

# 01 and 02: 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?

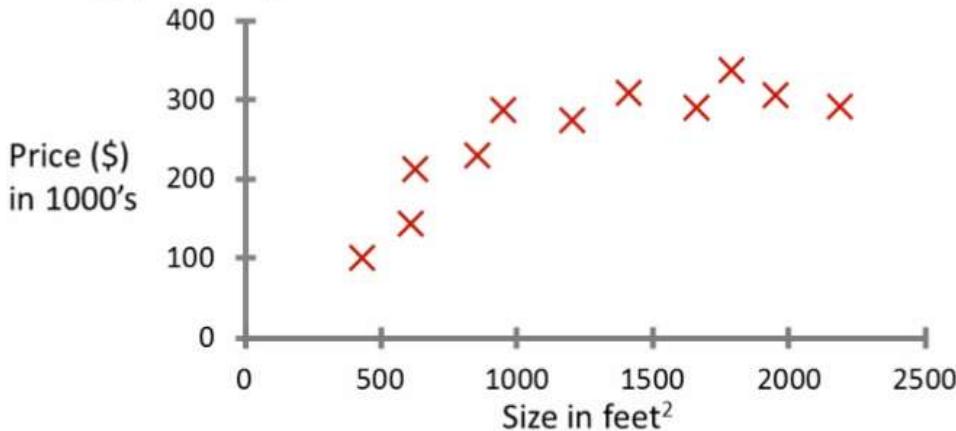
- Here we...
  - Define what it is

- 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

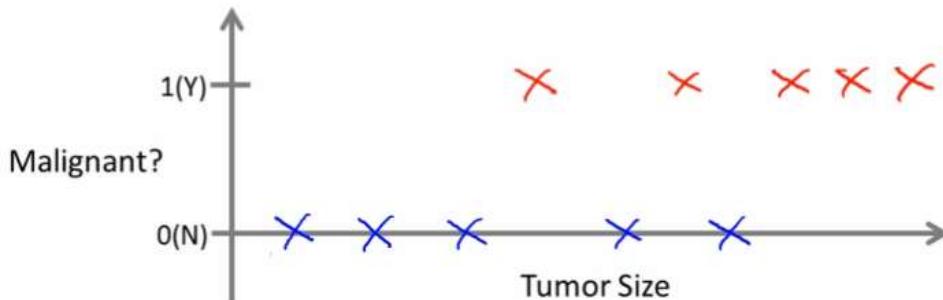
- Probably the most common problem type in machine learning
- Starting with an example
  - How do we predict housing prices
    - Collect data regarding housing prices and how they relate to size in feet

## 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

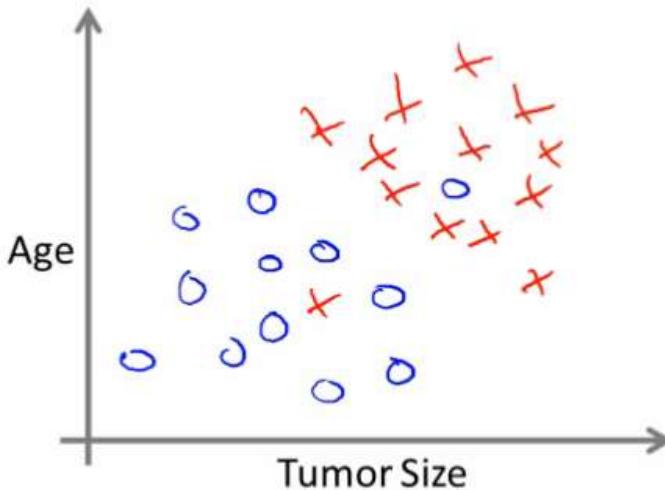
- The idea is we can learn what makes the price a certain value from the **training data**
- The algorithm should then produce more right answers based on new training data where we don't know the price already
  - i.e. predict the price
- We also call this a **regression problem**
  - Predict continuous 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



- Based on that data, you can try and define separate classes by
  - Drawing a straight line between the two groups
  - Using a more complex function to define the two groups (which we'll discuss later)

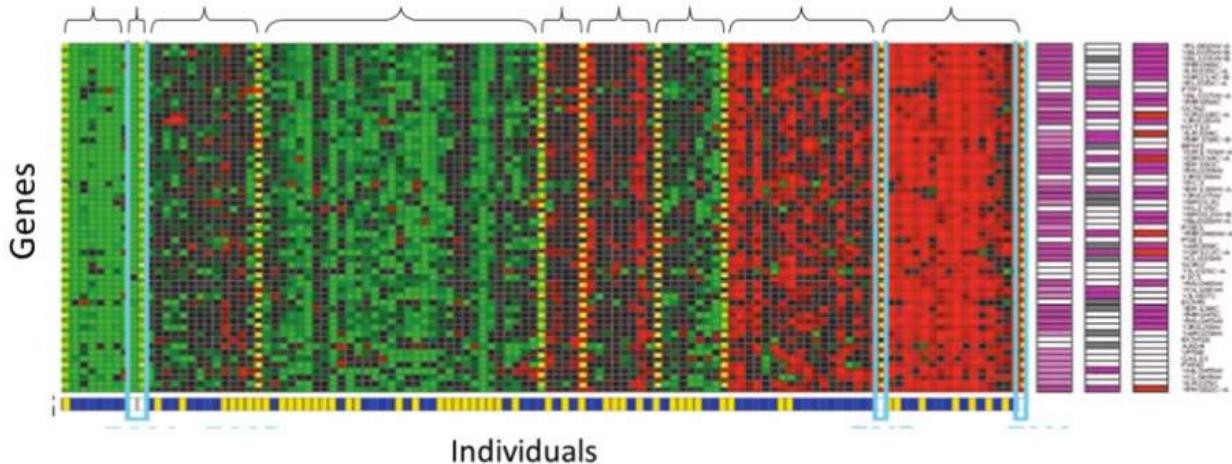
- Then, when you have an individual with a specific tumor size and who is a specific age, you can hopefully use that information to place them into one of your classes
- You might have many features to consider
  - Clump thickness
  - Uniformity of cell size
  - Uniformity of cell shape
- The most exciting 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

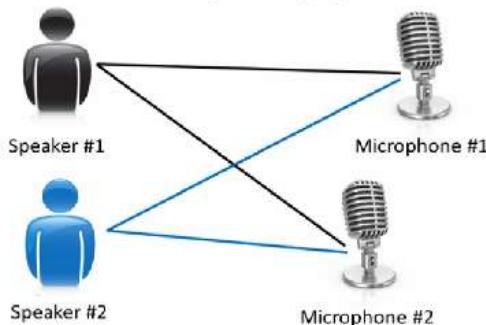


- Organize computer clusters
  - Identify potential weak spots or distribute workload effectively
- Social network analysis
  - Customer data
- Astronomical data analysis
  - Algorithms give amazing results
- Basically
  - Can you automatically generate structure
  - Because we don't give it the answer, 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
      - (x<sup>i</sup>, y<sup>j</sup>) - specific example (i<sup>th</sup> training example)
        - i is an index to training set

| Size in feet <sup>2</sup> (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  $x$ !
  - $\theta_i$  are **parameters**
    - $\theta_0$  is zero condition
    - $\theta_1$  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)

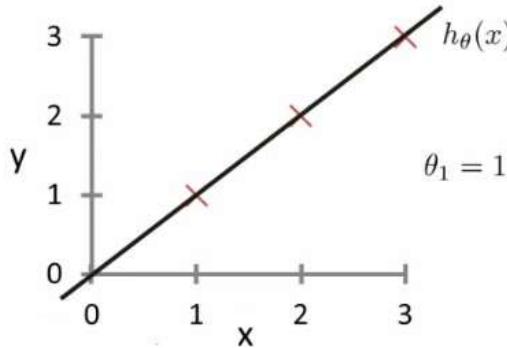
- A cost function lets us figure out how to fit the best straight line to our data
- Choosing values for  $\theta_i$  (parameters)
  - Different values give you different functions
  - If  $\theta_0$  is 1.5 and  $\theta_1$  is 0 then we get straight line parallel with  $X$  along 1.5 @  $y$
  - If  $\theta_1$  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
    - $1/m$  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  $\theta_0/\theta_1$  means we get the values of  $\theta_0$  and  $\theta_1$  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  $\theta$  values which make the hypothesis as accurate as possible

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

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

- 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  $\theta_0 = 0$

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

$\theta_0 = 0$

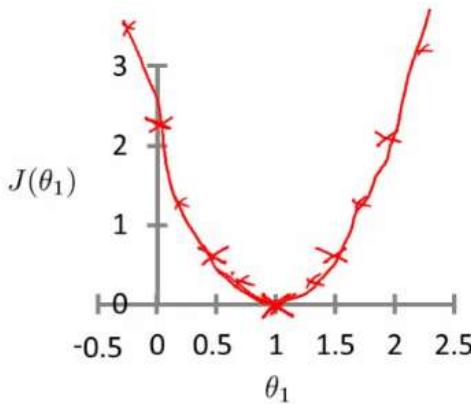
$$\underline{\theta_1}$$

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

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

- Cost function and goal here are very similar to when we have  $\theta_0$ , 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
  - $h_0(x)$ 
    - Hypothesis is a function of  $x$  - function of what the size of the house is

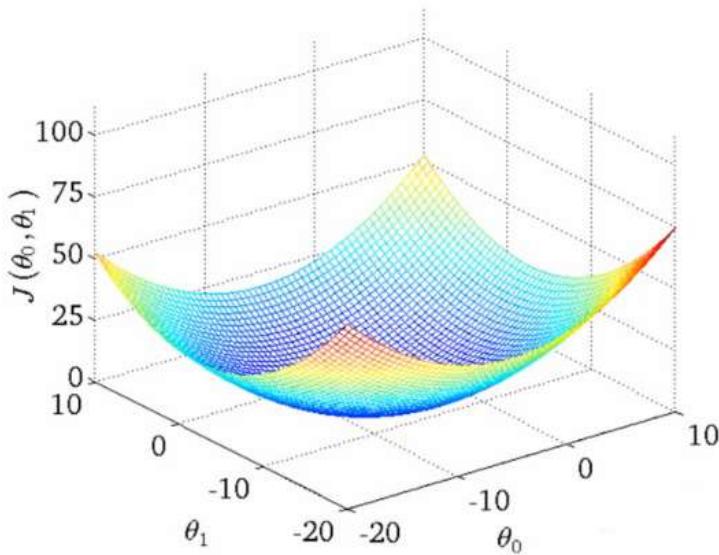
- $J(\theta_1)$ 
  - Is a function of the parameter of  $\theta_1$
- So for example
  - $\theta_1 = 1$
  - $J(\theta_1) = 0$
- Plot
  - $\theta_1$  vs  $J(\theta_1)$
  - Data
    - 1)
      - $\theta_1 = 1$
      - $J(\theta_1) = 0$
    - 2)
      - $\theta_1 = 0.5$
      - $J(\theta_1) = \sim 0.58$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



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

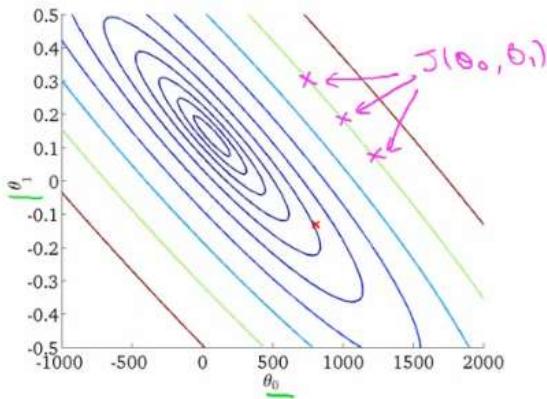
## A deeper insight into the cost function - simplified cost function

- 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
    - $\theta_1$  vs  $J(\theta_1)$
  - Now we have two parameters
    - Plot becomes a bit more complicated
    - Generates a 3D surface plot where axis are
      - $X = \theta_1$
      - $Z = \theta_0$
      - $Y = J(\theta_0, \theta_1)$



- 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  $\theta_1$  and  $\theta_0$  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  $\theta_0, \theta_1$ )



- Each point (like the red one above) represents a pair of parameter values for  $\theta_0$  and  $\theta_1$ 
  - 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  $\theta_0$  and  $\theta_1$

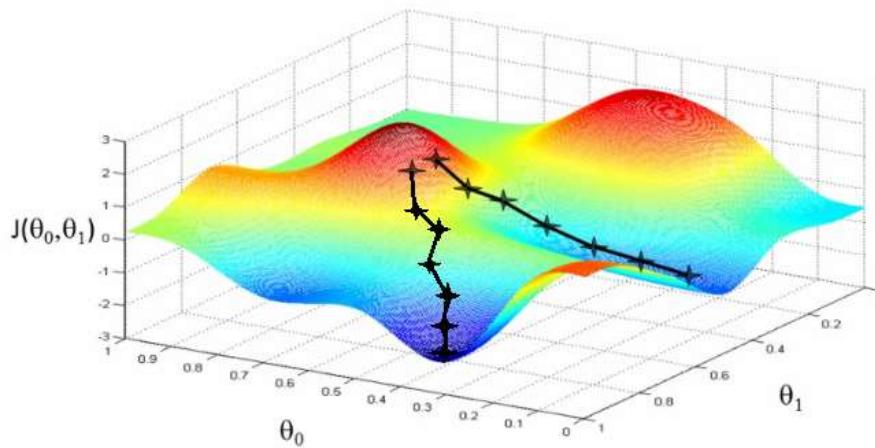
## Gradient descent algorithm

- 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  $\theta_0$  and  $\theta_1$  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  $\theta_j$  by setting it to  $(\theta_j - \alpha)$  times the partial derivative of the cost function with respect to  $\theta_j$
- Notation
  - $::=$ 
    - Denotes assignment
    - NB  $a = b$  is a *truth assertion*
  - $\alpha$  (alpha)
    - Is a number called the **learning rate**
    - Controls how big a step you take
      - If  $\alpha$  is big have an aggressive gradient descent
      - If  $\alpha$  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  $\theta_0$  and  $\theta_1$
  - For  $j = 0$  and  $j = 1$  means we **simultaneously** update both
  - How do we do this?
    - Compute the right hand side for both  $\theta_0$  and  $\theta_1$ 
      - So we need a temp value
      - Then, update  $\theta_0$  and  $\theta_1$  at the same time
      - We show this graphically below

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

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

$\theta_0 := \text{temp0}$

$\theta_1 := \text{temp1}$

- 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  $\theta_1$  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 ( $\alpha$ )
  - 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  $\theta_1$  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

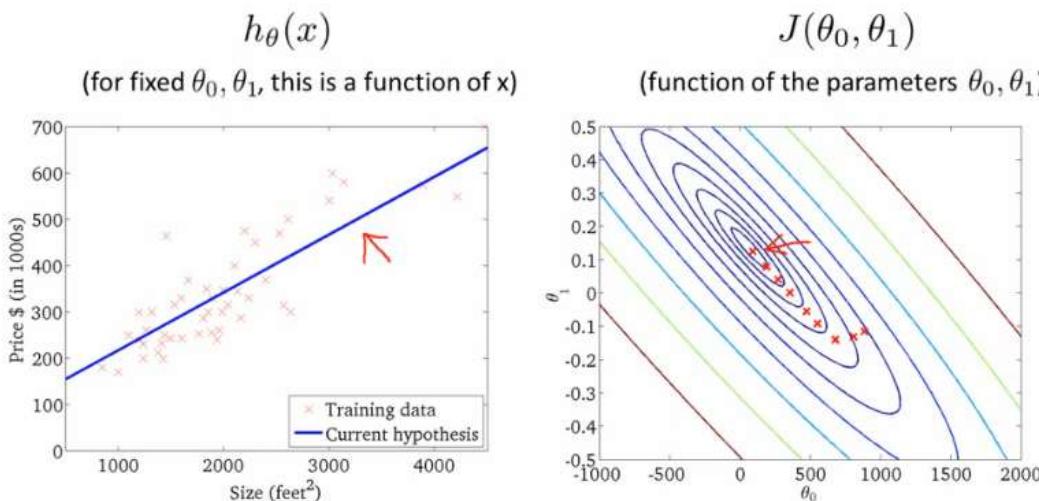
- Apply gradient descent to minimize the squared error cost function  $J(\theta_0, \theta_1)$
- Now we have a partial derivative

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

- 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  $\theta_0$  and  $\theta_1$  case
  - When we derive this expression in terms of  $j = 0$  and  $j = 1$  we get the following

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

- 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