

o1 and o2: Introduction, Regression Analysis, and Gradient Descent

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Introduction to the course

- We will learn about
 - State of the art
 - How to do the implementation
- Applications of machine learning include
 - Search
 - Photo tagging
 - Spam filters
- The AI dream of building machines as intelligent as humans
 - Many people believe best way to do that is mimic how humans learn
- What the course covers
 - Learn about state of the art algorithms
 - But the algorithms and math alone are no good
 - Need to know how to get these to work in problems
- Why is ML so prevalent?
 - Grew out of AI
 - Build intelligent machines
 - You can program a machine how to do some simple thing
 - For the most part hard-wiring AI is too difficult
 - Best way to do it is to have some way for machines to learn things themselves
 - A mechanism for learning - if a machine can learn from input then it does the hard work for you

Examples

- Database mining
 - Machine learning has recently become so big partly because of the huge amount of data being generated
 - Large datasets from growth of automation web
 - Sources of data include
 - Web data (click-stream or click through data)
 - Mine to understand users better
 - Huge segment of silicon valley
 - Medical records
 - Electronic records -> turn records in knowledges
 - Biological data
 - Gene sequences, ML algorithms give a better understanding of human genome
 - Engineering info
 - Data from sensors, log reports, photos etc
- Applications that we cannot program by hand
 - Autonomous helicopter
 - Handwriting recognition
 - This is very inexpensive because when you write an envelope, algorithms can automatically route envelopes through the post
 - Natural language processing (NLP)
 - AI pertaining to language
 - Computer vision
 - AI pertaining vision
- Self customizing programs
 - Netflix
 - Amazon
 - iTunes genius
 - Take users info
 - Learn based on your behavior
- Understand human learning and the brain
 - If we can build systems that mimic (or try to mimic) how the brain works, this may push our own understanding of the associated neurobiology

What is machine learning?

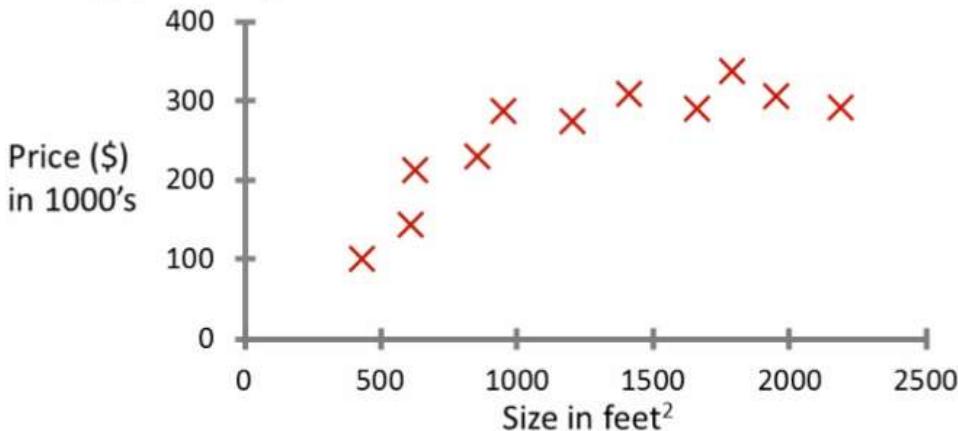
- Here we...
 - Define what it is

- When to use it
- Not a well defined definition
 - Couple of examples of how people have tried to define it
- Arthur Samuel (1959)
 - **Machine learning:** "Field of study that gives computers the ability to learn without being explicitly programmed"
 - Samuels wrote a checkers playing program
 - Had the program play 10000 games against itself
 - Work out which board positions were good and bad depending on wins/losses
- Tom Michel (1999)
 - **Well posed learning problem:** "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."
 - The checkers example,
 - E = 10000 games
 - T is playing checkers
 - P if you win or not
- Several types of learning algorithms
 - **Supervised learning**
 - Teach the computer how to do something, then let it use its new found knowledge to do it
 - **Unsupervised learning**
 - Let the computer learn how to do something, and use this to determine structure and patterns in data
 - Reinforcement learning
 - Recommender systems
- This course
 - Look at practical advice for applying learning algorithms
 - Learning a set of tools and **how** to apply them

Supervised learning - introduction

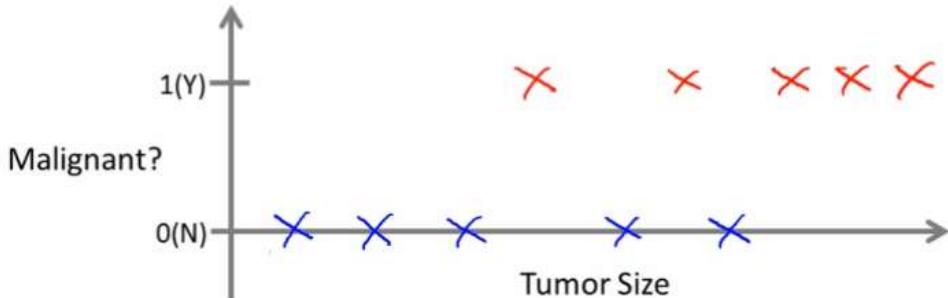
- Probably the most common problem type in machine learning
- Starting with an example
 - How do we predict housing prices
 - Collect data regarding housing prices and how they relate to size in feet

Housing price prediction.



- **Example problem:** "Given this data, a friend has a house 750 square feet - how much can they be expected to get?"
- What approaches can we use to solve this?
 - Straight line through data
 - Maybe \$150 000
 - Second order polynomial
 - Maybe \$200 000
 - One thing we discuss later - how to chose straight or curved line?
 - Each of these approaches represent a way of doing supervised learning
- **What does this mean?**
 - We gave the algorithm a data set where a "right answer" was provided
 - So we know actual prices for houses

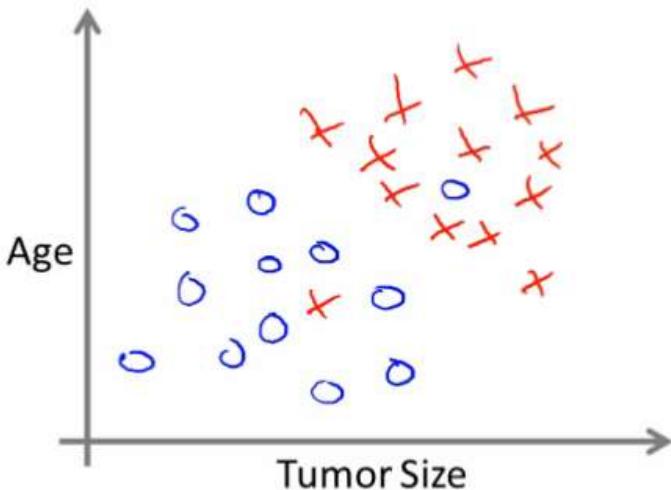
- The idea is we can learn what makes the price a certain value from the **training data**
- The algorithm should then produce more right answers based on new training data where we don't know the price already
 - i.e. predict the price
- We also call this a **regression problem**
 - Predict continuous valued output (price)
 - No real discrete delineation
- Another example
 - Can we define breast cancer as malignant or benign based on tumour size



- Looking at data
 - Five of each
 - Can you estimate prognosis based on tumor size?
 - This is an example of a **classification problem**
 - Classify data into one of two discrete classes - no in between, either malignant or not
 - In classification problems, can have a discrete number of possible values for the output
 - e.g. maybe have four values
 - 0 - benign
 - 1 - type 1
 - 2 - type 2
 - 3 - type 4
 - In classification problems we can plot data in a different way



- Use only one attribute (size)
 - In other problems may have multiple attributes
 - We may also, for example, know age and tumor size



- Then, when you have an individual with a specific tumor size and who is a specific age, you can hopefully use that information to place them into one of your classes
- You might have many features to consider
 - Clump thickness
 - Uniformity of cell size
 - Uniformity of cell shape
- The most exciting algorithms can deal with an infinite number of features
 - How do you deal with an infinite number of features?
 - Neat mathematical trick in support vector machine (which we discuss later)
 - If you have an infinitely long list - we can develop an algorithm to deal with that

- ***Summary***

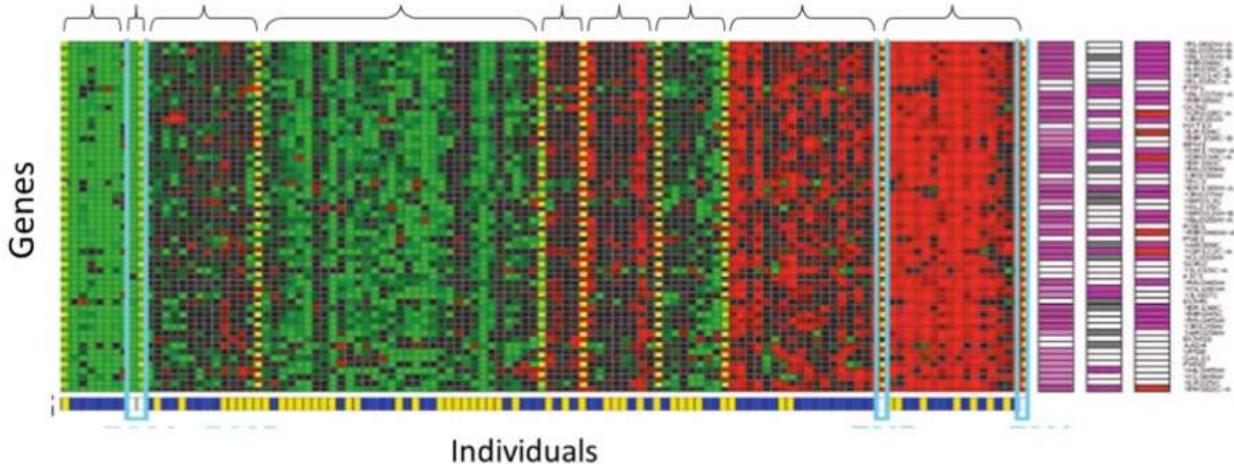
- Supervised learning lets you get the "right" data a
- Regression problem
- Classification problem

Unsupervised learning - introduction

- Second major problem type
- In unsupervised learning, we get unlabeled data
 - Just told - here is a data set, can you structure it
- One way of doing this would be to cluster data into groups
 - This is a **clustering algorithm**

Clustering algorithm

- Example of clustering algorithm
 - Google news
 - Groups news stories into cohesive groups
 - Used in any other problems as well
 - Genomics
 - Microarray data
 - Have a group of individuals
 - On each measure expression of a gene
 - Run algorithm to cluster individuals into types of people

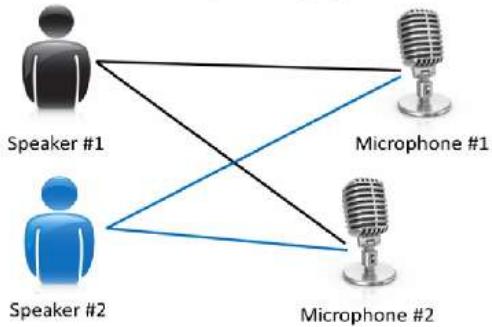


- Organize computer clusters
 - Identify potential weak spots or distribute workload effectively
- Social network analysis
 - Customer data
- Astronomical data analysis
 - Algorithms give amazing results
- Basically
 - Can you automatically generate structure
 - Because we don't give it the answer, it's unsupervised learning

Cocktail party algorithm

- Cocktail party problem
 - Lots of overlapping voices - hard to hear what everyone is saying
 - Two people talking
 - Microphones at different distances from speakers

Cocktail party problem



- Record slightly different versions of the conversation depending on where your microphone is
 - But overlapping none the less
- Have recordings of the conversation from each microphone
 - Give them to a cocktail party algorithm
 - Algorithm processes audio recordings
 - Determines there are two audio sources
 - Separates out the two sources
- Is this a very complicated problem
 - Algorithm can be done with one line of code!
 - `[W,s,v] = svd((repmat(sum(x.*x),1), size(x,1),1).*x)*x';`
 - Not easy to identify
 - But, programs can be short!
 - Using octave (or MATLAB) for examples
 - Often prototype algorithms in octave/MATLAB to test as it's very fast
 - Only when you show it works migrate it to C++
 - Gives a much faster agile development
- Understanding this algorithm
 - `svd` - linear algebra routine which is built into octave
 - In C++ this would be very complicated!
 - Shown that using MATLAB to prototype is a really good way to do this

Linear Regression

- Housing price data example used earlier
 - Supervised learning regression problem
- What do we start with?
 - Training set (this is your data set)
 - Notation (*used throughout the course*)
 - m = number of **training examples**
 - x's = input variables / features
 - y's = output variable "target" variables
 - (x,y) - single training example
 - (xⁱ, y^j) - specific example (ith training example)
 - i is an index to training set

Size in feet ² (x)	Price (\$) in 1000's (y)
2104	460
1416	232
1534	315
852	178
...	...

- With our training set defined - how do we used it?
 - Take training set
 - Pass into a learning algorithm

- Algorithm outputs a function (denoted h) ($h = \text{hypothesis}$)
 - This function takes an input (e.g. size of new house)
 - Tries to output the estimated value of Y
- How do we represent hypothesis h ?
 - Going to present h as;
 - $h_\theta(x) = \theta_0 + \theta_1 x$
 - $h(x)$ (shorthand)

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

- What does this mean?
 - Means Y is a linear function of x !
 - θ_i are **parameters**
 - θ_0 is zero condition
 - θ_1 is gradient
- This kind of function is a linear regression with one variable
 - Also called **univariate linear regression**
- So in summary
 - A hypothesis takes in some variable
 - Uses parameters determined by a learning system
 - Outputs a prediction based on that input

Linear regression - implementation (cost function)

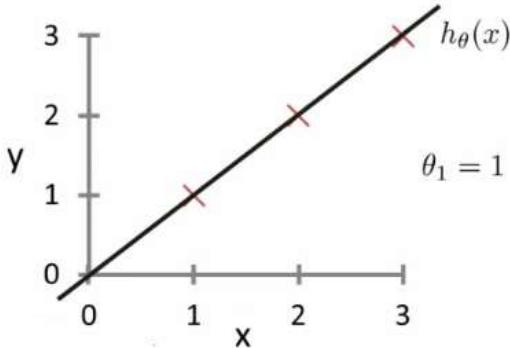
- A cost function lets us figure out how to fit the best straight line to our data
- Choosing values for θ_i (parameters)
 - Different values give you different functions
 - If θ_0 is 1.5 and θ_1 is 0 then we get straight line parallel with X along 1.5 @ y
 - If θ_1 is > 0 then we get a positive slope
- Based on our training set we want to generate parameters which make the straight line
 - Chosen these parameters so $h_\theta(x)$ is close to y for our training examples
 - Basically, uses xs in training set with $h_\theta(x)$ to give output which is as close to the actual y value as possible
 - Think of $h_\theta(x)$ as a "y imitator" - it tries to convert the x into y , and considering we already have y we can evaluate how well $h_\theta(x)$ does this
- To formalize this;
 - We want to solve a **minimization problem**
 - Minimize $(h_\theta(x) - y)^2$
 - i.e. minimize the difference between $h(x)$ and y for each/any/every example
 - Sum this over the training set

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

- Minimize squared difference between predicted house price and actual house price
 - $1/2m$
 - $1/m$ - means we determine the average
 - $1/2m$ the 2 makes the math a bit easier, and doesn't change the constants we determine at all (i.e. half the smallest value is still the smallest value!)
 - Minimizing θ_0/θ_1 means we get the values of θ_0 and θ_1 which find on average the minimal deviation of x from y when we use those parameters in our hypothesis function
 - More cleanly, this is a cost function

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

- And we want to minimize this cost function
 - Our cost function is (because of the summation term) inherently looking at ALL the data in the training set at any time
- So to recap
 - Hypothesis - is like your prediction machine, throw in an x value, get a putative y value



- Cost - is a way to, using your training data, determine values for your θ values which make the hypothesis as accurate as possible

$$\text{Minimize } J(\theta_0, \theta_1)$$

$\underbrace{\theta_0, \theta_1}_{\text{Cost Function}}$

- This cost function is also called the squared error cost function

- This cost function is reasonable choice for most regression functions
- Probably most commonly used function

- In case $J(\theta_0, \theta_1)$ is a bit abstract, going into what it does, why it works and how we use it in the coming sections

Cost function - a deeper look

- Lets consider some intuition about the cost function and why we want to use it
 - The cost function determines parameters
 - The value associated with the parameters determines how your hypothesis behaves, with different values generate different
- Simplified hypothesis
 - Assumes $\theta_0 = 0$

$$h_{\theta}(x) = \underline{\theta_1} x$$

$\theta_0 = 0$

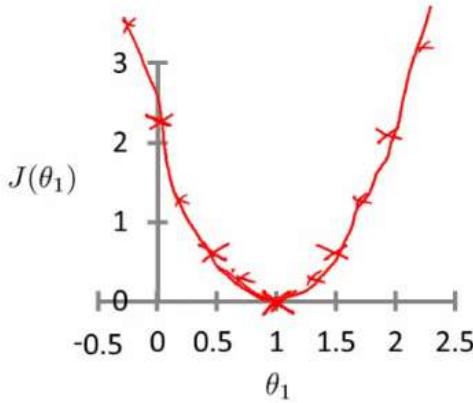
$$\underline{\theta_1}$$

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

$$\underset{\theta_1}{\text{minimize}} J(\theta_1)$$

- Cost function and goal here are very similar to when we have θ_0 , but with a simpler parameter
 - Simplified hypothesis makes visualizing cost function $J()$ a bit easier
- So hypothesis pass through 0,0
- Two key functions we want to understand
 - $h_{\theta}(x)$
 - Hypothesis is a function of x - function of what the size of the house is

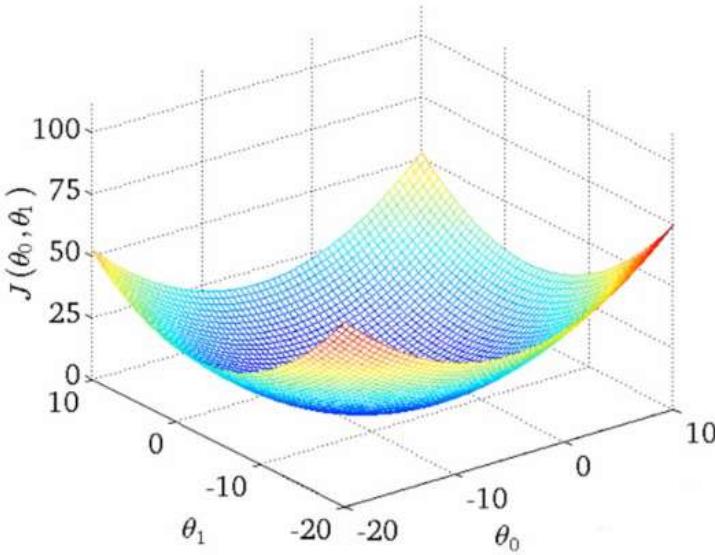
- $J(\theta_1)$
 - Is a function of the parameter of θ_1
- So for example
 - $\theta_1 = 1$
 - $J(\theta_1) = 0$
- Plot
 - θ_1 vs $J(\theta_1)$
 - Data
 - 1)
 - $\theta_1 = 1$
 - $J(\theta_1) = 0$
 - 2)
 - $\theta_1 = 0.5$
 - $J(\theta_1) = \sim 0.58$
 - 3)
 - $\theta_1 = 0$
 - $J(\theta_1) = \sim 2.3$
- If we compute a range of values plot
 - $J(\theta_1)$ vs θ_1 we get a polynomial (looks like a quadratic)



- The optimization objective for the learning algorithm is find the value of θ_1 which minimizes $J(\theta_1)$
 - So, here $\theta_1 = 1$ is the best value for θ_1

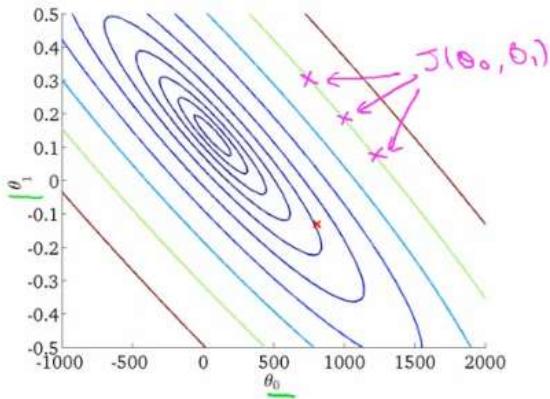
A deeper insight into the cost function - simplified cost function

- Assume you're familiar with contour plots or contour figures
 - Using same cost function, hypothesis and goal as previously
 - It's OK to skip parts of this section if you don't understand contour plots
- Using our original complex hypothesis with two variables,
 - So cost function is
 - $J(\theta_0, \theta_1)$
- Example,
 - Say
 - $\theta_0 = 50$
 - $\theta_1 = 0.06$
 - Previously we plotted our cost function by plotting
 - θ_1 vs $J(\theta_1)$
 - Now we have two parameters
 - Plot becomes a bit more complicated
 - Generates a 3D surface plot where axis are
 - X = θ_1
 - Z = θ_0
 - Y = $J(\theta_0, \theta_1)$



- We can see that the height (y) indicates the value of the cost function, so find where y is at a minimum
- Instead of a surface plot we can use a **contour figures/plots**
 - Set of ellipses in different colors
 - Each colour is the same value of $J(\theta_0, \theta_1)$, but obviously plot to different locations because θ_1 and θ_0 will vary
 - Imagine a bowl shape function coming out of the screen so the middle is the concentric circles

$J(\theta_0, \theta_1)$
(function of the parameters θ_0, θ_1)



- Each point (like the red one above) represents a pair of parameter values for θ_0 and θ_1
 - Our example here put the values at
 - $\theta_0 = \sim 800$
 - $\theta_1 = \sim -0.15$
 - Not a good fit
 - i.e. these parameters give a value on our contour plot far from the center
 - If we have
 - $\theta_0 = \sim 360$
 - $\theta_1 = 0$
 - This gives a better hypothesis, but still not great - not in the center of the countour plot
 - Finally we find the minimum, which gives the best hypothesis
- Doing this by eye/hand is a pain in the ass
 - What we really want is an efficient algorithm fro finding the minimum for θ_0 and θ_1

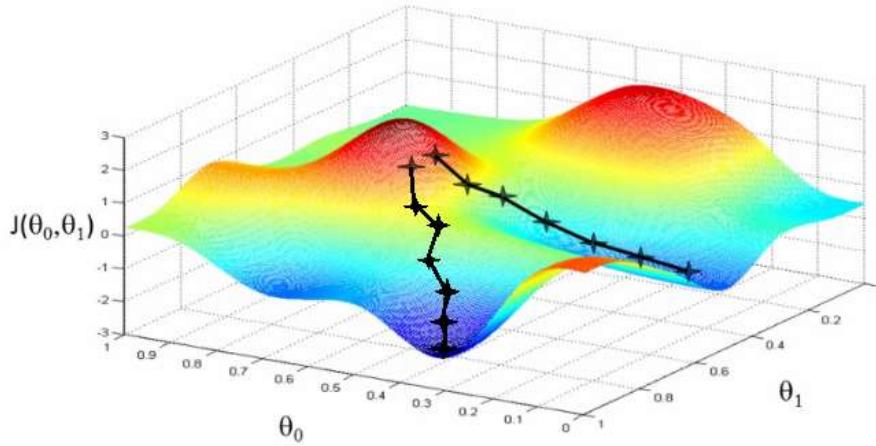
Gradient descent algorithm

- Minimize cost function J

- Gradient descent
 - Used all over machine learning for minimization
- Start by looking at a general $J()$ function
- Problem
 - We have $J(\theta_0, \theta_1)$
 - We want to get $\min J(\theta_0, \theta_1)$
- Gradient descent applies to more general functions
 - $J(\theta_0, \theta_1, \theta_2, \dots, \theta_n)$
 - $\min J(\theta_0, \theta_1, \theta_2, \dots, \theta_n)$

How does it work?

- Start with initial guesses
 - Start at $0,0$ (or any other value)
 - Keeping changing θ_0 and θ_1 a little bit to try and reduce $J(\theta_0, \theta_1)$
- Each time you change the parameters, you select the gradient which reduces $J(\theta_0, \theta_1)$ the most possible
- Repeat
- Do so until you converge to a local minimum
- Has an interesting property
 - Where you start can determine which minimum you end up



- Here we can see one initialization point led to one local minimum
- The other led to a different one

A more formal definition

- Do the following until convergence

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

- What does this all mean?
 - Update θ_j by setting it to $(\theta_j - \alpha)$ times the partial derivative of the cost function with respect to θ_j
- Notation
 - $:=$
 - Denotes assignment
 - NB $a = b$ is a *truth assertion*
 - α (alpha)
 - Is a number called the **learning rate**
 - Controls how big a step you take
 - If α is big have an aggressive gradient descent
 - If α is small take tiny steps

- Derivative term

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

- Not going to talk about it now, derive it later
- There is a subtlety about how this gradient descent algorithm is implemented
 - Do this for θ_0 and θ_1
 - For $j = 0$ and $j = 1$ means we **simultaneously** update both
 - How do we do this?
 - Compute the right hand side for both θ_0 and θ_1
 - So we need a temp value
 - Then, update θ_0 and θ_1 at the same time
 - We show this graphically below

```

temp0 :=  $\theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$ 
temp1 :=  $\theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$ 
 $\theta_0 := \text{temp0}$ 
 $\theta_1 := \text{temp1}$ 

```

- If you implement the non-simultaneous update it's not gradient descent, and will behave weirdly
 - But it might look sort of right - so it's important to remember this!

Understanding the algorithm

- To understand gradient descent, we'll return to a simpler function where we minimize one parameter to help explain the algorithm in more detail
 - $\min \theta_1 J(\theta_1)$ where θ_1 is a real number

- Two key terms in the algorithm

- Alpha
- Derivative term

- Notation nuances

- Partial derivative vs. derivative
 - Use partial derivative when we have multiple variables but only derive with respect to one
 - Use derivative when we are deriving with respect to all the variables

- Derivative term

$$\frac{\partial}{\partial \theta_j} J(\theta_1)$$

- Derivative says

- Lets take the tangent at the point and look at the slope of the line
- So moving towards the minimum (down) will create a negative derivative, alpha is always positive, so will update $j(\theta_1)$ to a smaller value
- Similarly, if we're moving up a slope we make $j(\theta_1)$ a bigger numbers

- Alpha term (α)

- What happens if alpha is too small or too large
- Too small
 - Take baby steps
 - Takes too long
- Too large
 - Can overshoot the minimum and fail to converge

- When you get to a local minimum

- Gradient of tangent/derivative is 0
- So derivative term = 0
- $\alpha * 0 = 0$
- So $\theta_1 = \theta_1 - 0$
- So θ_1 remains the same

- As you approach the global minimum the derivative term gets smaller, so your update gets smaller, even with alpha is fixed
 - Means as the algorithm runs you take smaller steps as you approach the minimum
 - So no need to change alpha over time

Linear regression with gradient descent

- Apply gradient descent to minimize the squared error cost function $J(\theta_0, \theta_1)$
- Now we have a partial derivative

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

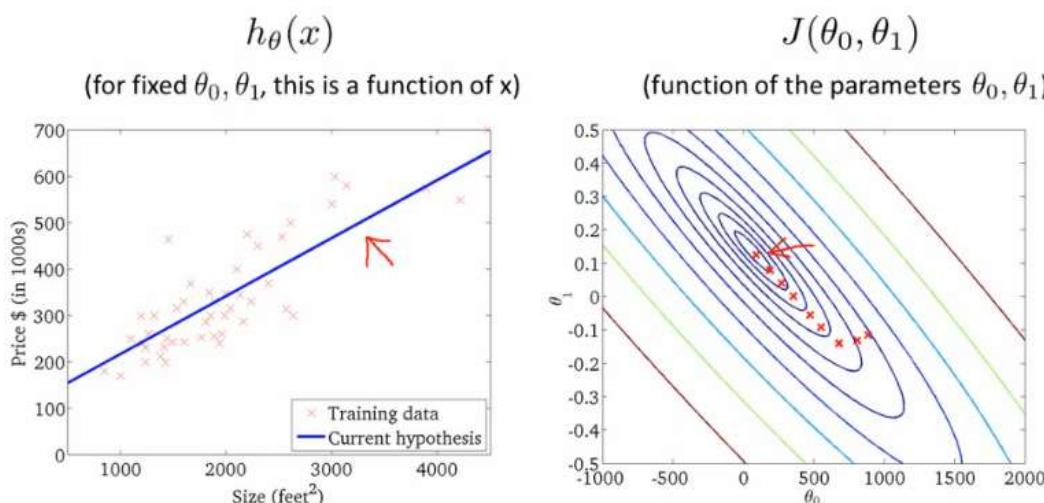
$$= \frac{2}{2m} \cdot \frac{1}{2m} \sum_{i=1}^m (\theta_0 + \theta_1 x^{(i)} - y^{(i)})^2$$

- So here we're just expanding out the first expression
 - $J(\theta_0, \theta_1) = 1/2m \dots$
 - $h_\theta(x) = \theta_0 + \theta_1 * x$
- So we need to determine the derivative for each parameter - i.e.
 - When $j = 0$
 - When $j = 1$
- Figure out what this partial derivative is for the θ_0 and θ_1 case
 - When we derive this expression in terms of $j = 0$ and $j = 1$ we get the following

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

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

- To check this you need to know multivariate calculus
 - So we can plug these values back into the gradient descent algorithm
- How does it work
 - Risk of meeting different local optimum
 - The linear regression cost function is always a **convex function** - always has a single minimum
 - Bowl shaped
 - One global optima
 - So gradient descent will always converge to global optima
 - In action
 - Initialize values to
 - $\theta_0 = 900$
 - $\theta_1 = -0.1$



- End up at a global minimum
- This is actually **Batch Gradient Descent**
 - Refers to the fact that over each step you look at all the training data
 - Each step compute over m training examples
 - Sometimes non-batch versions exist, which look at small data subsets

- We'll look at other forms of gradient descent (to use when m is too large) later in the course
- There exists a numerical solution for finding a solution for a minimum function
 - **Normal equations** method
 - Gradient descent scales better to large data sets though
 - Used in lots of contexts and machine learning

What's next - important extensions

Two extension to the algorithm

- **1) Normal equation for numeric solution**
 - To solve the minimization problem we can solve it [$\min J(\theta_0, \theta_1)$] exactly using a numeric method which avoids the iterative approach used by gradient descent
 - Normal equations method
 - Has advantages and disadvantages
 - Advantage
 - No longer an alpha term
 - Can be much faster for some problems
 - Disadvantage
 - Much more complicated
 - We discuss the normal equation in the **linear regression with multiple features** section
- **2) We can learn with a larger number of features**
 - So may have other parameters which contribute towards a prize
 - e.g. with houses
 - Size
 - Age
 - Number bedrooms
 - Number floors
 - x_1, x_2, x_3, x_4
 - With multiple features becomes hard to plot
 - Can't really plot in more than 3 dimensions
 - Notation becomes more complicated too
 - Best way to get around with this is the notation of linear algebra
 - Gives notation and set of things you can do with matrices and vectors
 - e.g. Matrix

$$X = \begin{bmatrix} 2104 & 5 & 1 & 45 \\ 1416 & 3 & 2 & 40 \\ 1534 & 3 & 2 & 30 \\ 852 & 2 & 1 & 36 \end{bmatrix} \quad y = \begin{bmatrix} 460 \\ 232 \\ 315 \\ 172 \end{bmatrix}$$

- We see here this matrix shows us
 - Size
 - Number of bedrooms
 - Number floors
 - Age of home
- All in one variable
 - Block of numbers, take all data organized into one big block
- Vector
 - Shown as y
 - Shows us the prices
- Need linear algebra for more complex linear regression models
- Linear algebra is good for making computationally efficient models (as seen later too)
 - Provide a good way to work with large sets of data sets
 - Typically vectorization of a problem is a common optimization technique