01 and 02: Introduction, Regression Analysis, and Gradient Descent

Next Index

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 party 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?

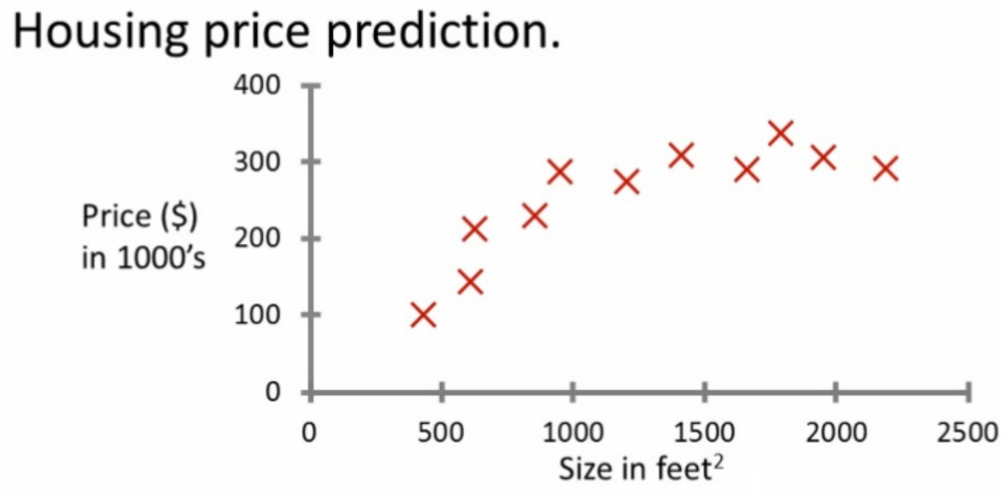
- Here we...
    - Define what it is
    - When to use it
- Not a well defined definition
    - Couple of examples of how people have tried to define it
- Arthur Samuel (1959)
    - ***Machine learning:*** **"Field of study that gives computers the ability to learn without being explicitly programmed"**
        - 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 = 10000s 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 it;s 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

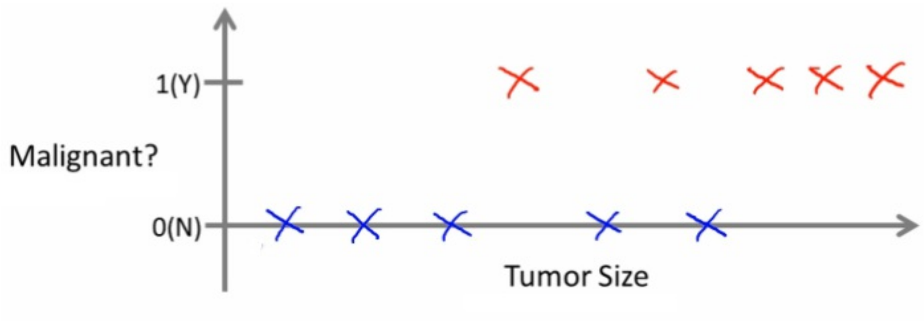
- Probably the most common problem type in machine learning
- Starting with an example
    - How do we predict housing prices
        - Collect data regarding housing prices and how they relate to size in feet



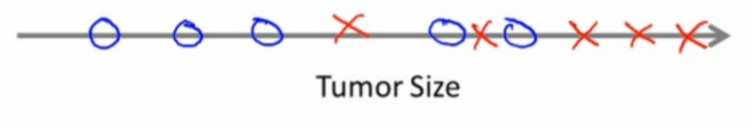
- **Example problem:** "Given this data, a friend has a house 750 square feet - how much can they be expected to get?"

- 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

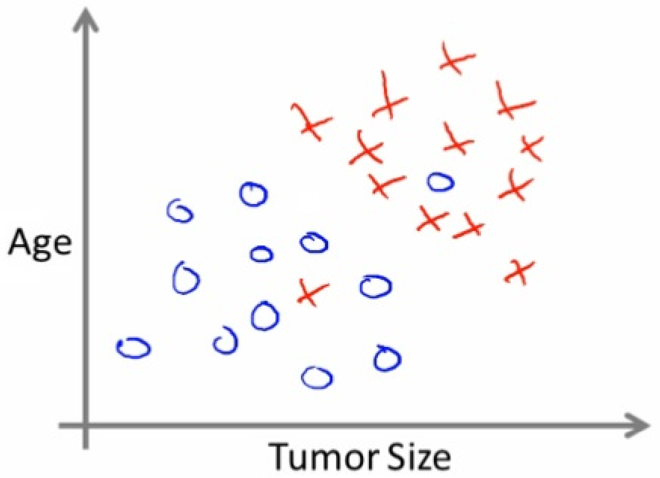
- Another example
    - Can we definer breast cancer as malignant or benign based on tumour size



- 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 and algorithm to deal with that

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

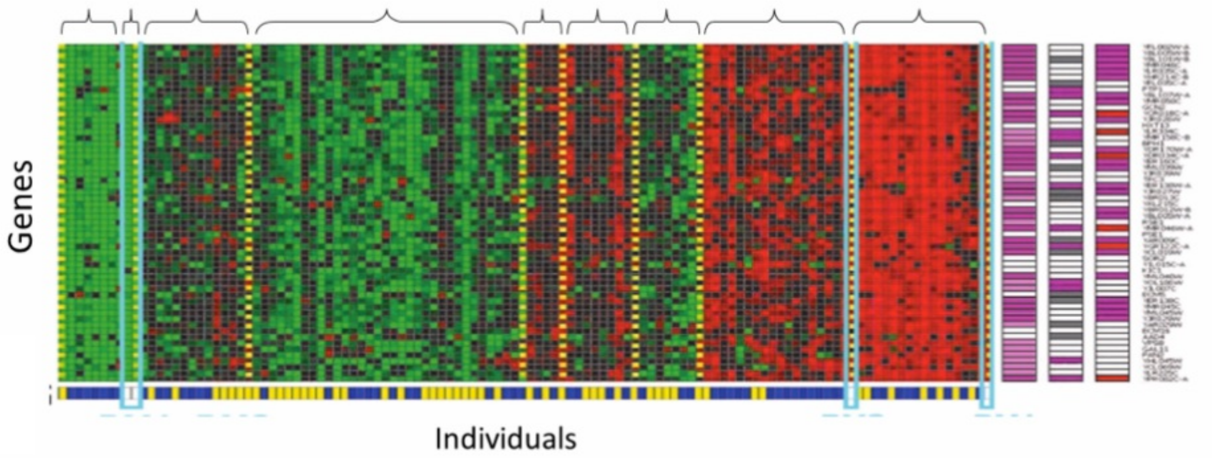
Unsupervised learning - introduction

- 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 to 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

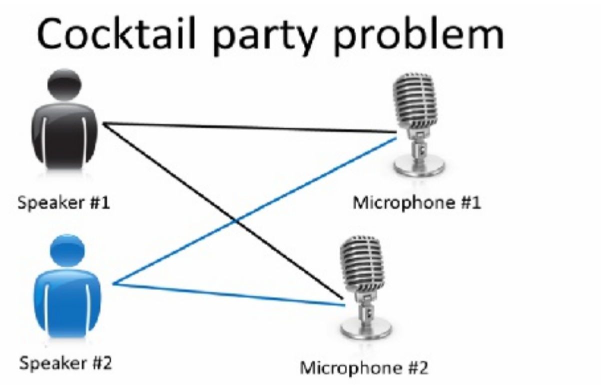


        - Organize computer clusters
            - Identify potential weak spots or distribute workload effectively
        - Social network analysis
            - Customer data
        - Astronomical data analysis
            - Algorithms give amazing results

- 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



- Record sightly 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^i, y^j) - specific example (i^{th} training example)
                - i is an index to training set

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

m = 47

- 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 = **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

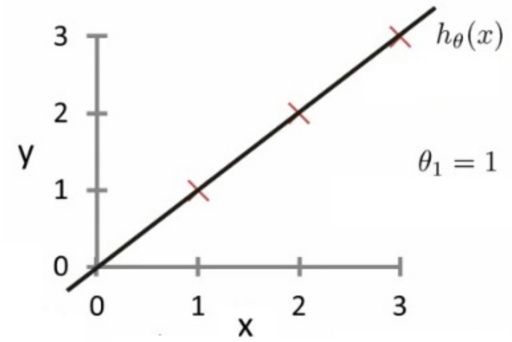
    - If θ_0 is 1.5 and θ_1 is 0 then we get straight line parallel with X along 1.5 @ y
    - If θ_1 is > 0 then we get a positive slope
- Based on our training set we want to generate parameters which make the straight line
    - Chosen these parameters so $h_\theta(x)$ is close to y for our training examples
        - 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 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

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

- Minimize squared different 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

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

- And we want to minimize this cost function
    - Our cost function is (because of the summartion 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

$$\underset{\theta_0,\theta_1}{\text{minimize}}\ \underbrace{J(\theta_0,\theta_1)}_{\text{Cost function}}$$

        - 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 $\theta_0 = 0$

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

$$\theta_0 = 0$$

$$\theta_1$$

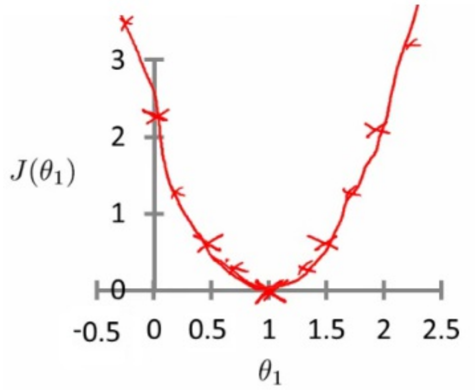
$$J(\theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

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

- 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 functins 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)

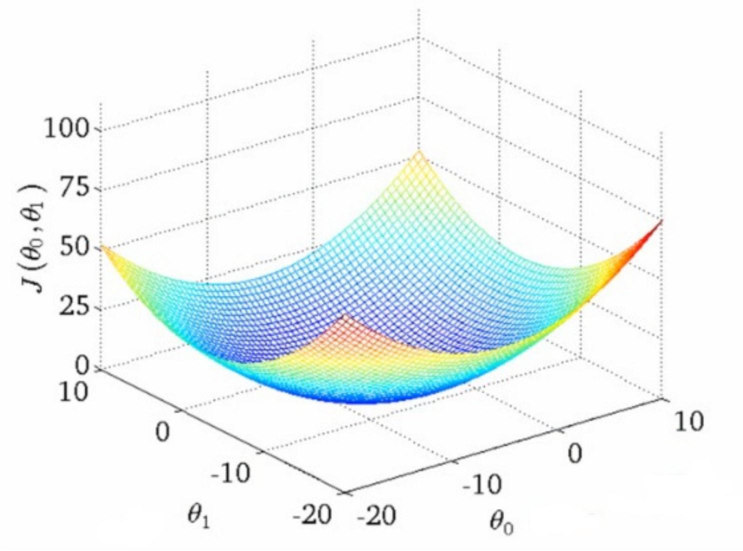


- The optimization objective for the learning algorithm is find the value of θ_1 which minimizes $J(\theta_1)$
    - So, here $\theta_1 = 1$ is the best value for θ_1

A deeper insight into the cost function - simplified cost function

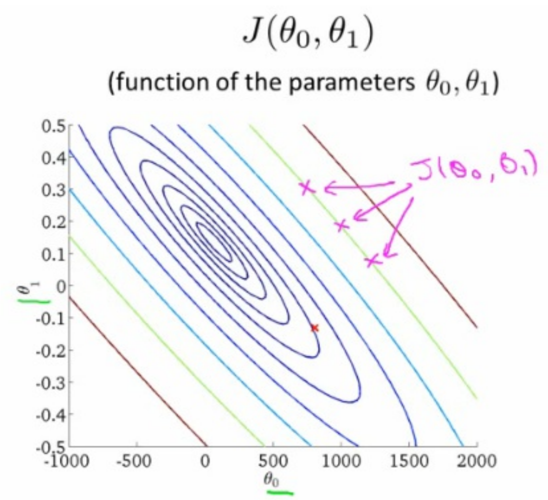
- Assume you're familiar with contour plots or contour figures
    - Using same cost function, hypothesis and goal as previously
    - It's OK to skip parts of this section if you don't understand cotour plots
- Using our original complex hyothesis with two pariables,

- 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
      - $X = \theta_1$
      - $Z = \theta_0$
      - $Y = J(\theta_0,\theta_1)$



- 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 θ_1 and θ_0 will vary
  - Imagine a bowl shape function coming out of the screen so the middle is the concentric circles



- Each point (like the red one above) represents a pair of parameter values for Ө0 and Ө1
  - 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

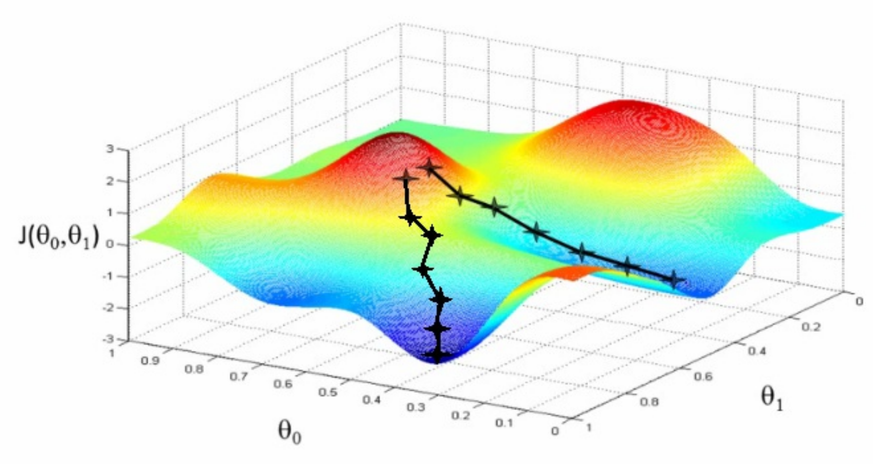
- Doing this by eye/hand is a pain in the ass
  - What we really want is an efficient algorithm fro finding the minimum for θ_0 and θ_1

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
  - $J(\theta_0, \theta_1, \theta_2 .... \theta_n)$
  - min $J(\theta_0, \theta_1, \theta_2 .... \theta_n)$

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 covergence

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

- What does this all mean?
  - Update θ_j by setting it to (θ_j - α) 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 subtly 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

$$\begin{aligned}
&\text{temp0} := \theta_0 - \alpha \tfrac{\partial}{\partial\theta_0} J(\theta_0, \theta_1) \\
&\text{temp1} := \theta_1 - \alpha \tfrac{\partial}{\partial\theta_1} J(\theta_0, \theta_1) \\
&\theta_0 := \text{temp0} \\
&\theta_1 := \text{temp1}
\end{aligned}$$

- 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 θ_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 mimum (down) will greate 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

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

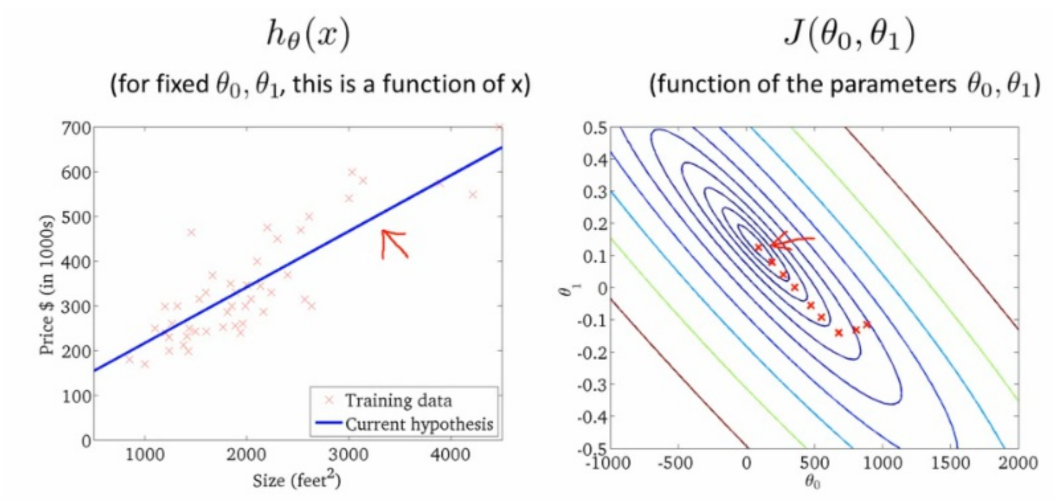
$$= \frac{\partial}{\partial\theta_j} \frac{1}{2m} \sum_{i=1}^{m} \left(\theta_0 + \theta_1 x^{(i)} - y^{(i)} \right)^2$$

- So here we're just expanding out the first expression
  - $J(\theta_0, \theta_1) = 1/2m....$
  - $h_\theta(x) = \theta_0 + \theta_1 * x$
- 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

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

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

- 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
        - x1, x2, x3, x4
    - 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

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

- 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 modles
- 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