Notation:

- **m** = Number of training examples
- **x**'s = "input" variable / features
- **y**'s = "output" variable / "target" variable

(x, y) - one training example

$(x^{(i)}, y^{(i)})$ - i^{th} training example

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H(x)= Theta0 + Theta1X

Cost Function is choosing the thetas to minimise difference between H(x) and Y

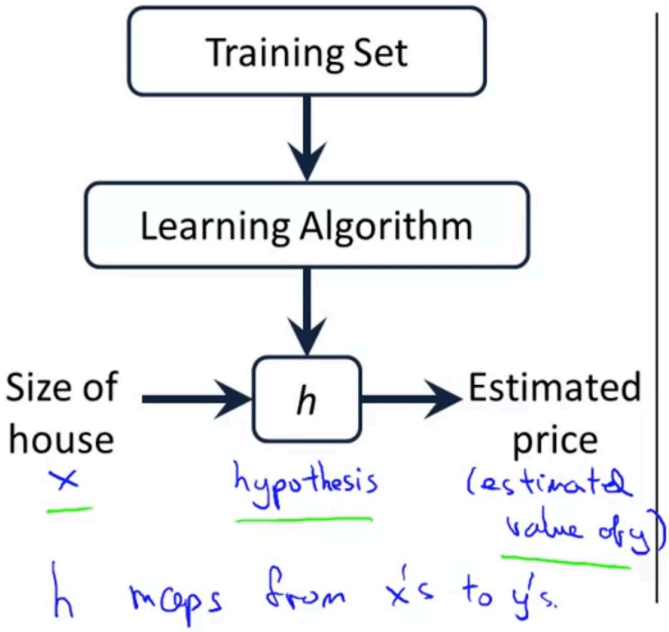
Cost Function

We can measure the accuracy of our hypothesis function by using a cost function. This takes an average difference (actually a fancier version of an average) of all the results of the hypothesis with inputs from x's and the actual output y's.

This function is otherwise called the "Squar

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (\hat{y}_i - y_i)^2 = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x_i) - y_i)^2$$

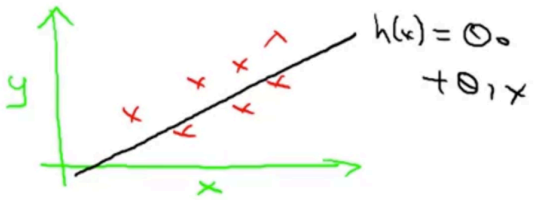
To break it apart, it is $\frac{1}{2}\ \bar{x}$ where $\bar{x}$ is the mean of the squares of $h_\theta(x_i) - y_i$, or the difference between the predicted



How do we represent *h* ?

$h_\theta(x) = \theta_0 + \theta_1 x$

Shorthand: $h(x)$



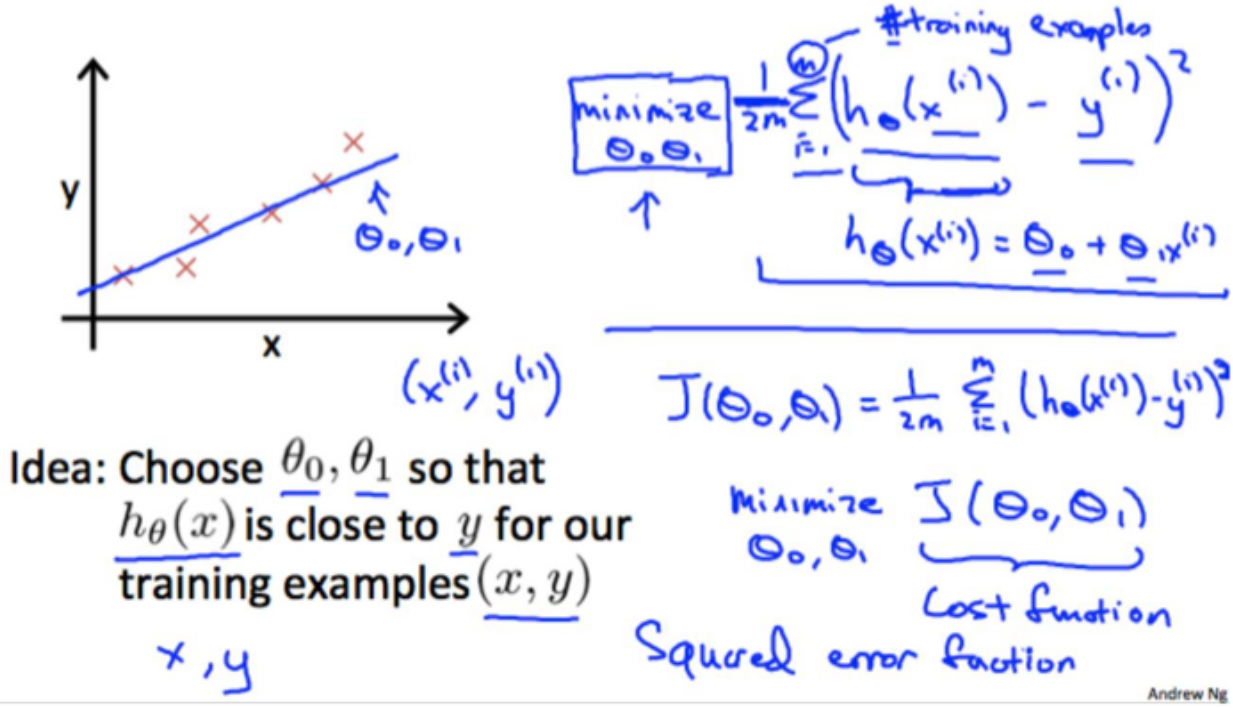
Linear regression with one variable. (x)

Univariate linear regression.

└ one variable

value and the actual value.

ed error function", or "Mean squared error". The mean is halved (½) as a convenience for the computation of the gradient descent, as the derivative term of the square function will cancel out the ½ term. The following image summarizes what the cost function does:



This function is otherwise called the "Squared error function", or "Mean squared error". The mean is halved $\left(\frac{1}{2}\right)$ convenience for the computation of the gradient descent, as the derivative term of the square function will ca the $\frac{1}{2}$ term. The following image summarizes what the cost function does:

Cost Function - Intuition I

If we try to think of it in visual terms, our training data set is scattered on the x-y plane. We are trying to make a straight line (defined by $h\theta(x)$) which passes through these scattered data points.

Our objective is to get the best possible line. The best possible line will be such so that the average squared vertical distances of the scattered points from the line will be the least. Ideally, the line should pass through all the points of our training data set. In such a case, the value of $J(\theta_0,\theta_1)$ will be 0. The following example shows the ideal situation where we have a cost function of 0.

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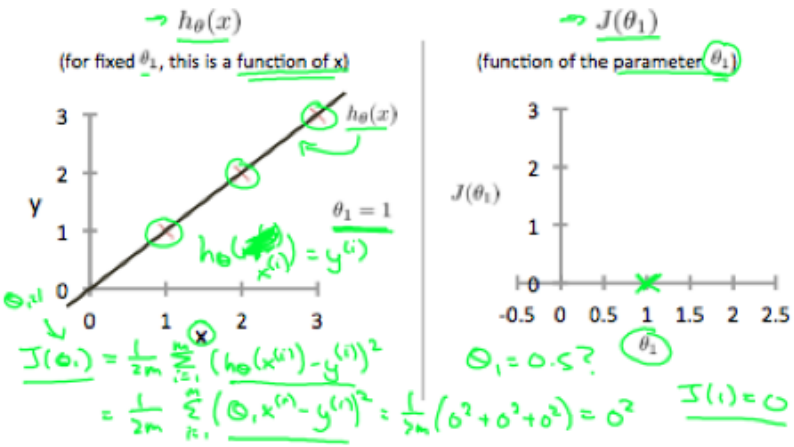
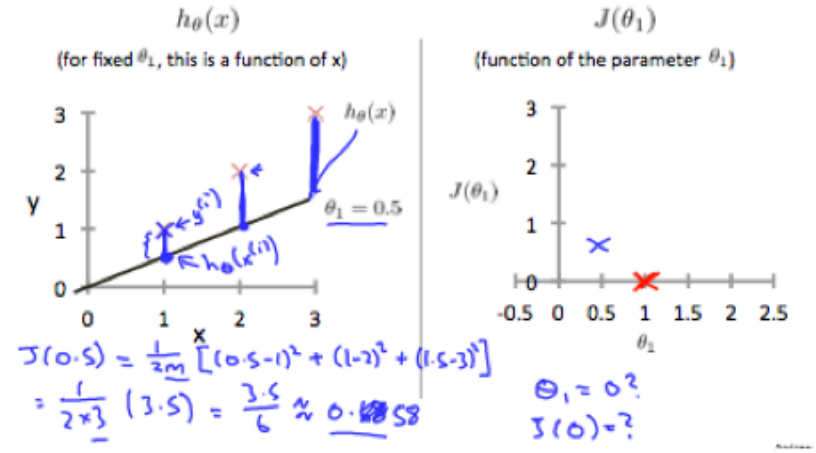
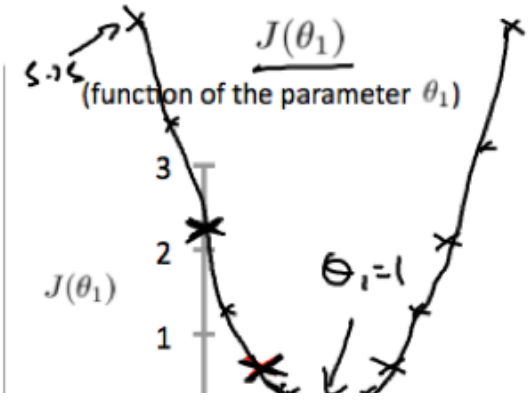
ncel out

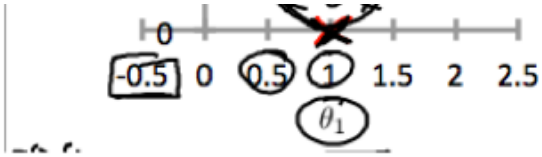


When $\theta_1=1$, we get a slope of 1 which goes through every single data point in our model. Conversely, when $\theta_1=0.5$, we see the vertical distance from our fit to the data points increase.



This increases our cost function to 0.58. Plotting several other points yields to the following graph:

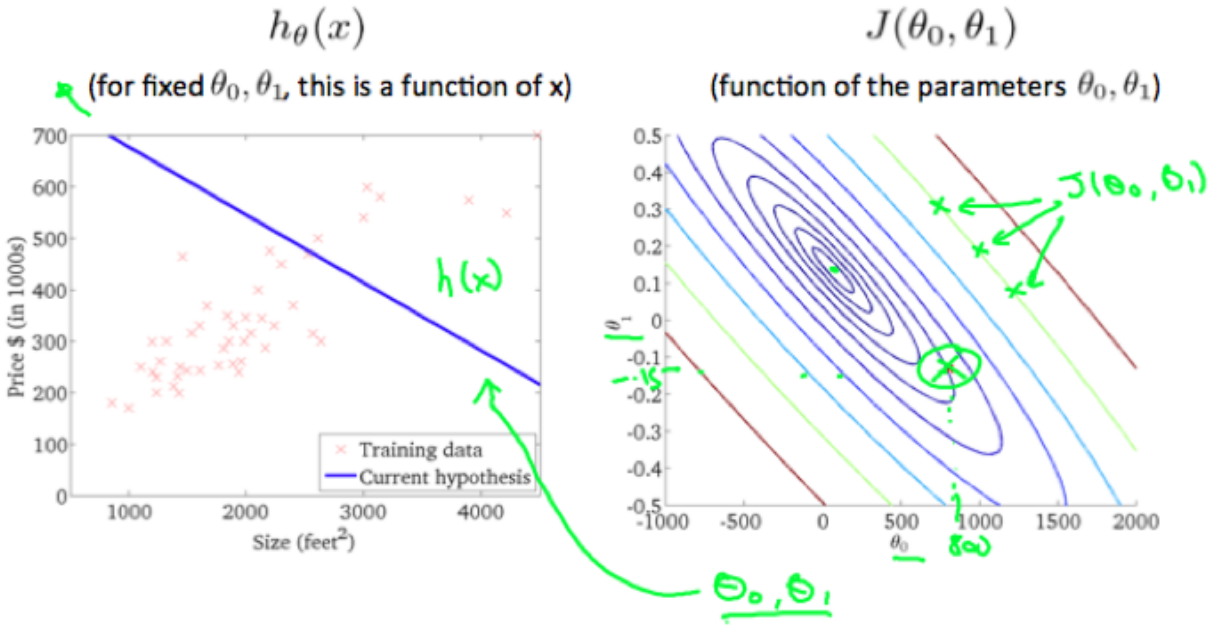




Thus as a goal, we should try to minimize the cost function. In this case, $\theta_1=1$ is our global minimum.

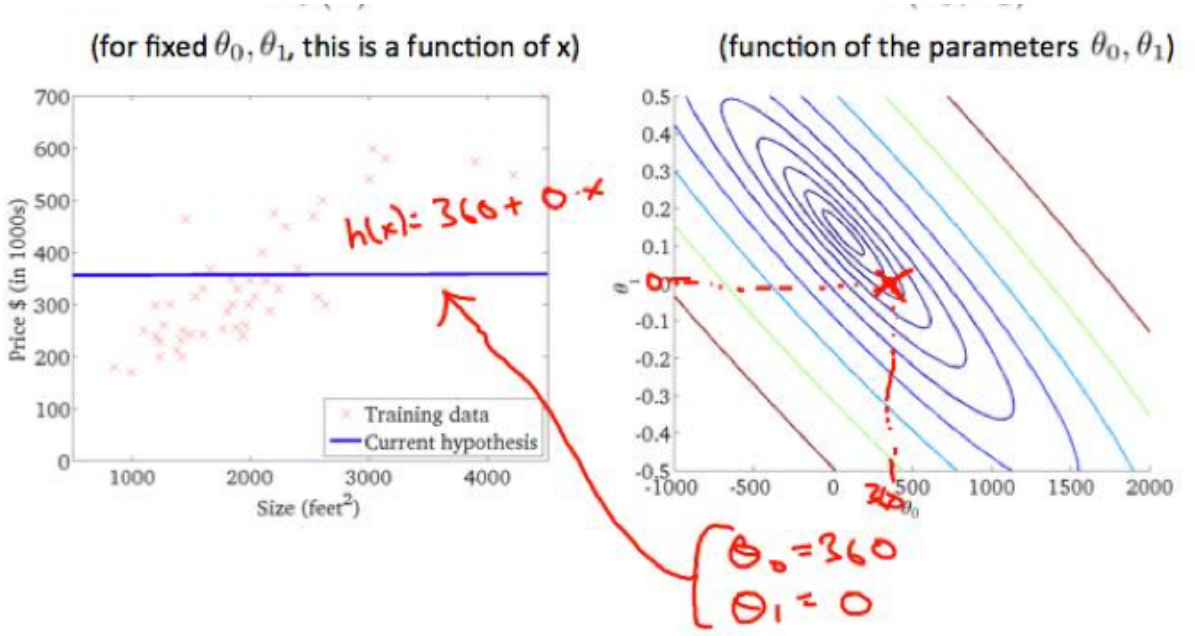
Cost Function - Intuition II

A contour plot is a graph that contains many contour lines. A contour line of a two variable function has a constant value at all points of the same line. An example of such a graph is the one to the right below.

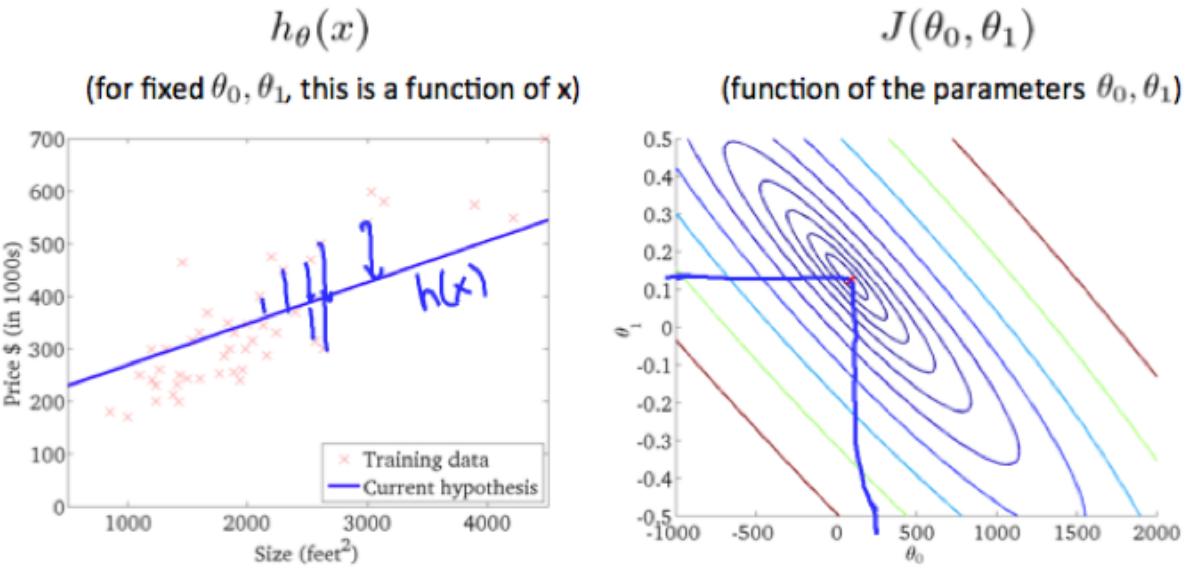


Taking any color and going along the 'circle', one would expect to get the same value of the cost function. For example, the three green points found on the green line above have the same value for $J(\theta_0,\theta_1)$ and as a result, they are found along the same line. The circled x displays the value of the cost function for the graph on the left when

θ_0= 800 and θ_1= -0.15. Taking another h(x) and plotting its contour plot, one gets the following graphs:



Whenθ_0= 360 andθ_1= 0, the value of$J(\theta_0,\theta_1)$ in the contour plot gets closer to the center thus reducing the cost function error. Now giving our hypothesis function a slightly positive slope results in a better fit of the data.



The graph above minimizes the cost function as much as possible and consequently, the result of θ_1 and θ_0 tend to be around 0.12 and 250 respectively. Plotting those values on our graph to the right seems to put our point in the center of the innermost 'circle'.

Gradient descent algorithm

Assignment
$a := b$

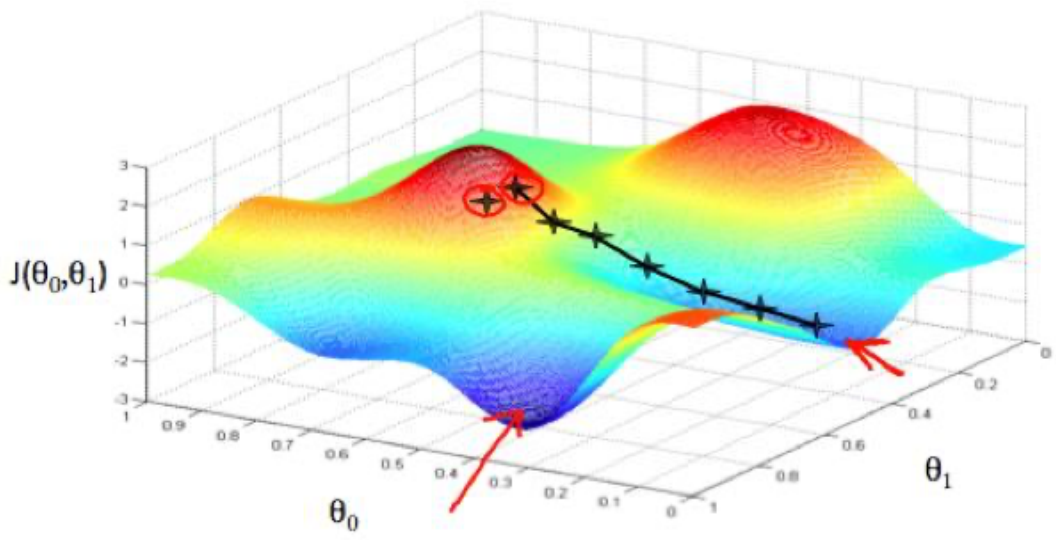
Truth assertion
$a = b$

Gradient Descent

So we have our hypothesis function and we have a way of measuring how well it fits into the data. Now we need to estimate the parameters in the hypothesis function. That's where gradient descent comes in.

Imagine that we graph our hypothesis function based on its fields $\theta_0$andθ_1(actually we are graphing the cost function as a function of the parameter estimates). We are not graphing x and y itself, but the parameter range of our hypothesis function and the cost resulting from selecting a particular set of parameters.

We put θ_0 on the x axis and θ_1 on the y axis, with the cost function on the vertical z axis. The points on our graph will be the result of the cost function using our hypothesis with those specific theta parameters. The graph below depicts such a setup.



We will know that we have succeeded when our cost function is at the very bottom of the pits in our graph, i.e. when its value is the minimum. The red arrows show the minimum points in the graph.

The way we do this is by taking the derivative (the tangential line to a function) of our cost function. The slope of the tangent is the derivative at that point and it will give us a direction to move towards. We make steps down the cost function in the direction with the steepest descent. The size of each step is determined by the parameter α, which is called the learning rate.

For example, the distance between each 'star' in the graph above represents a step determined by our parameter α. A smaller α would result in a smaller step and a larger α results in a larger step. The direction in which the step is taken is determined by the partial derivative of$J(\theta_0,\theta_1)$. Depending on where one starts on the graph, one could

repeat until convergence {

$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)$ (for $j = 0$ and $j = 1$)

}

learning rate

Simultaneously update θ_0 and θ_1

θ_0, θ_1

$a := a+1$ | $a = a+1$ ✗

Correct: Simultaneous update

$\text{temp0} := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$

$\text{temp1} := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$

$\theta_0 := \text{temp0}$

$\theta_1 := \text{temp1}$

Incorrect:

$\text{temp0} := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$

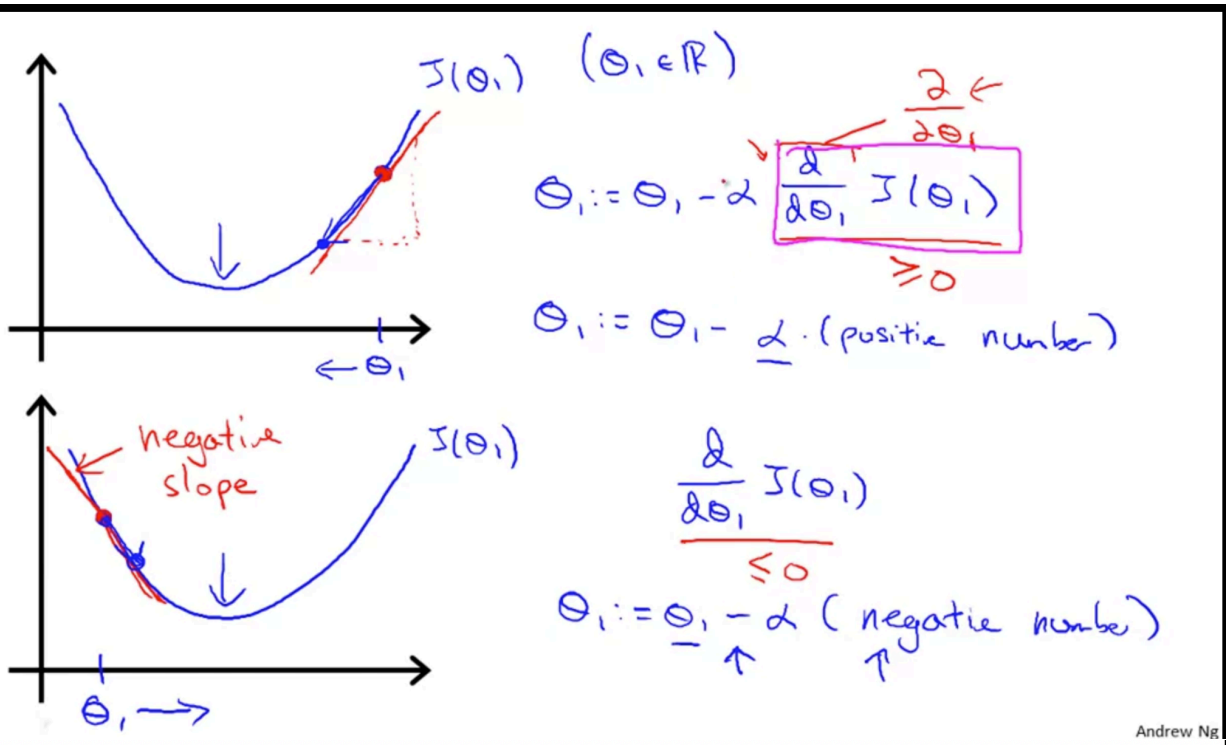
$\theta_0 := \text{temp0}$

$\text{temp1} := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$

$\theta_1 := \text{temp1}$

If slope is positive --> derivative is positive

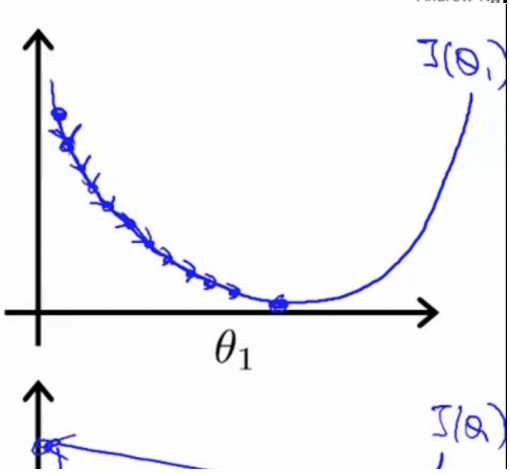
If slope is negative --> derivative is negative



Andrew Ng

$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$

If α is too small, gradient descent can be slow.

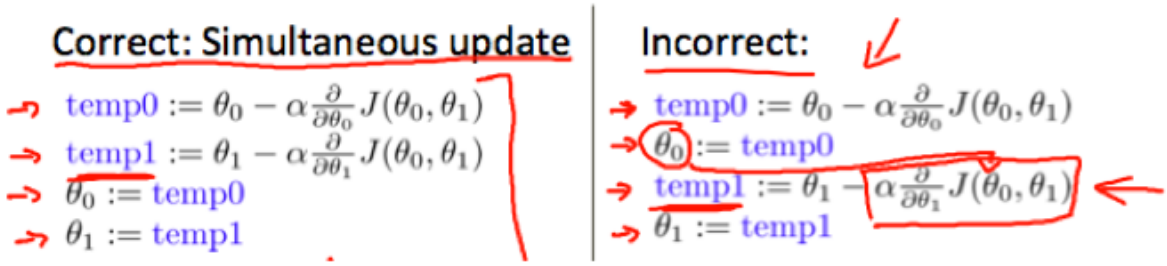


end up at different points. The image above shows us two different starting points that end up in two different places.The gradient descent algorithm is:repeat until convergence:

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)$$

where j=0,1 represents the feature index number.

At each iteration j, one should simultaneously update the parameters$\theta_1,\theta_2,...,\theta_n$. Updating a specific parameter prior to calculating another one on the$j_{(th)}$iteration would yield a wrong implementation.



Gradient Descent Intuition

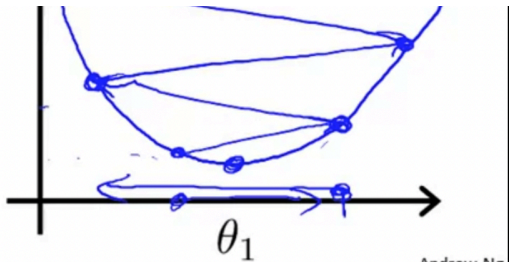
In this video we explored the scenario where we used one parameter$\theta_1$and plotted its cost function to implement a gradient descent. Our formula for a single parameter was :

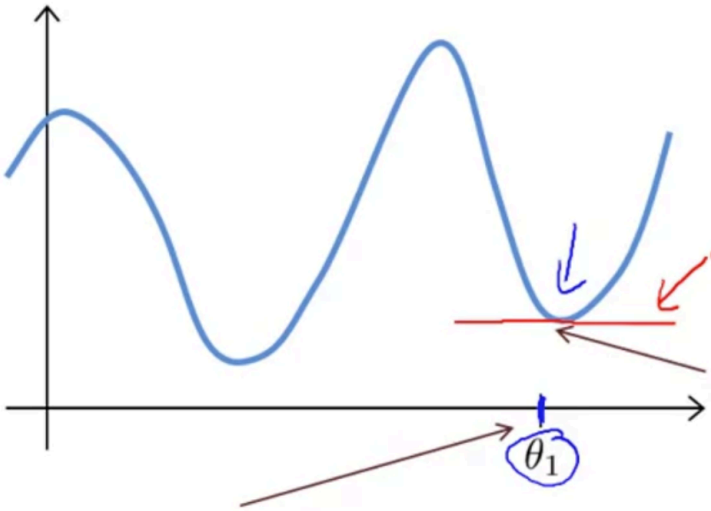
Repeat until convergence:

$$\theta_1 := \theta_1 - \alpha \frac{d}{d\theta_1} J(\theta_1)$$

Regardless of the slope's sign for $\frac{d}{d\theta_1} J(\theta_1)$, θ_1 eventually converges to its minimum value. The following graph shows that when the slope is negative, the value of θ_1 increases and when it is positive, the value of θ_1 decreases.

If α is too large, gradient descent can overshoot the minimum. It may fail to converge, or even diverge.





Current value of θ_1

$$\theta_1 := \theta_1 - \alpha \frac{d}{d\theta_1} J(\theta_1)$$

$$\theta_1 := \theta_1 - \alpha \cdot 0$$

$$\theta_1 := \theta_1$$

$$\frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) = \frac{\partial}{\partial \theta_j} \cdot \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2$$

$$= \frac{\partial}{\partial \theta_j} \frac{1}{2m} \sum_{i=1}^{m} \left(\theta_0 + \theta_1 x^{(i)} - y^{(i)} \right)^2$$

$$\theta_0 \; j = 0 : \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right)$$

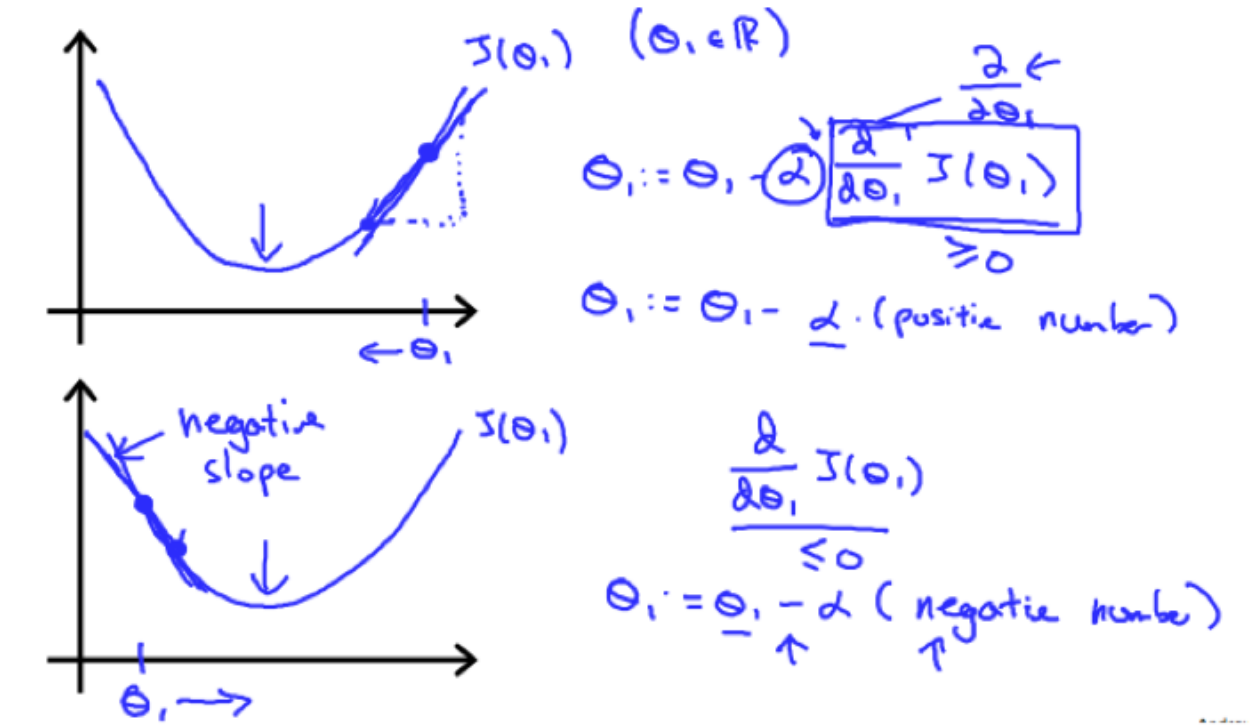
$$\theta_1 \; j = 1 : \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right) \cdot x^{(i)}$$

Gradient descent algorithm

$\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$

repeat until convergence {

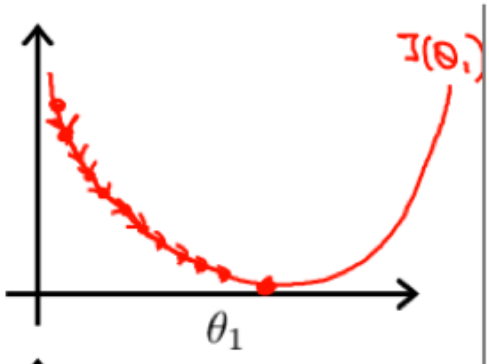
update



On a side note, we should adjust our parameter α to ensure that the gradient descent algorithm converges in a reasonable time. Failure to converge or too much time to obtain the minimum value imply that our step size is wrong.

$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

If α is too small, gradient descent can be slow.



If α is too large, gradient descent can overshoot the minimum. It may fail to converge, or even diverge.

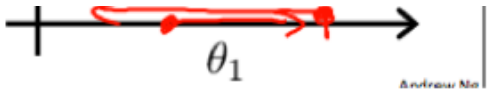
$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)$

$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right) \cdot x^{(i)}$

}

update θ_0 and θ_1 simultaneously

$\frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$



How does gradient descent converge with a fixed step size α?

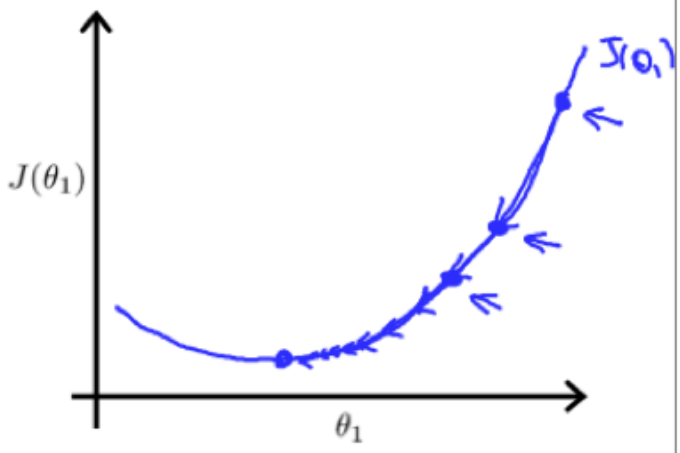
The intuition behind the convergence is that $\frac{d}{d\theta_1}J(\theta_1)$ approaches 0 as we approach the bottom of our convex function. At the minimum, the derivative will always be 0 and thus we get:

$$\theta_1 := \theta_1 - \alpha * 0$$

Gradient descent can converge to a local minimum, even with the learning rate α fixed.

$$\theta_1 := \theta_1 - \alpha \frac{d}{d\theta_1} J(\theta_1)$$

As we approach a local minimum, gradient descent will automatically take smaller steps. So, no need to decrease α over time.



Gradient Descent For Linear Regression

Note: [At 6:15 "h(x) = -900 - 0.1x" should be "h(x) = 900 - 0.1x"]

When specifically applied to the case of linear regression, a new form of the gradient descent equation can be derived. W substitute our actual cost function and our actual hypothesis function and modify the equation to :

repeat until convergence: {

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum^{m} (h_\theta(x_i) - y_i)$$

$$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^{m} \left((h_\theta(x_i) - y_i) x_i \right)$$

$$\}$$

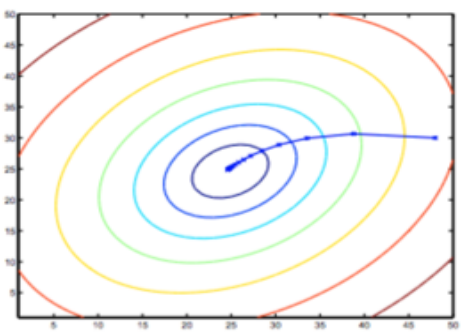
where m is the size of the training set, θ_0 a constant that will be changing simultaneously with θ_1 and x_i, y_i are values of given training set (data).

Note that we have separated out the two cases for θ_j into separate equations for θ_0 and θ_1; and that for θ_1 we are multiplying x_i at the end due to the derivative. The following is a derivation of $\frac{\partial}{\partial \theta_j} J(\theta)$ for a single example :

$$\begin{aligned}
\frac{\partial}{\partial \theta_j} J(\theta) &= \frac{\partial}{\partial \theta_j} \frac{1}{2} (h_\theta(x) - y)^2 \\
&= 2 \cdot \frac{1}{2} (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} (h_\theta(x) - y) \\
&= (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} \left(\sum_{i=0}^{n} \theta_i x_i - y \right) \\
&= (h_\theta(x) - y) \, x_j
\end{aligned}$$

The point of all this is that if we start with a guess for our hypothesis and then repeatedly apply these gradient desce equations, our hypothesis will become more and more accurate.

So, this is simply gradient descent on the original cost function J. This method looks at every example in the entire tra set on every step, and is called **batch gradient descent**. Note that, while gradient descent can be susceptible to local in general, the optimization problem we have posed here for linear regression has only one global, and no other local, optima; thus gradient descent always converges (assuming the learning rate α is not too large) to the global minimum Indeed, J is a convex quadratic function. Here is an example of gradient descent as it is run to minimize a quadratic fu



The ellipses shown above are the contours of a quadratic function. Also shown is the trajectory taken by gradient desc which was initialized at (48,30). The x's in the figure (joined by straight lines) mark the successive values of θ that grad descent went through as it converged to its minimum.

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minima

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Multiple Features

Note: [7:25 - θ^T is a 1 by (n+1) matrix and not an (n+1) by 1 matrix]

Linear regression with multiple variables is also known as "multivariate linear regression".

We now introduce notation for equations where we can have any number of input variables.

$$
\begin{aligned}
x_j^{(i)} &= \text{value of feature } j \text{ in the } i^{th} \text{ training example} \\
x^{(i)} &= \text{the input (features) of the } i^{th} \text{ training example} \\
m &= \text{the number of training examples} \\
n &= \text{the number of features}
\end{aligned}
$$

The multivariable form of the hypothesis function accommodating these multiple features is as follows:

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \cdots + \theta_n x_n$$

In order to develop intuition about this function, we can think about θ_0 as the basic price of a house, θ_1 as
per square meter, θ_2 as the price per floor, etc. x_1 will be the number of square meters in the house, x_2 th
of floors, etc.

Using the definition of matrix multiplication, our multivariable hypothesis function can be concisely repre

$$h_\theta(x) = \begin{bmatrix} \theta_0 & \theta_1 & \dots & \theta_n \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix} = \theta^T x$$

This is a vectorization of our hypothesis function for one training example; see the lessons on vectorizatio

Multiple features (variables).

Size (feet²) x_1	Number of bedrooms x_2	Number of floors x_3	Age of home (years) x_4	Price ($1000) y
2104	5	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178
...	...	...	...	...

$m = 47$

$x^{(2)} = \begin{bmatrix} 1416 \\ 3 \\ 2 \\ 40 \end{bmatrix}$

$x_3^{(2)} = 2$

Notation:

- n = number of features ($n = 4$)
- $x^{(i)}$ = input (features) of i^{th} training example.
- $x_j^{(i)}$ = value of feature j in i^{th} training example.

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$$

For convenience of notation, define $x_0 = 1$. ($x_0^{(i)} = 1$)

$x = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^{n+1}$ $\quad \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix} \in \mathbb{R}^{n+1}$

$h_\theta(x) = \theta_0 x_0 + \theta_1 x_1 + \cdots + \theta_n x_n$ ($x_0 = 1$)

$= \theta^T x$.

θ^T: $(n+1) \times 1$ matrix

$\theta^T x$

$x_0 = 1$

hould be ---> 1X(n+1)
theta^TϑT is a 1 by (n+1) matrix and not an (n+1) by 1
atrix]

more.

Gradient Descent for Multiple Variables

The gradient descent equation itself is generally the same form; we just have to repeat it for our 'n' features:

repeat until convergence: {

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x_0^{(i)}$$

$$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x_1^{(i)}$$

$$\theta_2 := \theta_2 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x_2^{(i)}$$

...

}

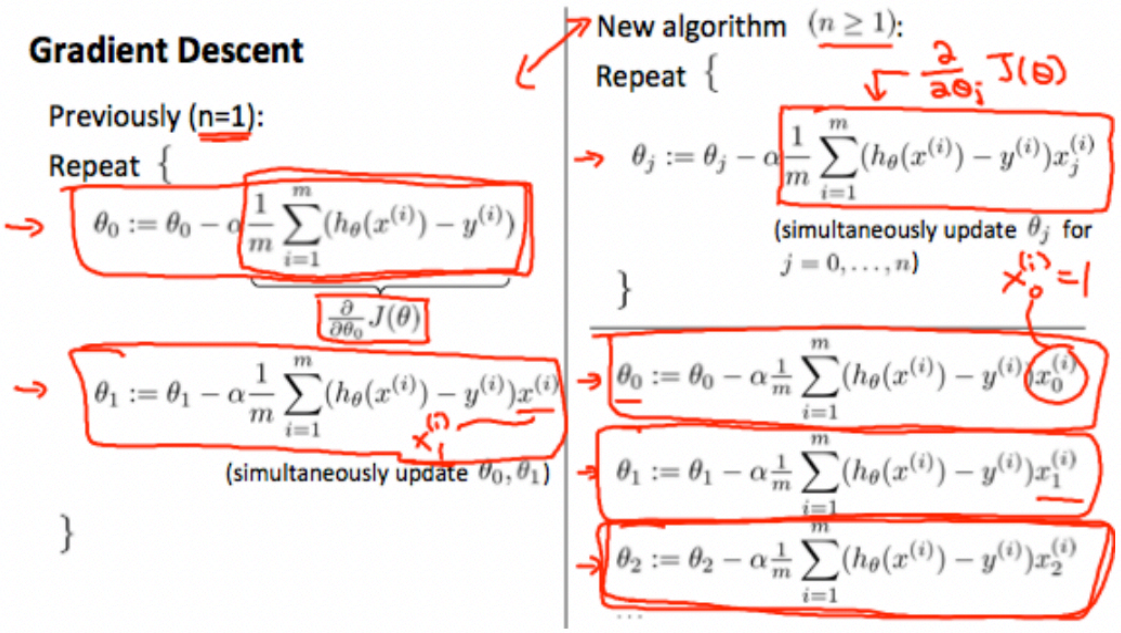
In other words:

repeat until convergence: {

$$\theta_j := \theta_j - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x_j^{(i)} \qquad \text{for j := 0...n}$$

}

The following image compares gradient descent with one variable to gradient descent with multiple variable



Hypothesis: $h_\theta(x) = \theta^T x = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$

Parameters: ~~$\theta_0, \theta_1, \ldots, \theta_n$~~ θ n+1 - dimensional vector

Cost function:

$$~~J(\theta_0, \theta_1, \ldots, \theta_n)~~ = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

$J(\theta)$

Gradient descent:

Repeat $\{$

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} ~~J(\theta_0, \ldots, \theta_n)~~ \; J(\theta)$$

$\}$

(simultaneously update for every $j = 0, \ldots, n$)

Gradient Descent in Practice I - Feature Scaling

Note: [6:20 - The average size of a house is 1000 but 100 is accidentally written instead]

We can speed up gradient descent by having each of our input values in roughly the same range. This is because θ wil descend quickly on small ranges and slowly on large ranges, and so will oscillate inefficiently down to the optimum when the variables are very uneven.

The way to prevent this is to modify the ranges of our input variables so that they are all roughly the same. Ideally:

$-1 \leq x_{(i)} \leq 1$

or

$-0.5 \leq x_{(i)} \leq 0.5$

These aren't exact requirements; we are only trying to speed things up. The goal is to get all input variables into roughly one of these ranges, give or take a few.

Two techniques to help with this are **feature scaling** and **mean normalization**. Feature scaling involves dividing the input values by the range (i.e. the maximum value minus the minimum value) of the input variable, resulting in a new range of just 1. Mean normalization involves subtracting the average value for an input variable from the values for th input variable resulting in a new average value for the input variable of just zero. To implement both of these techniques, adjust your input values as shown in this formula:

$$x_i := \frac{x_i - \mu_i}{s_i}$$

Where μ_i is the **average** of all the values for feature (i) and s_i is the range of values (max - min), or s_i is the standard deviation.

Note that dividing by the range, or dividing by the standard deviation, give different results. The quizzes in this course use range - the programming exercises use standard deviation.

For example, if x_i represents housing prices with a range of 100 to 2000 and a mean value of 1000, then, $x_i := \frac{price - 1000}{1900}$.

Gradient Descent in Practice II - Learning Rate

Note: [5:20 - the x -axis label in the right graph should be θ rather than No. of iterations]

Debugging gradient descent. Make a plot with *number of iterations* on the x-axis. Now plot the cost function, J(θ the number of iterations of gradient descent. If J(θ) ever increases, then you probably need to decrease α.

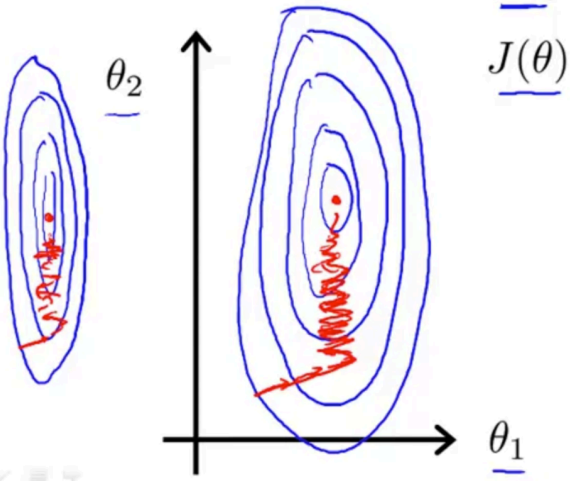
Automatic convergence test. Declare convergence if J(θ) decreases by less than E in one iteration, where E is sor

Feature Scaling

Idea: Make sure features are on a similar scale.

E.g. x_1 = size (0-2000 feet^2)

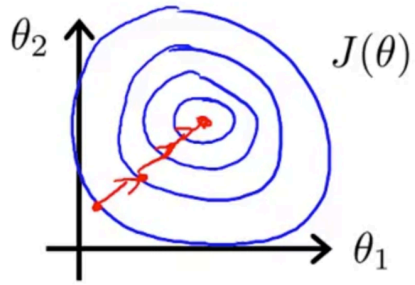
x_2 = number of bedrooms (1-5)



$$x_1 = \frac{\text{size (feet}^2)}{2000}$$

$$x_2 = \frac{\text{number of bedrooms}}{5}$$

$0 \le x_1 \le 1$ $\quad 0 \le x_2 \le 1$



Andrew N

Mean normalization

Replace x_i with $x_i - \mu_i$ to make features have approximately zero mean (Do not apply to $x_0 = 1$).

E.g. $x_1 = \frac{size - 1000}{2000}$

Average size = 1000

$x_2 = \frac{\#bedrooms - 2}{5}$

1-5 bedrooms

$-0.5 \le x_1 \le 0.5$ $\quad -0.5 \le x_2 \le 0.5$

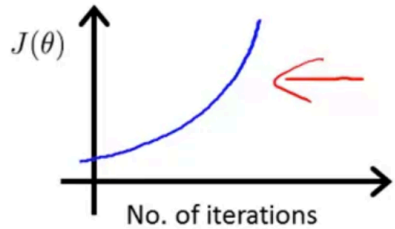
$x_1 \leftarrow \frac{x_1 - \mu_1}{s_1}$ $\quad x_2 \leftarrow \frac{x_2 - \mu_2}{s_2}$

μ_1: avg value of x_1 in training set

s_1: range (max - min) (or standard deviation)

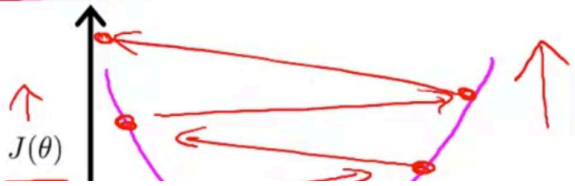
Andrew

Making sure gradient descent is working correctly.

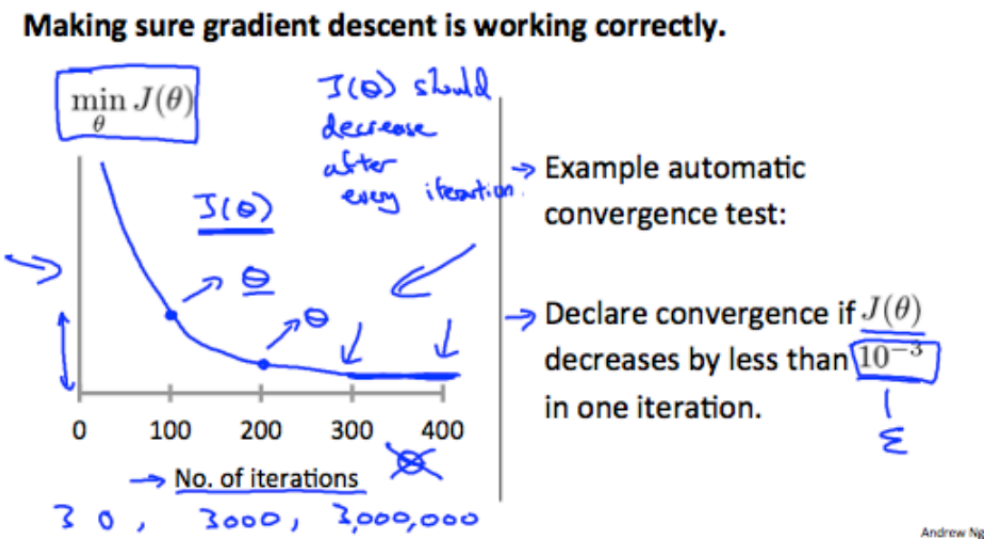


Gradient descent not working.

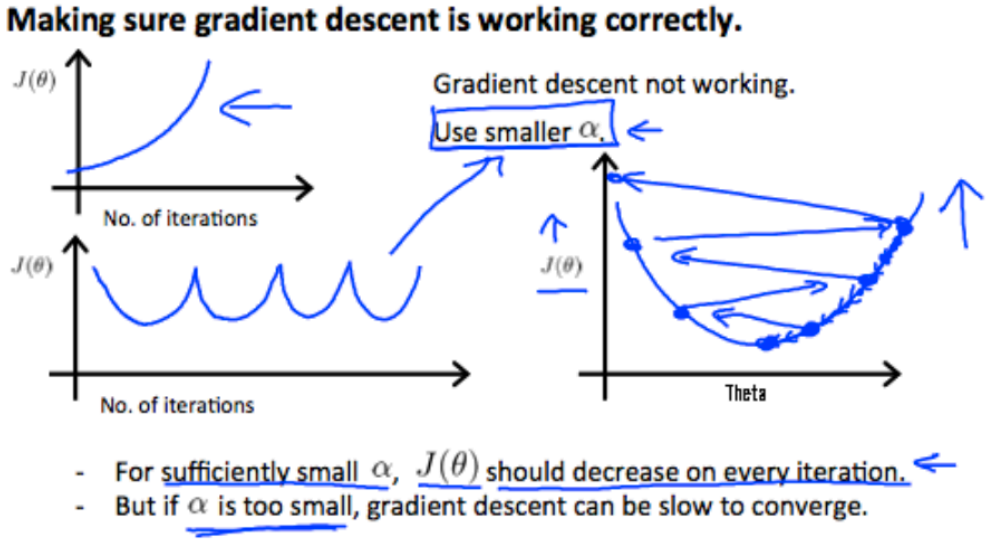
Use smaller α.



small value such as 10^{-3}. However in practice it's difficult to choose this threshold value.



It has been proven that if learning rate α is sufficiently small, then J(θ) will decrease on every iteration.



To summarize:

If α is too small: slow convergence.

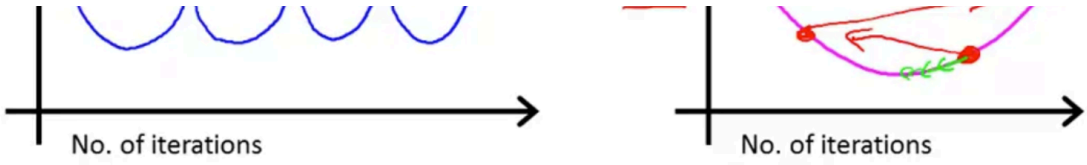
If α is too large: may not decrease on every iteration and thus may not converge.

Features and Polynomial Regression

We can improve our features and the form of our hypothesis function in a couple different ways.

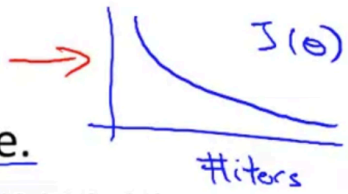
We can **combine** multiple features into one. For example, we can combine x_1 and x_2 into a new feature x_3 by tak
$x_1 \cdot x_2$.

Polynomial Regression



- For sufficiently small α, $J(\theta)$ should decrease on every iteration.
- But if α is too small, gradient descent can be slow to converge.

Summary:

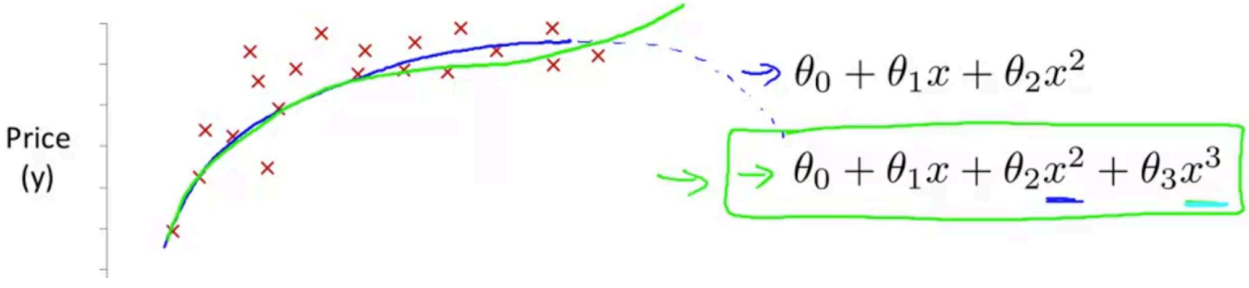


- If α is too small: slow convergence.
- If α is too large: $J(\theta)$ may not decrease on every iteration; may not converge. (Slow converge also possible)

To choose α, try

$$\ldots, 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1, \ldots$$

Polynomial regression



Polynomial Regression

Our hypothesis function need not be linear (a straight line) if that does not fit the data well.

We can **change the behavior or curve** of our hypothesis function by making it a quadratic, cubic or square root function (or any other form).

For example, if our hypothesis function is $h_\theta(x) = \theta_0 + \theta_1 x_1$ then we can create additional features based on x_1, to get the quadratic function $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_1^2$ or the cubic function $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^3$

In the cubic version, we have created new features x_2 and x_3 where $x_2 = x_1^2$ and $x_3 = x_1^3$.

To make it a square root function, we could do: $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 \sqrt{x_1}$

One important thing to keep in mind is, if you choose your features this way then feature scaling becomes very important.

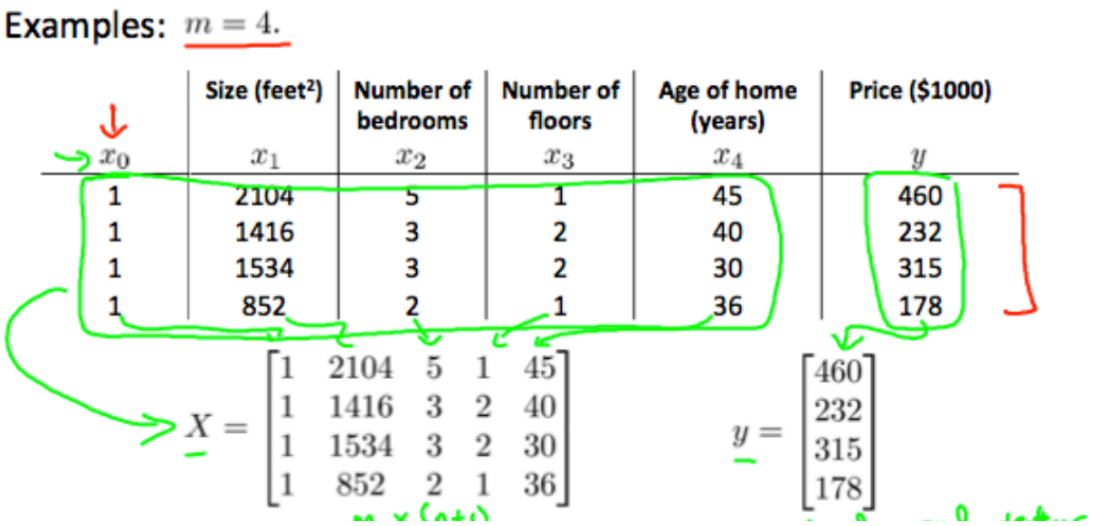
eg. if x_1 has range 1 - 1000 then range of x_1^2 becomes 1 - 1000000 and that of x_1^3 becomes 1 - 1000000000

Normal Equation

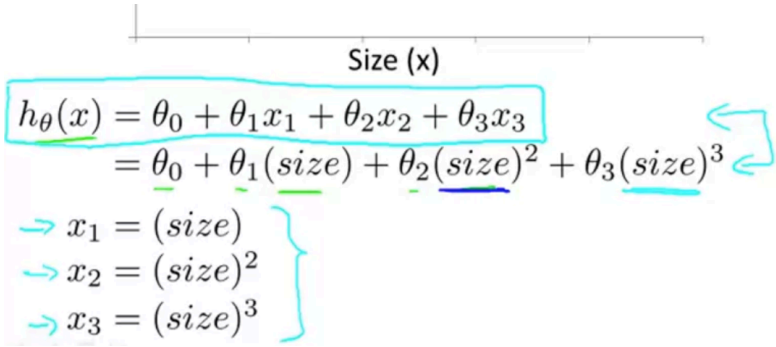
Note: [8:00 to 8:44 - The design matrix X (in the bottom right side of the slide) given in the example should have elements x with subscript 1 and superscripts varying from 1 to m because for all m training sets there are only 2 features x_0 and x_1. 12:56 - The X matrix is m by (n+1) and NOT n by n.]

Gradient descent gives one way of minimizing J. Let's discuss a second way of doing so, this time performing the minimization explicitly and without resorting to an iterative algorithm. In the "Normal Equation" method, we will minimize J by explicitly taking its derivatives with respect to the θj 's, and setting them to zero. This allows us to find the optimum theta without iteration. The normal equation formula is given below:

$$\theta = (X^T X)^{-1} X^T y$$



x_1, to



$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3$$
$$= \theta_0 + \theta_1(size) + \theta_2(size)^2 + \theta_3(size)^3$$

$x_1 = (size)$
$x_2 = (size)^2$
$x_3 = (size)^3$

Size: 1 - 1000
$Size^2$: 1 - 1000,000
$Size^3$: 1 - 10^9

Examples: $m = 4$.

x_0	Size (feet²) x_1	Number of bedrooms x_2	Number of floors x_3	Age of home (years) x_4	Price ($1000) y
1	2104	5	1	45	460
1	1416	3	2	40	232
1	1534	3	2	30	315
1	852	2	1	36	178

$$X = \begin{bmatrix} 1 & 2104 & 5 & 1 & 45 \\ 1 & 1416 & 3 & 2 & 40 \\ 1 & 1534 & 3 & 2 & 30 \\ 1 & 852 & 2 & 1 & 36 \end{bmatrix} \quad m \times (n+1)$$

$$y = \begin{bmatrix} 460 \\ 232 \\ 315 \\ 178 \end{bmatrix} \quad m\text{-dimensional vector}$$

$$\theta = (X^T X)^{-1} X^T y$$

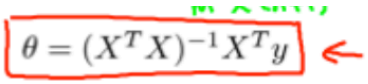
m training examples, n features.

Gradient Descent

- Need to choose α.
- Needs many iterations.
- Works well even when n is large.

Normal Equation

- No need to choose α.
- Don't need to iterate.
- Need to compute $(X^T X)^{-1}$ $n \times n$ $O(n^3)$



There is **no need** to do feature scaling with the normal equation.

The following is a comparison of gradient descent and the normal equation:

Gradient Descent	Normal Equation
Need to choose alpha	No need to choose alpha
Needs many iterations	No need to iterate
O (kn^2)	O (n^3), need to calculate inverse of $X^T X$
Works well when n is large	Slow if n is very large

With the normal equation, computing the inversion has complexity $\mathcal{O}(n^3)$. So if we have a very large numb features, the normal equation will be slow. In practice, when n exceeds 10,000 it might be a good time to go f normal solution to an iterative process.

Normal Equation Noninvertibility

When implementing the normal equation in octave we want to use the 'pinv' function rather than 'inv.' The function will give you a value of θ even if $X^T X$ is not invertible.

If $X^T X$ is **noninvertible,** the common causes might be having :

- Redundant features, where two features are very closely related (i.e. they are linearly dependent)
- Too many features (e.g. m ≤ n). In this case, delete some features or use "regularization" (to be explai later lesson).

Solutions to the above problems include deleting a feature that is linearly dependent with another or delet more features when there are too many features.

Classification

Classification

To attempt classification, one method is to use linear regression and map all predictions greater than 0.5 as a less than 0.5 as a 0. However, this method doesn't work well because classification is not actually a linear fur

$n = 10^6$

- Slow if n is very large.

$n = 100$
$n = 1000$
$\cdots$ $n = 10000$

What if $X^T X$ is non-invertible?

- Redundant features (linearly dependent).
  E.g. x_1 = size in feet^2
  ~~x_2 = size in m^2~~
  $x_1 = (3.28)^2 x_2$

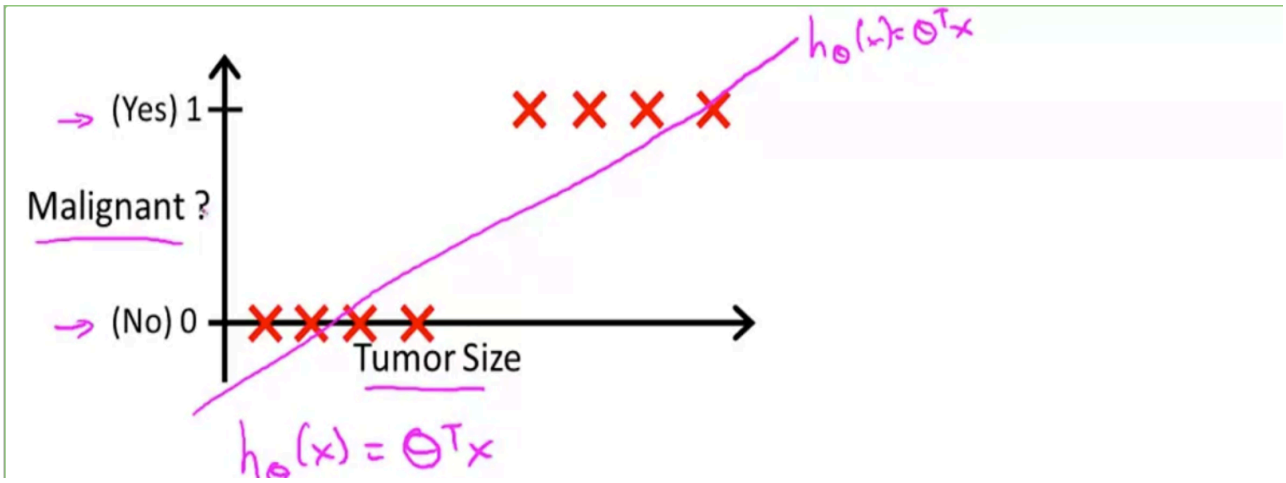
  $1\,m = 3.28$ feet

  $\rightarrow m = 10$
  $\rightarrow n = 100$

  $\theta \in \mathbb{R}^{101}$

- Too many features (e.g. $m \leq n$).
  - Delete some features, or use regularization.

  ↓ later



The classification problem is just like the regression problem, except that the values we now want to predict only a small number of discrete values. For now, we will focus on the **binary classification problem** in which take on only two values, 0 and 1. (Most of what we say here will also generalize to the multiple-class case.) Fo if we are trying to build a spam classifier for email, then $x^{(i)}$ may be some features of a piece of email, and y it is a piece of spam mail, and 0 otherwise. Hence, y∈{0,1}. 0 is also called the negative class, and 1 the positiv and they are sometimes also denoted by the symbols "-" and "+." Given $x^{(i)}$, the corresponding $y^{(i)}$ is also c label for the training example.

Hypothesis Representation

We could approach the classification problem ignoring the fact that y is discrete-valued, and use our old linea regression algorithm to try to predict y given x. However, it is easy to construct examples where this method very poorly. Intuitively, it also doesn't make sense for $h_\theta(x)$ to take values larger than 1 or smaller than 0 wh know that y ∈ {0, 1}. To fix this, let's change the form for our hypotheses $h_\theta(x)$ to satisfy $0 \leq h_\theta(x) \leq 1$. T accomplished by plugging $\theta^T x$ into the Logistic Function.

Our new form uses the "Sigmoid Function," also called the "Logistic Function":

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

$$z = \theta^T x$$

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

The following image shows us what the sigmoid function looks like:

→ Threshold classifier output $h_\theta(x)$ at 0.5:

If $h_\theta(x) \geq 0.5$, predict "y = 1"

If $h_\theta(x) < 0.5$, predict "y = 0"

Classification: y = 0 or 1

$h_\theta(x)$ can be > 1 or < 0

Logistic Regression: $0 \leq h_\theta(x) \leq 1$

(Classification)

Logistic Regression Model

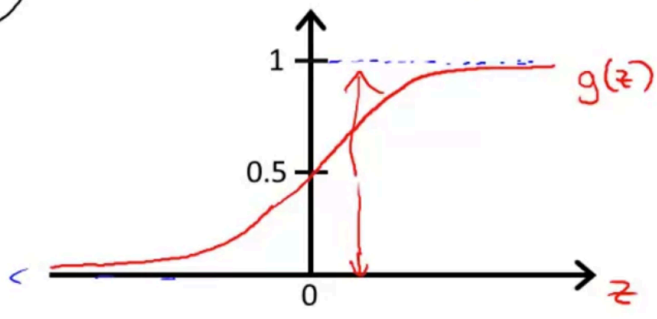
Want $0 \leq h_\theta(x) \leq 1$

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

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

$z = \theta^T x$

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



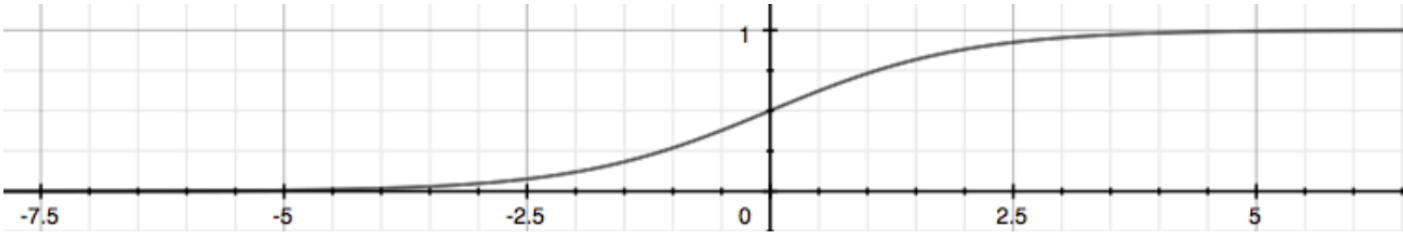
→ Sigmoid function

→ Logistic function

Parameters θ.

Interpretation of Hypothesis Output $h_\theta(x)$

$h_\theta(x)$ = estimated probability that y = 1 on input x



The function g(z), shown here, maps any real number to the (0, 1) interval, making it useful for transforming a arbitrary-valued function into a function better suited for classification.

$h_\theta(x)$ will give us the **probability** that our output is 1. For example, $h_\theta(x) = 0.7$ gives us a probability of 7 our output is 1. Our probability that our prediction is 0 is just the complement of our probability that it is 1 (e probability that it is 1 is 70%, then the probability that it is 0 is 30%).

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

Decision Boundary

Decision Boundary

In order to get our discrete 0 or 1 classification, we can translate the output of the hypothesis function as follo

$$h_\theta(x) \geq 0.5 \rightarrow y = 1$$
$$h_\theta(x) < 0.5 \rightarrow y = 0$$

The way our logistic function g behaves is that when its input is greater than or equal to zero, its output is gre or equal to 0.5:

$$g(z) \geq 0.5$$
$$when\ z \geq 0$$

Remember.

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

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

$h_\theta(x)$ – estimated probability that $y = 1$ on input x

Example: If $x = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ \text{tumorSize} \end{bmatrix}$

$h_\theta(x) = 0.7$ $\quad y=1$

Tell patient that 70% chance of tumor being malignant

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

$y = 0$ or 1

"probability that y = 1, given x, parameterized by θ"

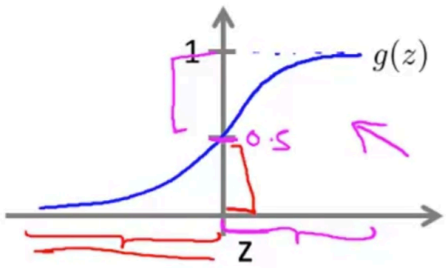
$\rightarrow P(y=0|x;\theta) + P(y=1|x;\theta) = 1$

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

Logistic regression

$\rightarrow h_\theta(x) = g(\theta^T x) = P(y=1|x;\theta)$

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



Suppose predict "$y = 1$" if $h_\theta(x) \geq 0.5$

$\theta^T x \geq 0$

$g(z) \geq 0.5$ when $z \geq 0$

$h_\theta(x) = g(\theta^T x) \geq 0.5$ whenever $\theta^T x \geq 0$

predict "$y = 0$" if $h_\theta(x) \leq 0.5$

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

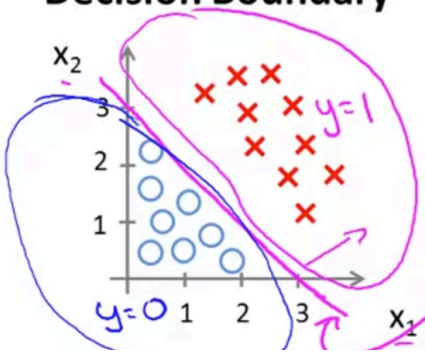
$\theta^T x < 0$

$g(z) < 0.5$

Andrew Ng

Decision Boundary

$\theta = \begin{bmatrix} -3 \\ 1 \\ 1 \end{bmatrix}$



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

$-3 \quad 1 \quad 1$

Decision boundary

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

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 hyp function.

Example:

$$\theta = \begin{bmatrix} 5 \\ -1 \\ 0 \end{bmatrix}$$
$$y = 1\ if\ 5 + (-1)x_1 + 0x_2 \geq 0$$
$$5 - x_1 \geq 0$$
$$-x_1 \geq -5$$
$$x_1 \leq 5$$

In this case, our decision boundary is a straight vertical line placed on the graph where $x_1 = 5$, and everythi left of that denotes y = 1, while everything to the right denotes y = 0.

Again, the input to the sigmoid function g(z) (e.g. $\theta^T X$) doesn't need to be linear, and could be a function tha describes a circle (e.g. $z = \theta_0 + \theta_1 x_1^2 + \theta_2 x_2^2$) or any shape to fit our data.

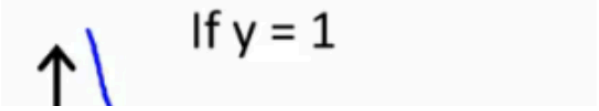
Cost Function

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

Instead, our cost function for logistic regression looks like:

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \text{Cost}(h_\theta(x^{(i)}), y^{(i)})$$
$$\text{Cost}(h_\theta(x), y) = -\log(h_\theta(x)) \qquad \text{if y} = 1$$
$$\text{Cost}(h_\theta(x), y) = -\log(1 - h_\theta(x)) \qquad \text{if y} = 0$$

When y = 1, we get the following plot for $J(\theta)$ vs $h_\theta(x)$:



Predict "$y = 1$" if $-3 + x_1 + x_2 \geq 0$

$\theta^T x$

$x_1 + x_2 \geq 3$

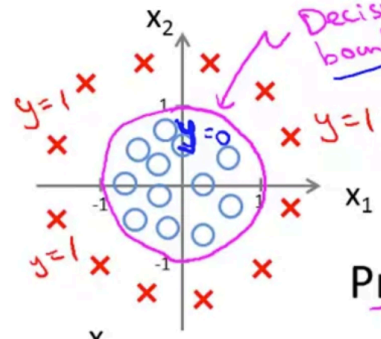
$h_\theta(x) = 0.5$

$x_1 + x_2 = 3$

$x_1 + x_2 < 3$

$y = 0$

Non-linear decision boundaries



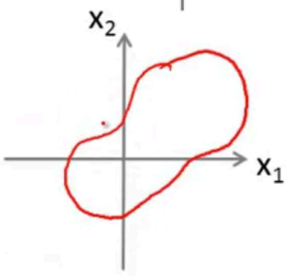
$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2)$$

$\theta = \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$

Predict "$y = 1$" if $-1 + x_1^2 + x_2^2 \geq 0$

$x_1^2 + x_2^2 = 1$

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



$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_1^2 x_2 + \theta_5 x_1^2 x_2^2 + \theta_6 x_1^3 x_2 + \dots)$$

Andrew Ng

Cost function

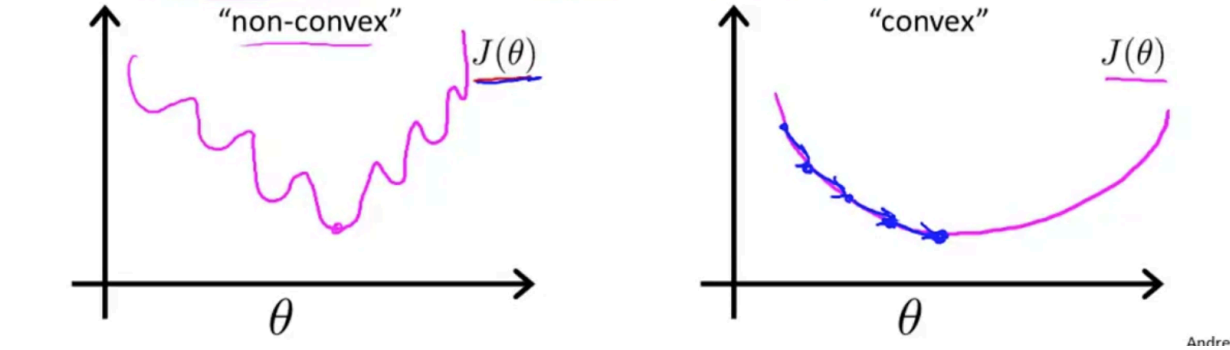
Linear regression: $J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \frac{1}{2} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$

Logistic

$\text{cost}(h_\theta(x^{(i)}), y)$

$\text{Cost}(h_\theta(x), y) = \frac{1}{2} \left(h_\theta(x) - y\right)^2$

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



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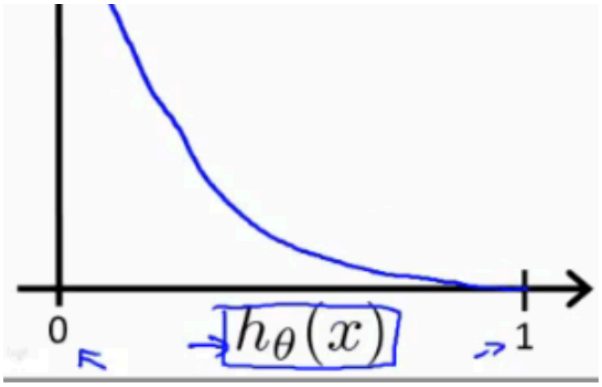
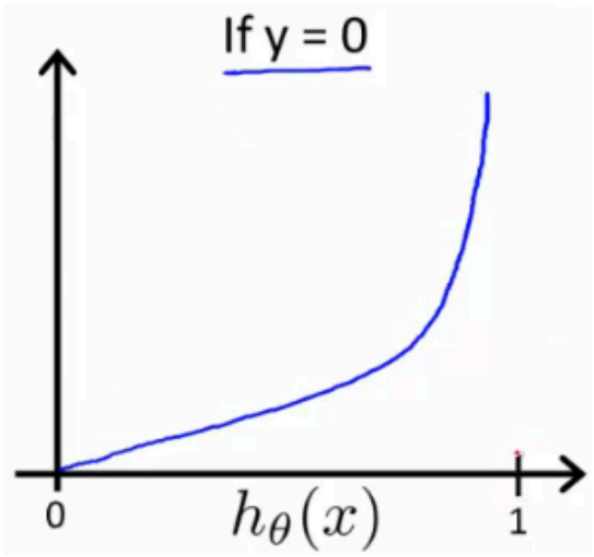
Logistic regression cost function



Similarly, when y = 0, we get the following plot for $J(\theta)$ vs $h_\theta(x)$:



$$\text{Cost}(h_\theta(x), y) = 0 \text{ if } h_\theta(x) = y$$
$$\text{Cost}(h_\theta(x), y) \to \infty \text{ if } y = 0 \text{ and } h_\theta(x) \to 1$$
$$\text{Cost}(h_\theta(x), y) \to \infty \text{ if } y = 1 \text{ and } h_\theta(x) \to 0$$

If our correct answer 'y' is 0, then the cost function will be 0 if our hypothesis function also outputs 0. If our
approaches 1, then the cost function will approach infinity.

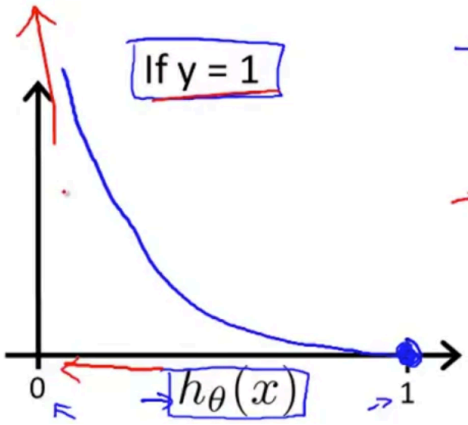
If our correct answer 'y' is 1, then the cost function will be 0 if our hypothesis function outputs 1. If our hypo
approaches 0, then the cost function will approach infinity.

Note that writing the cost function in this way guarantees that J(θ) is convex for logistic regression.

Simplified Cost Function and Gradient Descent

Logistic regression cost function

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



- $\text{Cost} = 0$ if $y = 1, h_\theta(x) = 1$
  But as $h_\theta(x) \to 0$
  $Cost \to \infty$
- Captures intuition that if $h_\theta(x) = 0$, (predict $P(y = 1|x; \theta) = 0$), but $y = 1$, we'll penalize learning algorithm by a very large cost.

hypothesis

othesis

Logistic regression cost function

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

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

Simplified Cost Function and Gradient Descent

Note: [6:53 - the gradient descent equation should have a 1/m factor]

We can compress our cost function's two conditional cases into one case:

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

Notice that when y is equal to 1, then the second term $(1 - y) \log(1 - h_\theta(x))$ will be zero and will not affec result. If y is equal to 0, then the first term $-y \log(h_\theta(x))$ will be zero and will not affect the result.

We can fully write out our entire cost function as follows:

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

A vectorized implementation is:

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

Gradient Descent

Remember that the general form of gradient descent is:

$$\begin{aligned} &Repeat \ \{ \\ &\quad \theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta) \\ &\} \end{aligned}$$

We can work out the derivative part using calculus to get:

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

Notice that this algorithm is identical to the one we used in linear regression. We still have to simultaneously values in theta.

A vectorized implementation is:

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

Note: $y = 0$ or 1 always

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

If $y=1$: $\text{Cost}(h_\theta(x), y) = -\log h_\theta(x)$

If $y=0$: $\text{Cost}(h_\theta(x), y) = -\log(1 - h_\theta(x))$

Logistic regression cost function

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

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

To fit parameters θ:

$$\min_\theta J(\theta)$$

Get θ

To make a prediction given new x:

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

$p(y=1 \mid x; \theta)$

Gradient Descent

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

Want $\min_\theta J(\theta)$:

$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix}$

Repeat {

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

(simultaneously update all θ_j)

}

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

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

Algorithm looks identical to linear regression!

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

Advanced Optimization

Note: [7:35 - '100' should be 100 instead. The value provided should be an integer and not a character string

"Conjugate gradient", "BFGS", and "L-BFGS" are more sophisticated, faster ways to optimize θ that can be us
of gradient descent. We suggest that you should not write these more sophisticated algorithms yourself (unl
an expert in numerical computing) but use the libraries instead, as they're already tested and highly optimiz
provides them.

We first need to provide a function that evaluates the following two functions for a given input value θ:

$$J(\theta)$$
$$\frac{\partial}{\partial \theta_j} J(\theta)$$

We can write a single function that returns both of these:

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

Then we can use octave's "fminunc()" optimization algorithm along with the "optimset()" function that crea
object containing the options we want to send to "fminunc()". (Note: the value for MaxIter should be an integ
character string - errata in the video at 7:30)

```
options = optimset('GradObj', 'on', 'MaxIter', 100);
initialTheta = zeros(2,1);
   [optTheta, functionVal, exitFlag] = fminunc(@costFunction, initialTheta, options);

```

We give to the function "fminunc()" our cost function, our initial vector of theta values, and the "options" ob
we created beforehand.

Multiclass Classification: One-vs-all

Now we will approach the classification of data when we have more than two categories. Instead of y = {0,1} we
expand our definition so that y = {0,1...n}.

Since y = {0,1...n}, we divide our problem into n+1 (+1 because the index starts at 0) binary classification proble

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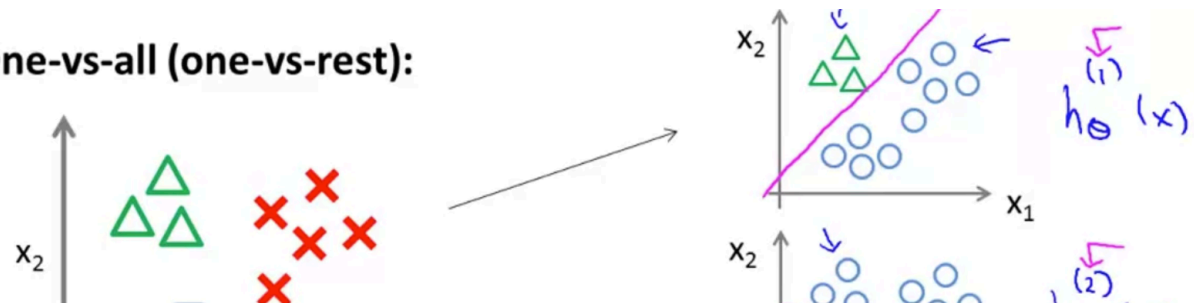
One-vs-all (one-vs-rest):



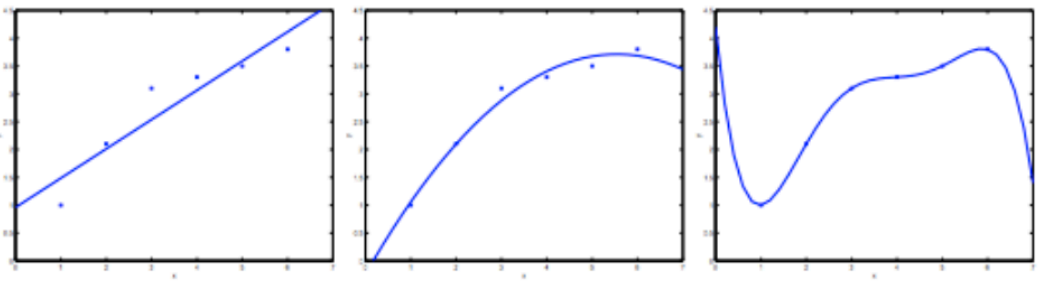
Since y = {0,1...n}, we divide our problem into n+1 (+1 because the index starts at 0) binary classification problem each one, we predict the probability that 'y' is a member of one of our classes.

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

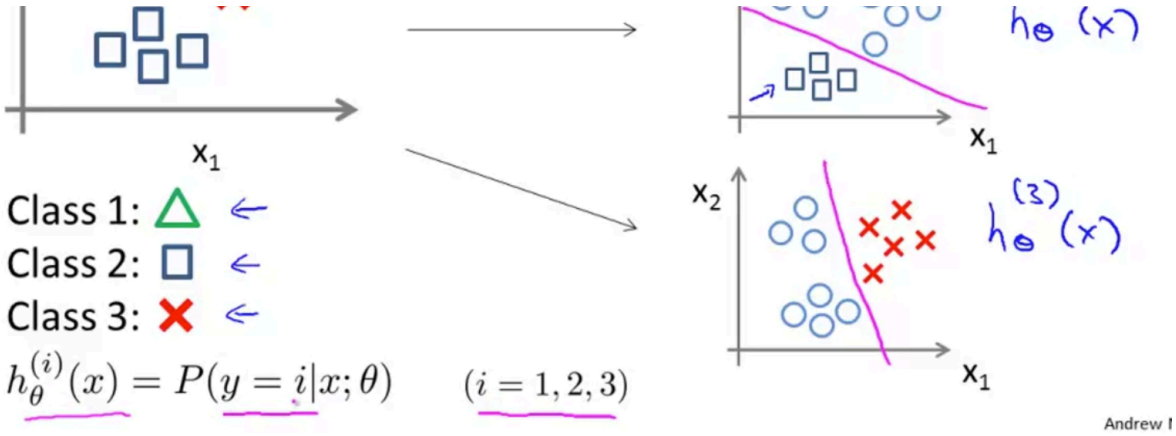
We are basically choosing one class and then lumping all the others into a single second class. We do this repea applying binary logistic regression to each case, and then use the hypothesis that returned the highest value as prediction.

The Problem of Overfitting

Consider the problem of predicting y from x ∈ R. The leftmost figure below shows the result of fitting a $y = \theta$ a dataset. We see that the data doesn't really lie on straight line, and so the fit is not very good.



Instead, if we had added an extra feature x^2 , and fit $y = \theta_0 + \theta_1 x + \theta_2 x^2$, then we obtain a slightly bet data (See middle figure). Naively, it might seem that the more features we add, the better. However, there is danger in adding too many features: The rightmost figure is the result of fitting a 5^{th} order polynomial $y = \sum_{j=0}^{5} \theta_j x^j$. We see that even though the fitted curve passes through the data perfectly, we would not exp



Andrew N

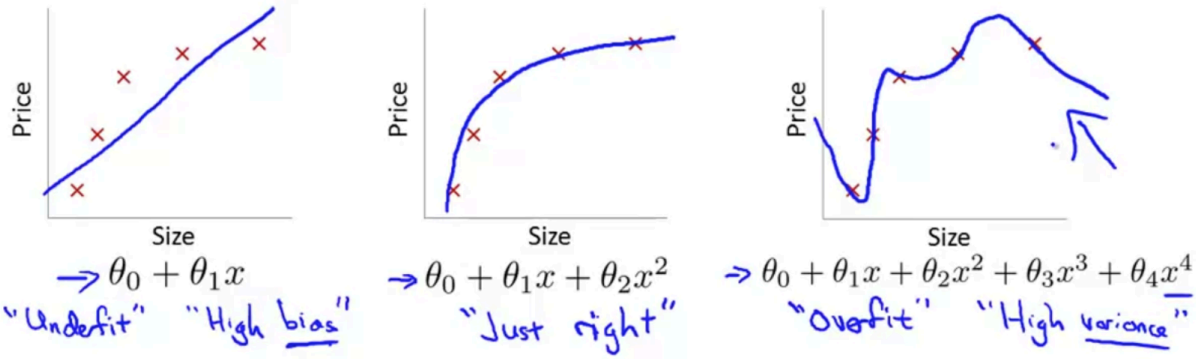
One-vs-all

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

$$\max_i h_\theta^{(i)}(x)$$

Example: Linear regression (housing prices)



$\rightarrow \theta_0 + \theta_1 x$ "Underfit" "High bias"

$\rightarrow \theta_0 + \theta_1 x + \theta_2 x^2$ "Just right"

$\rightarrow \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$ "Overfit" "High variance"

Overfitting: If we have too many features, the learned hypothesis may fit the training set very well ($J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 \approx 0$), but fail to generalize to new examples (predict prices on new examples).

Example: Logistic regression

be a very good predictor of, say, housing prices (y) for different living areas (x). Without formally defining wh
terms mean, we'll say the figure on the left shows an instance of **underfitting**—in which the data clearly sho
structure not captured by the model—and the figure on the right is an example of **overfitting**.

Underfitting, or high bias, is when the form of our hypothesis function h maps poorly to the trend of the dat
usually caused by a function that is too simple or uses too few features. At the other extreme, overfitting, or
variance, is caused by a hypothesis function that fits the available data but does not generalize well to predi
data. It is usually caused by a complicated function that creates a lot of unnecessary curves and angles unre
data.

> This terminology is applied to both linear and logistic regression. There are two main options to address the
> overfitting:
>
> 1) Reduce the number of features:
>
> - Manually select which features to keep.
> - Use a model selection algorithm (studied later in the course).
>
> 2) Regularization
>
> - Keep all the features, but reduce the magnitude of parameters θ_j.
> - Regularization works well when we have a lot of slightly useful features.

Cost Function

Note: [5:18 - There is a typo. It should be $\sum_{j=1}^{n} \theta_j^2$ instead of $\sum_{i=1}^{n} \theta_j^2$]

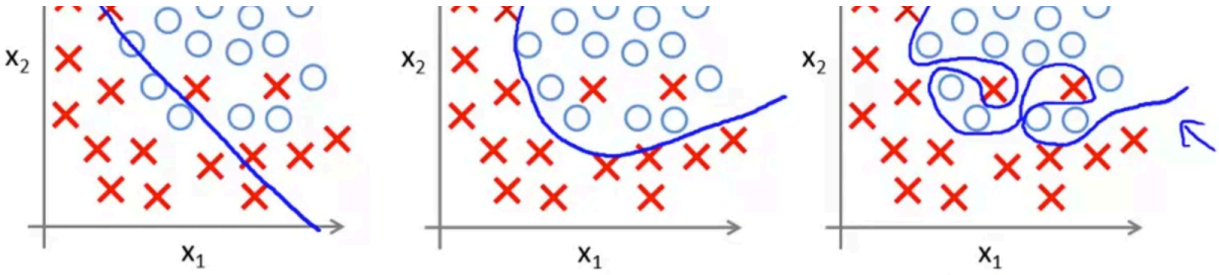
If we have overfitting from our hypothesis function, we can reduce the weight that some of the terms in our fu
carry by increasing their cost.

Say we wanted to make the following function more quadratic:

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

We'll want to eliminate the influence of $\theta_3 x^3$ and $\theta_4 x^4$. Without actually getting rid of these features or chan
form of our hypothesis, we can instead modify our **cost function**:

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



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

(g = sigmoid function)

"Underfit"

$g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2 + \theta_5 x_1 x_2)$

$g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 + \theta_5 x_1^2 x_2^3 + \theta_6 x_1^3 x_2 + \dots)$

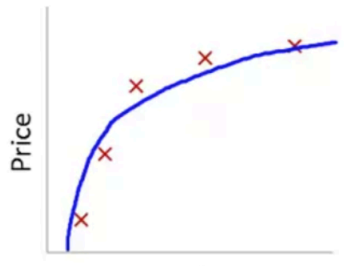
"Overfit"

Addressing overfitting:

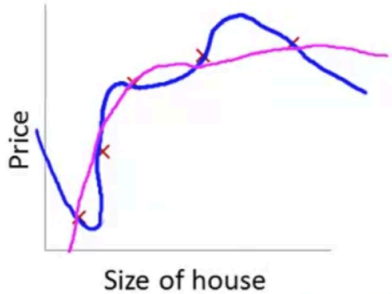
Options:

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

Intuition



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

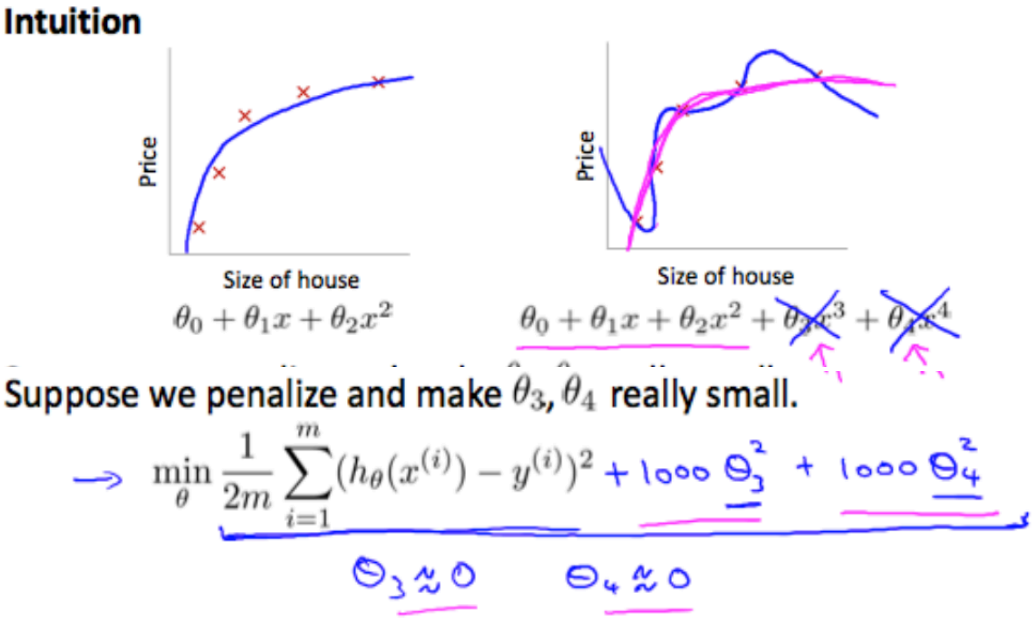


$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

Suppose we penalize and make θ_3, θ_4 really small.

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

We've added two extra terms at the end to inflate the cost of θ_3 and θ_4. Now, in order for the cost function to g to zero, we will have to reduce the values of θ_3 and θ_4 to near zero. This will in turn greatly reduce the values o and $\theta_4 x^4$ in our hypothesis function. As a result, we see that the new hypothesis (depicted by the pink curve) a quadratic function but fits the data better due to the extra small terms $\theta_3 x^3$ and $\theta_4 x^4$.



We could also regularize all of our theta parameters in a single summation as:

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

The λ, or lambda, is the **regularization parameter**. It determines how much the costs of our theta paramete inflated.

Using the above cost function with the extra summation, we can smooth the output of our hypothesis functi reduce overfitting. If lambda is chosen to be too large, it may smooth out the function too much and cause underfitting. Hence, what would happen if $\lambda = 0$ or is too small ?

Regularized Linear Regression

Note: [8:43 - It is said that X is non-invertible if m $\leq$ n. The correct statement should be that X is non-invertib and may be non-invertible if m = n.

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

Gradient Descent

We will modify our gradient descent function to separate out θ_0 from the rest of the parameters because we

Regularization.

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

Housing:
- Features: $x_1, x_2, \ldots, x_{100}$
- Parameters: $\theta_0, \theta_1, \theta_2, \ldots, \theta_{100}$

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

In regularized linear regression, we choose θ to minimize

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

What if λ is set to an extremely large value (perhaps for too large for our problem, say $\lambda = 10^{10}$)?

$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

$\theta_1, \theta_2, \theta_3, \theta_4 \approx 0$

$h_\theta(x) = \theta_0$

Gradient descent

Repeat {

$$\theta_0 := \theta_0 - \alpha \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha\left[\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)} + \frac{\lambda}{m}\theta_j\right] \quad (j = 1, 2, 3, \ldots, n)$$

}

We will modify our gradient descent function to separate out θ_0 from the rest of the parameters because we want to penalize θ_0.

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

The term $\frac{\lambda}{m}\theta_j$ performs our regularization. With some manipulation our update rule can also be represented

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

The first term in the above equation, $1 - \alpha\frac{\lambda}{m}$ will always be less than 1. Intuitively you can see it as reducin of θ_j by some amount on every update. Notice that the second term is now exactly the same as it was before

Normal Equation

Now let's approach regularization using the alternate method of the non-iterative normal equation.

To add in regularization, the equation is the same as our original, except that we add another term insid parentheses:

$$
\begin{aligned}
&\theta = \left(X^T X + \lambda \cdot L \right)^{-1} X^T y \\
&\text{where } \ L = \begin{bmatrix} 0 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix}
\end{aligned}
$$

L is a matrix with 0 at the top left and 1's down the diagonal, with 0's everywhere else. It should have dim (n+1)×(n+1). Intuitively, this is the identity matrix (though we are not including x_0), multiplied with a sin number λ.

Recall that if m < n, then $X^T X$ is non-invertible. However, when we add the term λ·L, then $X^T X$ + λ· invertible.

Regularized Logistic Regression

We can regularize logistic regression in a similar way that we regularize linear regression. As a result, we c overfitting. The following image shows how the regularized function, displayed by the pink line, is less lik

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

$1 - \alpha\frac{\lambda}{m} < 1$ 0.99 $\theta_j \times 0.99$

Non-invertibility (optional/advanced).

Suppose $m \leq n$,
(#examples) (#features)

$$\theta = (X^T X)^{-1} X^T y$$

non-invertible / singular

pinv inv

If $\lambda > 0$,

$$\theta = \left(X^T X + \lambda \begin{bmatrix} 0 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix} \right)^{-1} X^T y$$

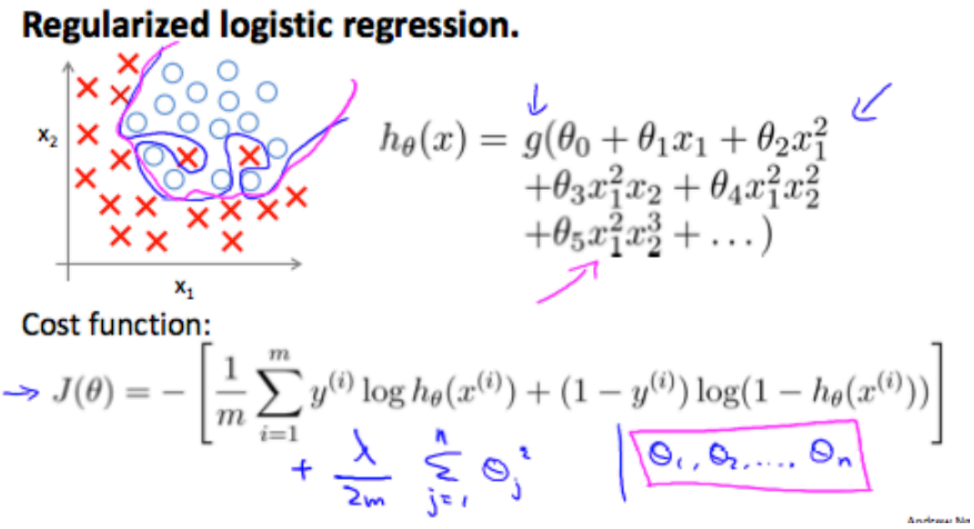
invertible.

Gradient descent

Repeat {

$$\theta_0 := \theta_0 - \alpha\frac{1}{m}\sum(h_\theta(x^{(i)}) - y^{(i)})x_0^{(i)}$$

overfitting. The following image shows how the regularized function, displayed by the pink line, is less ti
than the non-regularized function represented by the blue line:



Cost Function

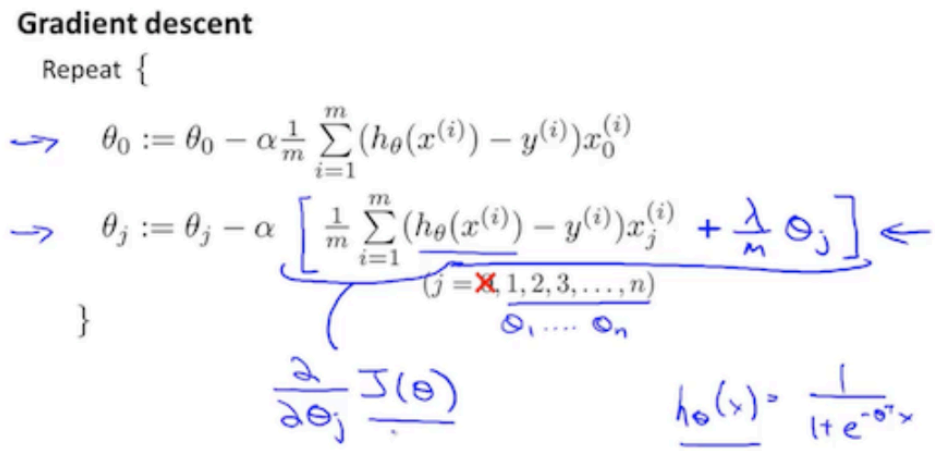
Recall that our cost function for logistic regression was:

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

We can regularize this equation by adding a term to the end:

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

The second sum, $\sum_{j=1}^{n} \theta_j^2$ **means to explicitly exclude** the bias term, θ_0. I.e. the θ vector is indexed from 0 t
(holding n+1 values, θ_0 through θ_n), and this sum explicitly skips θ_0, by running from 1 to n, skipping 0. Thus,
computing the equation, we should continuously update the two following equations:



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

$$(j = \cancel{0}, 1, 2, 3, \ldots, n)$$

$\theta_1 \ldots \theta_n$

$$\frac{\partial}{\partial \theta_j} J(\theta)$$

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

}

θ_j^2

o n

when