03: Linear Algebra - Review

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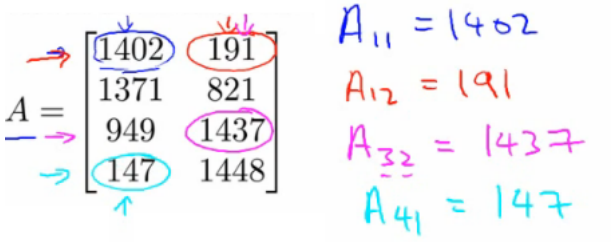
Matrices - overview

- Rectangular array of numbers written between square brackets
  - 2D array
  - Named as capital letters (A,B,X,Y)
- Dimension of a matrix are [Rows x Columns]
  - Start at top left
  - To bottom left
  - To bottom right
  - $R^{[r \times c]}$ means a matrix which has r rows and c columns

$$A = \begin{bmatrix} 1402 & 191 \\ 1371 & 821 \\ 949 & 1437 \\ 147 & 1448 \end{bmatrix}$$

    - Is a [4 x 2] matrix

- Matrix elements
  - $A_{(i,j)}$ = entry in i^{th} row and jth column



- Provides a way to organize, index and access a lot of data

Vectors - overview

- Is an n by 1 matrix
  - Usually referred to as a lower case letter
  - n rows
  - 1 column
  - e.g.

$$y = \begin{bmatrix} 460 \\ 232 \\ 315 \\ 178 \end{bmatrix}$$

- Is a 4 dimensional vector
  - Refer to this as a vector R4
- Vector elements
  - v_i = i^{th} element of the vector
  - Vectors can be 0-indexed (C++) or 1-indexed (MATLAB)
  - In math 1-indexed is most common
    - But in machine learning 0-index is useful
  - Normally assume using 1-index vectors, but be aware sometimes these will (explicitly) be 0 index ones

Matrix manipulation

- ***Addition***
  - Add up elements one at a time
  - Can only add matrices of the *same dimensions*
    - Creates a new matrix of the same dimensions of the ones added

$$\begin{bmatrix} 1 & 0 \\ 2 & 5 \\ 3 & 1 \end{bmatrix} + \begin{bmatrix} 4 & 0.5 \\ 2 & 5 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 5 & 0.5 \\ 4 & 10 \\ 3 & 2 \end{bmatrix}$$

- ***Multiplication by scalar***
  - Scalar = real number
  - Multiply each element by the scalar
  - Generates a matrix of the same size as the original matrix

$$3 \times \begin{bmatrix} 1 & 0 \\ 2 & 5 \\ 3 & 1 \end{bmatrix} = \begin{bmatrix} 3 & 0 \\ 6 & 15 \\ 9 & 3 \end{bmatrix}$$

- ***Division by a scalar***
  - Same as multiplying a matrix by 1/4
  - Each element is divided by the scalar
- ***Combination of operands***
  - Evaluate multiplications first

$$3 \times \begin{bmatrix} 1 \\ 4 \\ 2 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 5 \end{bmatrix} - \begin{bmatrix} 3 \\ 0 \\ 2 \end{bmatrix} /3$$

- **Matrix by vector multiplication**
  - [3 x 2] matrix * [2 x 1] vector
    - New matrix is [3 x 1]
      - More generally if [a x b] * [b x c]
        - Then new matrix is [a x c]
    - How do you do it?
      - Take the two vector numbers and multiply them with the first row of the matrix
        - Then add results together - this number is the first number in the new vector
      - The multiply second row by vector and add the results together
      - Then multiply final row by vector and add them together

$$\begin{bmatrix} 1 & 3 \\ 4 & 0 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 5 \end{bmatrix} = \begin{bmatrix} 16 \\ 4 \\ 7 \end{bmatrix}$$

3×2 2×1

$1 \times 1 + 3 \times 5 = 16$

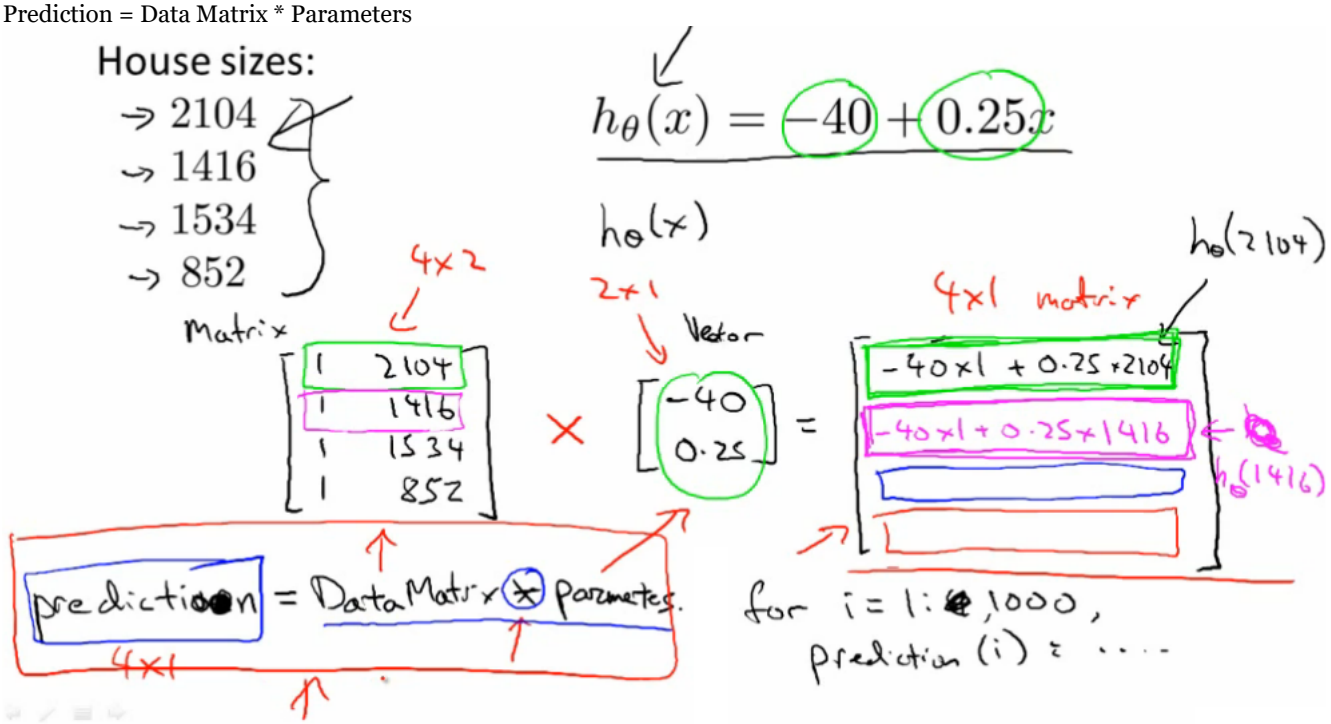
$4 \times 1 + 0 \times 5 = 4$

$2 \times 1 + 1 \times 5 = 7$

- Detailed explanation
  - A * x = y
    - A is m x n matrix
    - x is n x 1 matrix
    - n must match between vector and matrix
      - i.e. inner dimensions must match
    - Result is an m-dimensional vector

- To get y_i - multiply A's i^{th} row with all the elements of vector x and add them up

- Neat trick
  - Say we have a data set with four values
  - Say we also have a hypothesis $h_\theta(x) = -40 + 0.25x$
    - Create your data as a matrix which can be multiplied by a vector
    - Have the parameters in a vector which your matrix can be multiplied by
  - Means we can do
    - Prediction = Data Matrix * Parameters



  - Here we add an extra column to the data with 1s - this means our θ_0 values can be calculated and expressed

- The diagram above shows how this works
  - This can be far more efficient computationally than lots of for loops
  - This is also easier and cleaner to code (assuming you have appropriate libraries to do matrix multiplication)

- ***Matrix-matrix multiplication***
  - General idea
    - Step through the second matrix one column at a time
    - Multiply each column vector from second matrix by the entire first matrix, each time generating a vector
    - The final product is these vectors combined (not added or summed, but literally just put together)
  - Details
    - A x B = C
      - A = [m x n]
      - B = [n x o]
      - C = [m x o]
        - With vector multiplications o = 1
    - Can only multiply matrix where columns in A match rows in B
  - Mechanism
    - Take column 1 of B, treat as a vector
    - Multiply A by that column - generates an [m x 1] vector
    - Repeat for each column in B
      - There are o columns in B, so we get o columns in C
  - Summary
    - *The i^{th} column of matrix C is obtained by multiplying A with the i^{th} column of B*
  - Start with an example
  - A x B

$$\begin{bmatrix} 1 & 3 & 2 \\ 4 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 3 \\ 0 & 1 \\ 5 & 2 \end{bmatrix}$$

- Initially
  - Take matrix A and multiply by the first column vector from B
  - Take the matrix A and multiply by the second column vector from B

$$\begin{bmatrix}1 & 3 & 2\\4 & 0 & 1\end{bmatrix} \times \begin{bmatrix}1\\0\\5\end{bmatrix} = \begin{bmatrix}11\\9\end{bmatrix}$$

$$\begin{bmatrix}1 & 3 & 2\\4 & 0 & 1\end{bmatrix} \times \begin{bmatrix}3\\1\\2\end{bmatrix} = \begin{bmatrix}10\\14\end{bmatrix}$$

- 2 x 3 times 3 x 2 gives you a 2 x 2 matrix

Implementation/use

- House prices, but now we have three hypothesis and the same data set
- To apply all three hypothesis to all data we can do this efficiently using matrix-matrix multiplication
  - Have
    - Data matrix
    - Parameter matrix
  - Example
    - Four houses, where we want to predict the prize
    - Three competing hypotheses
    - Because our hypothesis are one variable, to make the matrices match up we make our data (houses sizes) vector into a 4x2 matrix by adding an extra column of 1s

House sizes:

$$\begin{Bmatrix}2104\\1416\\1534\\852\end{Bmatrix}$$

Have 3 competing hypotheses:

1. $h_\theta(x) = -40 + 0.25x$
2. $h_\theta(x) = 200 + 0.1x$
3. $h_\theta(x) = -150 + 0.4x$

Matrix

$$\begin{bmatrix}1 & 2104\\1 & 1416\\1 & 1534\\1 & 852\end{bmatrix}$$

$\times$ Matrix

$$\begin{bmatrix}-40 & 200 & -150\\0.25 & 0.1 & 0.4\end{bmatrix} = \begin{bmatrix}486 & 410 & 692\\314 & 342 & 416\\344 & 353 & 464\\173 & 285 & 191\end{bmatrix}$$

Prediction of first ho

Predictions of 2nd ho

- What does this mean
  - Can quickly apply three hypotheses at once, making 12 predictions
  - Lots of good linear algebra libraries to do this kind of thing very efficiently

Matrix multiplication properties

- Can pack a lot into one operation
  - However, should be careful of how you use those operations
  - Some interesting properties
- **Commutativity**
  - When working with raw numbers/scalars multiplication is commutative
    - 3 * 5 == 5 * 3
  - This is not true for matrix
    - A x B != B x A
    - **Matrix multiplication is not commutative**
- **Associativity**
  - 3 x 5 x 2 == 3 x 10 = 15 x 2
    - Associative property
  - **Matrix multiplications is associative**
    - A x (B x C) == (A x B) x C
- **Identity matrix**
  - 1 is the identity for any scalar
    - i.e. 1 x z = z

        - for any real number
    - In matrices we have an identity matrix called I
        - Sometimes called $I_{\{n \times n\}}$

$$\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}_{2\times 2} \qquad \begin{bmatrix}1 & 0 & 0\\0 & 1 & 0\\0 & 0 & 1\end{bmatrix}_{3\times 3} \qquad \begin{bmatrix}1 & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 0 & 1 & 0\\0 & 0 & 0 & 1\end{bmatrix}_{4\times 4}$$

- See some identity matrices above
    - Different identity matrix for each set of dimensions
    - Has
        - 1s along the diagonals
        - 0s everywhere else
    - 1x1 matrix is just "1"

- Has the property that any matrix A which can be multiplied by an identity matrix gives you matrix A back
    - So if A is [m x n] then
        - A * I
            - I = n x n
        - I * A
            - I = m x m
        - (To make inside dimensions match to allow multiplication)
- Identity matrix dimensions are implicit
- Remember that matrices are not commutative AB != BA
    - Except when B is the identity matrix
    - Then AB == BA

Inverse and transpose operations

- **Matrix inverse**
    - How does the concept of "the inverse" relate to real numbers?
        - 1 = "identity element" (as mentioned above)
            - Each number has an inverse
                - This is the number you multiply a number by to get the identify element
                - i.e. if you have x, x * 1/x = 1
        - e.g. given the number 3
            - $3 * 3^{-1} = 1$ (the identity number/matrix)
        - In the space of real numbers **not everything has an inverse**
            - e.g. 0 does not have an inverse
    - What is the inverse of a matrix
        - If A is an m x m matrix, then A inverse = A^{-1}
        - So $A*A^{-1} = I$
        - Only matrices which are m x m have inverses
            - Square matrices only!
    - Example
        - 2 x 2 matrix

$$\underbrace{\begin{bmatrix}3 & 4\\2 & 16\end{bmatrix}}_{A} \underbrace{\begin{bmatrix}0.4 & -0.1\\-0.05 & 0.075\end{bmatrix}}_{A^{-1}} = \underbrace{\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}}_{A^{-1}A} = I_{2\times 2}$$

        - How did you find the inverse
            - Turns out that you can sometimes do it by hand, although this is very hard
            - Numerical software for computing a matrices inverse
                - Lots of open source libraries
    - If A is all zeros then there is no inverse matrix
        - Some others don't, intuition should be matrices that don't have an inverse are a singular matrix or a degenerate matrix (i.e. when it's too close to 0)
        - So if all the values of a matrix reach zero, this can be described as reaching singularity

- **Matrix transpose**
    - Have matrix A (which is [n x m]) how do you change it to become [m x n] while keeping the same values
        - i.e. swap rows and columns!
    - How you do it;
        - Take first row of A - becomes 1st column of A^T
        - Second row of A - becomes 2nd column...
    - A is an m x n matrix
        - B is a transpose of A
        - Then B is an n x m matrix

- $A_{(i,j)} = B_{(j,i)}$

6/14

$$\underline{A} = \begin{bmatrix} 1 & 2 & 0 \\ 3 & 5 & 9 \end{bmatrix} \quad \underline{A^T} = \begin{bmatrix} 1 & 3 \\ 2 & 5 \\ 0 & 9 \end{bmatrix}$$

04: Linear Regression with Multiple Variables

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Linear regression with multiple features

New version of linear regression with multiple features

- Multiple variables = multiple features
- In original version we had
  - X = house size, use this to predict
  - y = house price
- If in a new scheme we have more variables (such as number of bedrooms, number floors, age of the home)
  - x_1, x_2, x_3, x_4 are the four features
    - x_1 - size (feet squared)
    - x_2 - Number of bedrooms
    - x_3 - Number of floors
    - x_4 - Age of home (years)
  - y is the output variable (price)
- More notation
  - **n**
    - number of features (n = 4)
  - **m**
    - number of examples (i.e. number of rows in a table)
  - **x^i**
    - vector of the input for an example (so a vector of the four parameters for the i^{th} input example)
    - i is an index into the training set
    - So
      - x is an n-dimensional feature vector
      - x^3 is, for example, the 3rd house, and contains the four features associated with that house
  - **x_j^i**
    - The value of feature j in the ith training example
    - So
      - x_2^3 is, for example, the number of bedrooms in the third house
- Now we have multiple features
  - What is the form of our hypothesis?
  - Previously our hypothesis took the form;
    - $h_\theta(x) = \theta_0 + \theta_1 x$
      - Here we have two parameters (theta 1 and theta 2) determined by our cost function
      - One variable x
  - Now we have multiple features
    - $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \theta_4 x_4$
  - For example
    - $h_\theta(x) = 80 + 0.1x_1 + 0.01x_2 + 3x_3 - 2x_4$
      - An example of a hypothesis which is trying to predict the price of a house
      - Parameters are still determined through a cost function
  - For convenience of notation, $x_0 = 1$
    - For every example i you have an additional 0th feature for each example
    - So now your **feature vector** is n + 1 dimensional feature vector indexed from 0
      - This is a column vector called x
      - Each example has a column vector associated with it
      - So let's say we have a new example called "X"
    - **Parameters** are also in a 0 indexed n+1 dimensional vector
      - This is also a column vector called θ
      - This vector is the same for each example
  - Considering this, hypothesis can be written
    - $h_\theta(x) = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \theta_4 x_4$

- If we do
  - $h_\theta(x) = \theta^T X$
    - θ^T is an [1 x n+1] matrix
    - In other words, because θ is a column vector, the transposition operation transforms it into a row vector
    - So before
      - θ was a matrix [n + 1 x 1]
    - Now
      - θ^T is a matrix [1 x n+1]
    - Which means the inner dimensions of θ^T and X match, so they can be multiplied together as
      - [1 x n+1] * [n+1 x 1]
      - = $h_\theta(x)$
      - So, in other words, the transpose of our parameter vector * an input example X gives you a predicted hypothesis which is [1 x 1] dimensions (i.e. a single value)
  - This $x_0 = 1$ lets us write this like this
- This is an example of multivariate linear regression

Gradient descent for multiple variables

- Fitting parameters for the hypothesis with gradient descent
  - Parameters are θ_0 to θ_n
  - Instead of thinking about this as n separate values, think about the parameters as a single vector (θ)
    - Where θ is n+1 dimensional
- Our cost function is

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

- Similarly, instead of thinking of J as a function of the n+1 numbers, J() is just a function of the parameter vector
  - J(θ)
- **Gradient descent**

Repeat {

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

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

- Once again, this is
  - $\theta_j = \theta_j$ - learning rate (α) times the partial derivative of J(θ) with respect to $\theta_{J(...)}$
  - We do this through a **simultaneous update** of every θ_j value
- Implementing this algorithm
  - When n = 1

Repeat {

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

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

(simultaneously update θ_0, θ_1) }

- Above, we have slightly different update rules for θ_0 and θ_1
  - Actually they're the same, except the end has a previously undefined $x_0^{(i)}$ as 1, so wasn't shown
- We now have an almost identical rule for multivariate gradient descent

New algorithm $(n \geq 1)$:

Repeat $\{$

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

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

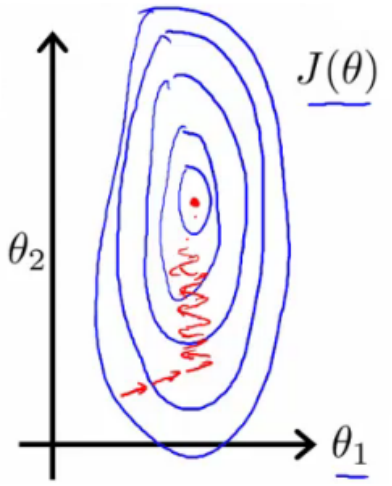
- What's going on here?
  - We're doing this for each j (0 until n) as a simultaneous update (like when n = 1)
  - So, we re-set θ_j to
    - θ_j minus the learning rate (α) times the partial derivative of of the θ vector with respect to θ_j
    - In non-calculus words, this means that we do
      - Learning rate
      - Times 1/m (makes the maths easier)
      - Times the sum of
        - The hypothesis taking in the variable vector, minus the actual value, times the j-th value in that variable vector for EACH example
  - It's important to remember that

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

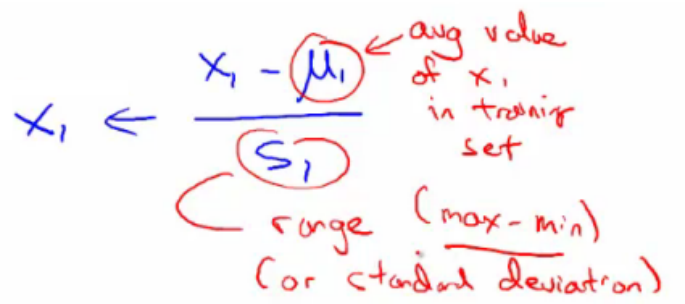
- These algorithm are highly similar

Gradient Decent in practice: 1 Feature Scaling

- Having covered the theory, we now move on to learn about some of the practical tricks
- Feature scaling
  - If you have a problem with multiple features
  - You should make sure those features have a similar scale
    - Means gradient descent will converge more quickly
  - e.g.
    - x1 = size (0 - 2000 feet)
    - x2 = number of bedrooms (1-5)
    - Means the contours generated if we plot θ_1 vs. θ_2 give a very tall and thin shape due to the huge range difference
  - Running gradient descent on this kind of cost function can take a long time to find the global minimum



- Pathological input to gradient descent
  - So we need to rescale this input so it's more effective
  - So, if you define each value from x1 and x2 by dividing by the max for each feature
  - Contours become more like circles (as scaled between 0 and 1)
- May want to get everything into -1 to +1 range (approximately)
  - Want to avoid large ranges, small ranges or very different ranges from one another
  - Rule a thumb regarding acceptable ranges
    - -3 to +3 is generally fine - any bigger bad
    - -1/3 to +1/3 is ok - any smaller bad
- Can do **mean normalization**
  - Take a feature x_i
    - Replace it by (x_i - mean)/max
    - So your values all have an average of about 0



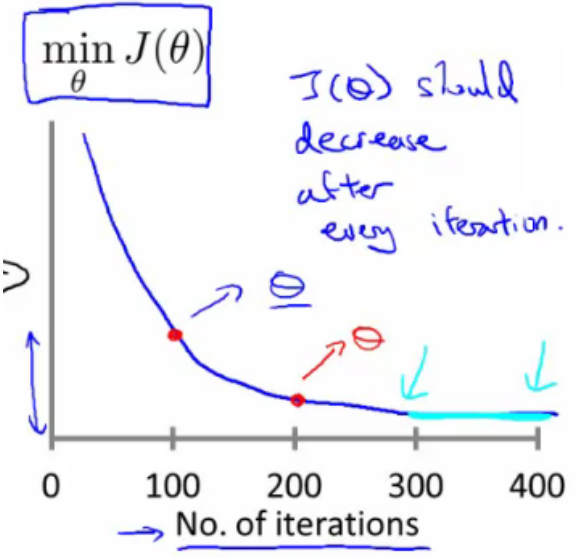
- Instead of max can also use standard deviation

Learning Rate α

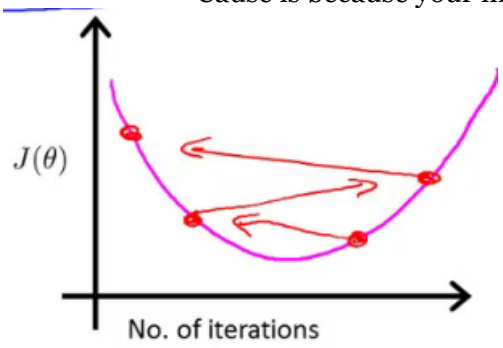
- Focus on the learning rate (α)
- Topics
  - Update rule
  - Debugging
  - How to chose α

Make sure gradient descent is working

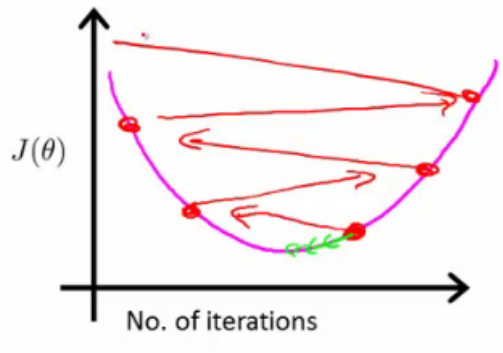
- Plot min J(θ) vs. no of iterations
  - (i.e. plotting J(θ) over the course of gradient descent
- If gradient descent is working then J(θ) should decrease after every iteration
- Can also show if you're not making huge gains after a certain number
  - Can apply heuristics to reduce number of iterations if need be
  - If, for example, after 1000 iterations you reduce the parameters by nearly nothing you could chose to only run 1000 iterations in the future
  - Make sure you don't accidentally hard-code thresholds like this in and then forget about why they're their though!



- Number of iterations varies a lot
  - 30 iterations
  - 3000 iterations
  - 3000 000 iterations
  - Very hard to tel in advance how many iterations will be needed
  - Can often make a guess based a plot like this after the first 100 or so iterations
- Automatic convergence tests
  - Check if J(θ) changes by a small threshold or less
    - Choosing this threshold is hard
    - So often easier to check for a straight line
      - Why? - Because we're seeing the straightness in the context of the whole algorithm
      - Could you design an automatic checker which calculates a threshold based on the systems preceding progress?
- Checking its working
  - If you plot J(θ) vs iterations and see the value is increasing - means you probably need a smaller α
    - Cause is because your minimizing a function which looks like this



- But you overshoot, so reduce learning rate so you actually reach the minimum (green line)



- So, use a smaller α

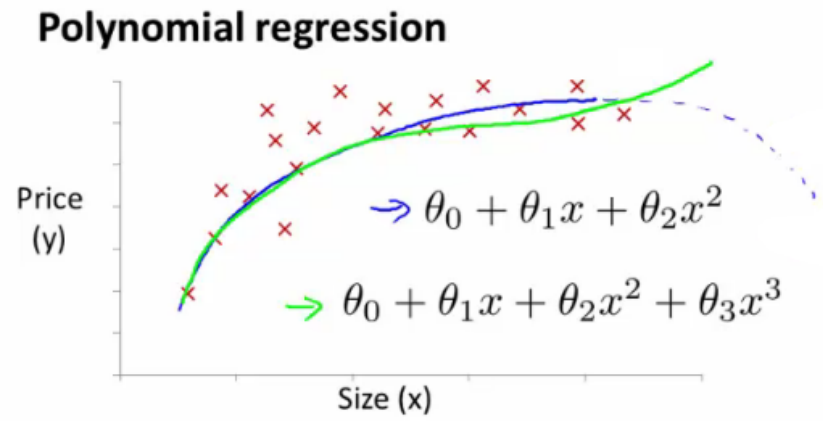
- Another problem might be if J(θ) looks like a series of waves
  - Here again, you need a smaller α
- However
  - If α is small enough, J(θ) will decrease on every iteration
  - BUT, if α is too small then rate is too slow

        - A less steep incline is indicative of a slow convergence, because we're decreasing by less on each iteration than a steeper slope
- Typically
    - Try a range of alpha values
    - Plot J(θ) vs number of iterations for each version of alpha
    - Go for roughly threefold increases
        - 0.001, 0.003, 0.01, 0.03. 0.1, 0.3

Features and polynomial regression

- Choice of features and how you can get different learning algorithms by choosing appropriate features
- Polynomial regression for non-linear function

- Example
    - House price prediction
        - Two features
            - Frontage - width of the plot of land along road (x_1)
            - Depth - depth away from road (x_2)
    - You don't have to use just two features
        - **Can create new features**
    - Might decide that an important feature is the land area
        - So, create a new feature = frontage * depth (x_3)
        - $h(x) = \theta_0 + \theta_1 x_3$
            - Area is a better indicator
    - Often, by defining new features you may get a better model
- Polynomial regression
    - May fit the data better
    - $\theta_0 + \theta_1 x + \theta_2 x^2$ e.g. here we have a quadratic function
    - For housing data could use a quadratic function
        - But may not fit the data so well - inflection point means housing prices decrease when size gets really big
        - So instead must use a cubic function

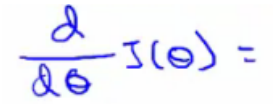


- How do we fit the model to this data
    - To map our old linear hypothesis and cost functions to these polynomial descriptions the easy thing to do is set
        - $x_1 = x$
        - $x_2 = x^2$
        - $x_3 = x^3$
    - By selecting the features like this and applying the linear regression algorithms you can do polynomial linear regression
    - Remember, feature scaling becomes even more important here
- Instead of a conventional polynomial you could do variable ^(1/something) - i.e. square root, cubed root etc
- Lots of features - later look at developing an algorithm to chose the best features

Normal equation

- For some linear regression problems the normal equation provides a better solution
- So far we've been using gradient descent
  - Iterative algorithm which takes steps to converse
- Normal equation solves θ analytically
  - Solve for the optimum value of theta
- Has some advantages and disadvantages

How does it work?

- Simplified cost function
  - $J(\theta) = a\theta^2 + b\theta + c$
    - θ is just a real number, not a vector
  - Cost function is a quadratic function
  - How do you minimize this?
    - Do
    - 
      - Take derivative of J(θ) with respect to θ
      - Set that derivative equal to 0
      - Allows you to solve for the value of θ which minimizes J(θ)
- In our more complex problems;
  - Here θ is an n+1 dimensional vector of real numbers
  - Cost function is a function of the vector value
    - How do we minimize this function
      - Take the partial derivative of J(θ) with respect θ_j and set to 0 for every j
      - Do that and solve for θ_0 to θ_n
      - This would give the values of θ which minimize J(θ)
  - If you work through the calculus and the solution, the derivation is pretty complex
    - Not going to go through here
    - Instead, what do you need to know to implement this process

Example of normal equation

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

- Here
  - m = 4
  - n = 4
- To implement the normal equation
  - Take examples
  - Add an extra column (x_0 feature)
  - Construct a matrix (X - **the design matrix**) which contains all the training data features in an [m x n+1] matrix
  - Do something similar for y
    - Construct a column vector y vector [m x 1] matrix
  - Using the following equation (X transpose * X) inverse times X transpose y

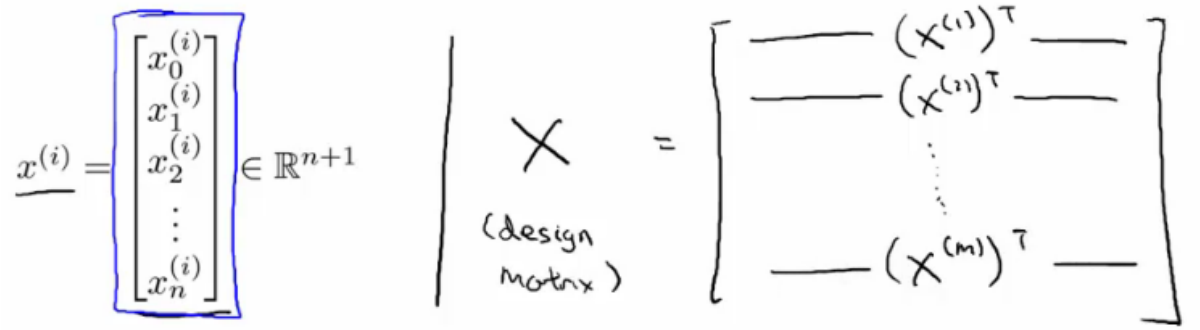
$$\theta = (X^T X)^{-1} X^T y$$

$$\left(\begin{bmatrix} 1 & 1 & 1 & 1 \\ 2104 & 1416 & 1534 & 852 \\ 5 & 3 & 3 & 2 \\ 1 & 2 & 2 & 1 \\ 45 & 40 & 30 & 36 \end{bmatrix} \times \begin{bmatrix} 1 & 2104 & 5 & 1 & 45 \\ 1 & 1416 & 3 & 2 & 40 \\ 1 & 1534 & 3 & 2 & 30 \\ 1 & 852 & 2 & 1 & 36 \end{bmatrix} \right)^{-1} \times \begin{bmatrix} 1 & 1 & 1 & 1 \\ 2104 & 1416 & 1534 & 852 \\ 5 & 3 & 3 & 2 \\ 1 & 2 & 2 & 1 \\ 45 & 40 & 30 & 36 \end{bmatrix} \times \begin{bmatrix} 460 \\ 232 \\ 315 \\ 178 \end{bmatrix}$$

- If you compute this, you get the value of theta which minimize the cost function

General case

- Have m training examples and n features
  - The **design matrix** (X)
    - Each training example is a n+1 dimensional feature column vector
    - X is constructed by taking each training example, determining its transpose (i.e. column -> row) and using it for a row in the design A
    - This creates an [m x (n+1)] matrix



  - **Vector y**
    - Used by taking all the y values into a column vector

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

- What is this equation?!
  - $(X^T * X)^{-1}$
    - What is this --> the inverse of the matrix $(X^T * X)$
      - i.e. $A = X^T X$
      - $A^{-1} = (X^T X)^{-1}$
- In octave and MATLAB you could do;

```
pinv(X'*x)*x'*y
```

    - X' is the notation for X transpose
    - pinv is a function for the inverse of a matrix
- In a previous lecture discussed feature scaling
  - If you're using the normal equation then no need for feature scaling

When should you use gradient descent and when should you use feature scaling?

  - ***Gradient descent***
    - Need to chose learning rate
    - Needs many iterations - could make it slower
    - Works well even when *n* is massive (millions)
      - Better suited to big data

        - What is a big *n* though
            - 100 or even a 1000 is still (relativity) small
            - If n is 10 000 then look at using gradient descent
    - ***Normal equation***
        - No need to chose a learning rate
        - No need to iterate, check for convergence etc.
        - Normal equation needs to compute $(X^T X)^{-1}$
            - This is the inverse of an n x n matrix
            - With most implementations computing a matrix inverse grows by $O(n^3)$
                - So not great
        - Slow of *n* is large
            - Can be much slower

Normal equation and non-invertibility

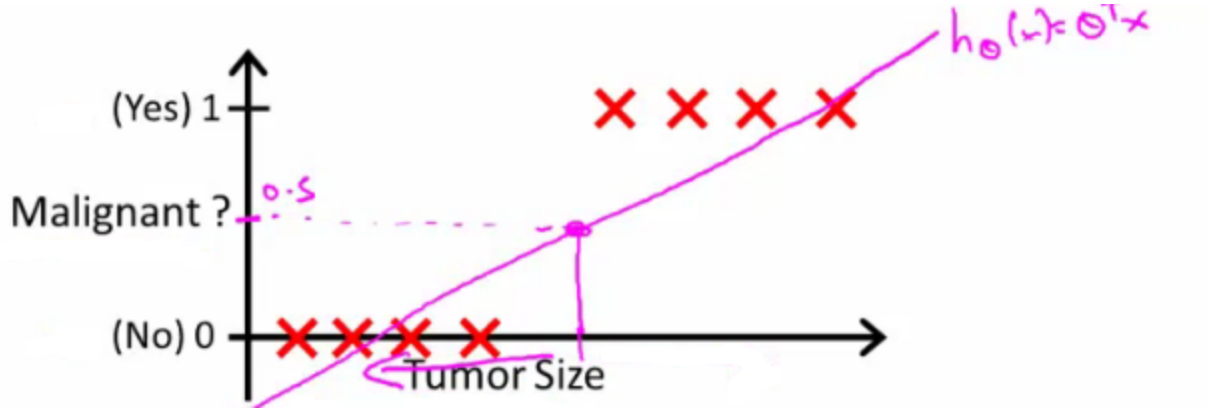
- Advanced concept
    - Often asked about, but quite advanced, perhaps optional material
    - Phenomenon worth understanding, but not probably necessary
- When computing $(X^T X)^{-1} * X^T * y$)
    - What if $(X^T X)$ is non-invertible (singular/degenerate)
        - Only some matrices are invertible
        - This should be quite a rare problem
            - Octave can invert matrices using
                - pinv (pseudo inverse)
                    - This gets the right value even if $(X^T X)$ is non-invertible
                - inv (inverse)
    - What does it mean for $(X^T X)$ to be non-invertible
        - Normally two common causes
            - **Redundant features** in learning model
                - e.g.
                    - x_1 = size in feet
                    - x_2 = size in meters squared
            - **Too many features**
                - e.g. m <= n (m is much larger than n)
                    - m = 10
                    - n = 100
                - Trying to fit 101 parameters from 10 training examples
                - Sometimes work, but not always a good idea
                - Not enough data
                - Later look at *why* this may be too little data
                - To solve this we
                    - Delete features
                    - Use **regularization** (let's you use lots of features for a small training set)
    - If you find $(X^T X)$ to be non-invertible
        - Look at features --> are features linearly dependent?
            - So just delete one, will solve problem

06: Logistic Regression

Previous Next Index

Classification

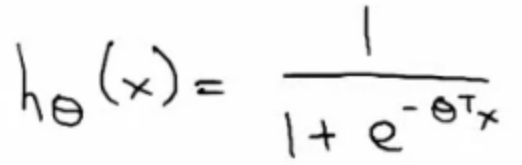
- Where y is a discrete value
  - Develop the logistic regression algorithm to determine what class a new input should fall into
- Classification problems
  - Email -> spam/not spam?
  - Online transactions -> fraudulent?
  - Tumor -> Malignant/benign
- Variable in these problems is Y
  - Y is either 0 or 1
    - 0 = negative class (absence of something)
    - 1 = positive class (presence of something)
- Start with **binary class problems**
  - Later look at multiclass classification problem, although this is just an extension of binary classification
- How do we develop a classification algorithm?
  - Tumour size vs malignancy (0 or 1)
  - We *could* use linear regression
    - Then threshold the classifier output (i.e. anything over some value is yes, else no)
    - In our example below linear regression with thresholding seems to work



- We can see above this does a reasonable job of stratifying the data points into one of two classes
  - But what if we had a single Yes with a very small tumour
  - This would lead to classifying all the existing yeses as nos
- Another issues with linear regression
  - We know Y is 0 or 1
  - Hypothesis can give values large than 1 or less than 0
- So, logistic regression generates a value where is always either 0 or 1
  - Logistic regression is a **classification algorithm** - don't be confused

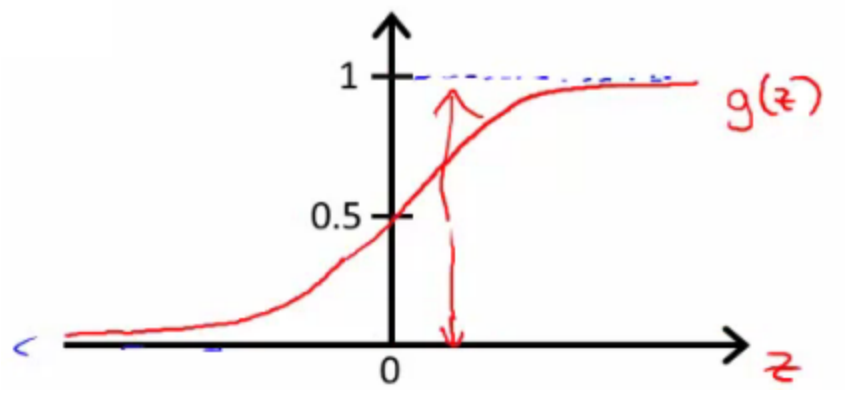
Hypothesis representation

- What function is used to represent our hypothesis in classification
- We want our classifier to output values between 0 and 1
  - When using linear regression we did $h_\theta(x) = (\theta^T x)$
  - For classification hypothesis representation we do $h_\theta(x) = g((\theta^T x))$
    - Where we define g(z)
      - z is a real number
    - $g(z) = 1/(1 + e^{-z})$
      - This is the **sigmoid function**, or the **logistic function**
    - If we combine these equations we can write out the hypothesis as



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

- What does the sigmoid function look like
- Crosses 0.5 at the origin, then flattens out]
  - Asymptotes at 0 and 1



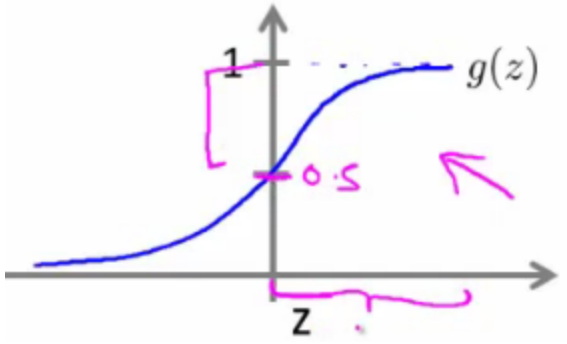
- Given this we need to fit θ to our data

Interpreting hypothesis output

- When our hypothesis ($h_\theta(x)$) outputs a number, we treat that value as the estimated probability that y=1 on input x
  - Example
    - If X is a feature vector with $x_0 = 1$ (as always) and x_1 = tumourSize
    - $h_\theta(x) = 0.7$
      - Tells a patient they have a 70% chance of a tumor being malignant
  - We can write this using the following notation
    - $h_\theta(x) = P(y=1|x\,;\,\theta)$
  - What does this mean?
    - Probability that y=1, given x, parameterized by θ
- Since this is a binary classification task we know y = 0 or 1
  - So the following must be true
    - $P(y=1|x\,;\,\theta) + P(y=0|x\,;\,\theta) = 1$
    - $P(y=0|x\,;\,\theta) = 1 - P(y=1|x\,;\,\theta)$

Decision boundary

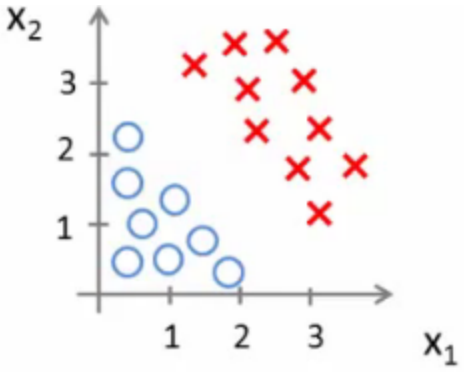
- Gives a better sense of what the hypothesis function is computing
- Better understand of what the hypothesis function looks like
  - One way of using the sigmoid function is;
    - When the probability of y being 1 is greater than 0.5 then we can predict y = 1
    - Else we predict y = 0
  - When is it exactly that $h_\theta(x)$ is greater than 0.5?
    - Look at sigmoid function
      - g(z) is greater than or equal to 0.5 when z is greater than or equal to 0



    - So if z is positive, g(z) is greater than 0.5
      - $z = (\theta^T x)$
    - So when
      - $\theta^T x >= 0$
    - Then $h_\theta >= 0.5$
- So what we've shown is that the hypothesis predicts y = 1 when $\theta^T x >= 0$
  - The corollary of that when $\theta^T x <= 0$ then the hypothesis predicts y = 0
  - Let's use this to better understand how the hypothesis makes its predictions

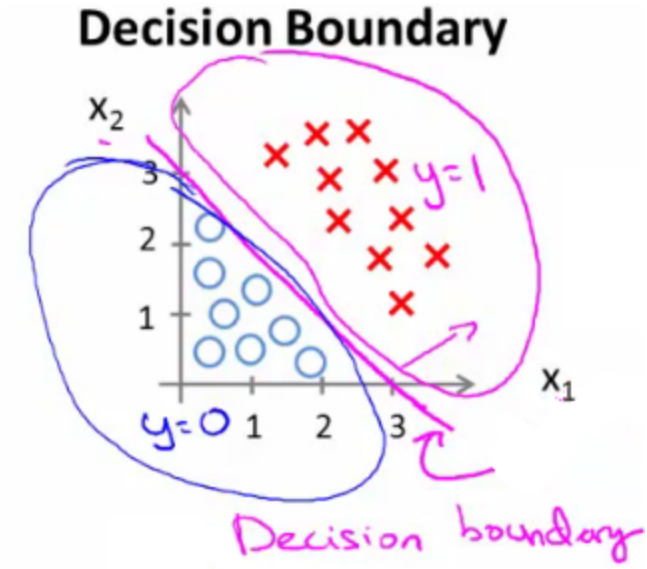
Decision boundary

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



- So, for example
  - $\theta_0 = -3$

  - $\theta_1 = 1$
  - $\theta_2 = 1$
- So our parameter vector is a column vector with the above values
  - So, θ^T is a row vector = [-3,1,1]
- What does this mean?
  - The z here becomes $\theta^T x$
  - We predict "y = 1" if
    - $-3x_0 + 1x_1 + 1x_2 >= 0$
    - $-3 + x_1 + x_2 >= 0$
- We can also re-write this as
  - If ($x_1 + x_2 >= 3$) then we predict y = 1
  - If we plot
    - $x_1 + x_2 = 3$ we graphically plot our **decision boundary**



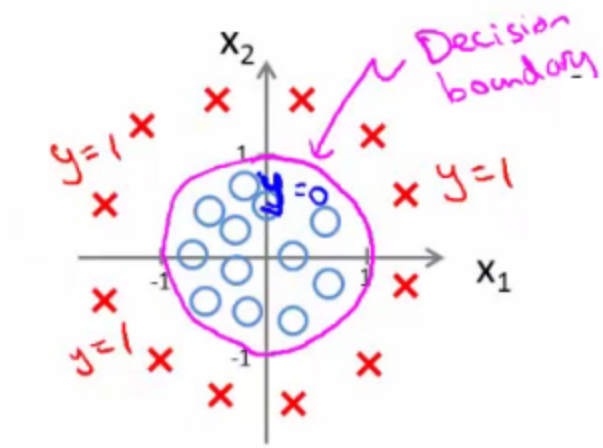
- Means we have these two regions on the graph
  - Blue = false
  - Magenta = true
  - Line = decision boundary
    - Concretely, the straight line is the set of points where $h_\theta(x) = 0.5$ exactly
  - The decision boundary is a property of the hypothesis
    - Means we can create the boundary with the hypothesis and parameters without any data
      - Later, we use the data to determine the parameter values
    - i.e. y = 1 if
      - $5 - x_1 > 0$
      - $5 > x_1$

Non-linear decision boundaries

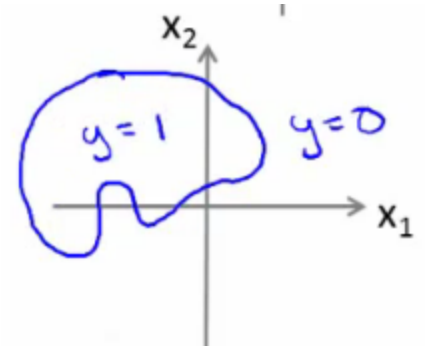
- Get logistic regression to fit a complex non-linear data set
  - Like polynomial regress add higher order terms
  - So say we have

- $h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_3 x_1^2 + \theta_4 x_2^2)$
- We take the transpose of the θ vector times the input vector
  - Say θ^T was [-1,0,0,1,1] then we say;
  - Predict that "y = 1" *if*
    - $-1 + x_1^2 + x_2^2 >= 0$

      or
    - $x_1^2 + x_2^2 >= 1$
  - If we plot $x_1^2 + x_2^2 = 1$
    - This gives us a circle with a radius of 1 around 0



- Mean we can build more complex decision boundaries by fitting complex parameters to this (relatively) simple hypothesis
- More complex decision boundaries?
  - By using higher order polynomial terms, we can get even more complex decision boundaries



Cost function for logistic regression

- Fit θ parameters
- Define the optimization object for the cost function we use the fit the parameters
  - Training set of *m* training examples
    - Each example has is n+1 length column vector

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

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

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

- This is the situation
  - Set of m training examples
  - Each example is a feature vector which is n+1 dimensional
  - $x_0 = 1$
  - $y \in \{0,1\}$
  - Hypothesis is based on parameters (θ)
    - Given the training set how to we chose/fit θ?
- Linear regression uses the following function to determine θ

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

- Instead of writing the squared error term, we can write
  - If we define "cost()" as;
    - $\text{cost}(h_\theta(x^i), y) = 1/2(h_\theta(x^i) - y^i)^2$
    - Which evaluates to the cost for an individual example using the same measure as used in linear regression
  - We can **redefine J(θ) as**

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

    - Which, appropriately, is the sum of all the individual costs over the training data (i.e. the same as linear regression)
- To further simplify it we can get rid of the superscripts
  - So

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

- What does this actually mean?

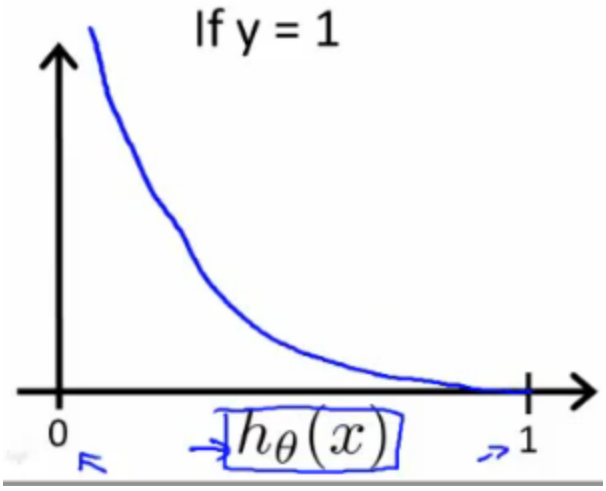
  - This is the cost you want the learning algorithm to pay if the outcome is $h_\theta(x)$ and the actual outcome is y
  - If we use this function for logistic regression this is a **non-convex function** for parameter optimization
    - Could work....
- What do we mean by non convex?
  - We have some function - J(θ) - for determining the parameters
  - Our hypothesis function has a non-linearity (sigmoid function of $h_\theta(x)$)
    - This is a complicated non-linear function
  - If you take $h_\theta(x)$ and plug it into the Cost() function, and them plug the Cost() function into J(θ) and plot J(θ) we find many local optimum -> *non convex function*
  - Why is this a problem
    - Lots of local minima mean gradient descent may not find the global optimum - may get stuck in a global minimum
  - We would like a convex function so if you run gradient descent you converge to a global minimum

A convex logistic regression cost function

- To get around this we need a different, convex Cost() function which means we can apply gradient descent

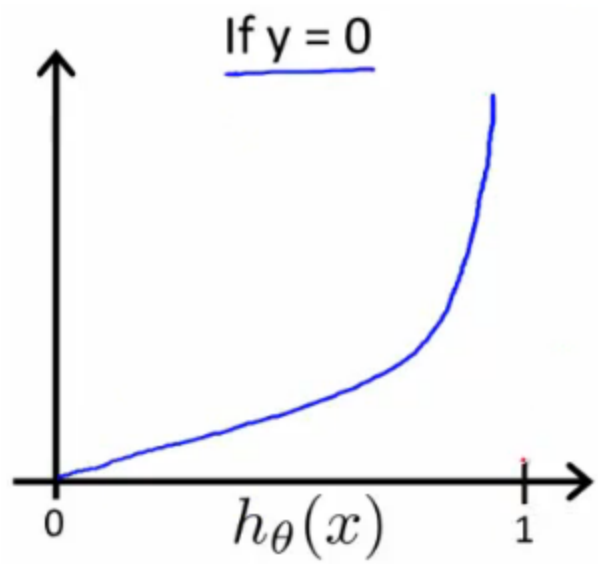
$$\text{Cost}(h_\theta(x), y) = \begin{cases} -\log(h_\theta(x)) & \text{if } y = 1 \\ -\log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$

- **This is our logistic regression cost function**
  - This is the penalty the algorithm pays
  - Plot the function
- Plot y = 1
  - So $h_\theta(x)$ evaluates as $-\log(h_\theta(x))$



- So when we're right, cost function is 0

    - Else it slowly increases cost function as we become "more" wrong
    - X axis is what we predict
    - Y axis is the cost associated with that prediction
- This cost functions has some interesting properties
    - If y = 1 and $h_\theta(x) = 1$
        - If hypothesis predicts exactly 1 and thats exactly correct then that corresponds to 0 (exactly, not nearly 0)
    - As $h_\theta(x)$ goes to 0
        - Cost goes to infinity
        - This captures the intuition that if $h_\theta(x) = 0$ (predict $P(y=1|x;\theta) = 0$) but y = 1 this will penalize the learning algorithm with a massive cost
- What about if y = 0
- then cost is evaluated as $-\log(1- h_\theta(x))$
    - Just get inverse of the other function



- Now it goes to plus infinity as $h_\theta(x)$ goes to 1
- With our particular cost functions $J(\theta)$ is going to be convex and avoid local minimum

Simplified cost function and gradient descent

- Define a simpler way to write the cost function and apply gradient descent to the logistic regression
    - By the end should be able to implement a fully functional logistic regression function
- Logistic regression cost function is as follows

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

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

Note: $y = 0$ or 1 always

- This is the cost for a single example
  - For binary classification problems y is always 0 or 1
    - Because of this, we can have a simpler way to write the cost function
      - Rather than writing cost function on two lines/two cases
      - Can compress them into one equation - more efficient
  - Can write cost function is
    - **$\text{cost}(h_\theta, (x), y) = -y\log(h_\theta(x)) - (1-y)\log(1 - h_\theta(x))$**
      - This equation is a more compact of the two cases above
  - We know that there are only two possible cases
    - y = 1
      - Then our equation simplifies to
        - $-\log(h_\theta(x)) - (0)\log(1 - h_\theta(x))$
          - $-\log(h_\theta(x))$
          - Which is what we had before when y = 1
    - y = 0
      - Then our equation simplifies to
        - $-(0)\log(h_\theta(x)) - (1)\log(1 - h_\theta(x))$
        - $= -\log(1- h_\theta(x))$
        - Which is what we had before when y = 0
    - Clever!
- So, in summary, our cost function for the θ parameters can be defined as

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

- Why do we chose this function when other cost functions exist?
  - This cost function can be derived from statistics using the principle of **maximum likelihood estimation**
    - Note this does mean there's an underlying Gaussian assumption relating to the distribution of features
  - Also has the nice property that it's convex
- To fit parameters θ:
  - Find parameters θ which minimize J(θ)
  - This means we have a set of parameters to use in our model for future predictions
- Then, if we're given some new example with set of features x, we can take the θ which we generated, and output our prediction using

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

- This result is
  - p(y=1 | x ; θ)
    - Probability y = 1, given x, parameterized by θ

How to minimize the logistic regression cost function

- Now we need to figure out how to minimize J(θ)
  - Use gradient descent as before
  - Repeatedly update each parameter using a learning rate

Repeat {

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

(simultaneously update all θ_j)

}

- If you had *n* features, you would have an n+1 column vector for θ
- This equation is the same as the linear regression rule
  - The only difference is that our definition for the hypothesis has changed
- Previously, we spoke about how to monitor gradient descent to check it's working
  - Can do the same thing here for logistic regression
- When implementing logistic regression with gradient descent, we have to update all the θ values (θ_0 to θ_n) simultaneously
  - Could use a for loop
  - Better would be a vectorized implementation
- Feature scaling for gradient descent for logistic regression also applies here

Advanced optimization

- Previously we looked at gradient descent for minimizing the cost function
- Here look at advanced concepts for minimizing the cost function for logistic regression
  - Good for large machine learning problems (e.g. huge feature set)
- *What is gradient descent actually doing?*
  - We have some cost function J(θ), and we want to minimize it
  - We need to write code which can take θ as input and compute the following
    - J(θ)
    - Partial derivative if J(θ) with respect to j (where j=0 to j = n)

$J(\theta)$

$\frac{\partial}{\partial \theta_j} J(\theta)$ (for $j = 0, 1, \ldots, n$)

- Given code that can do these two things
  - Gradient descent repeatedly does the following update

$$\text{Repeat } \{ \theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta) \}$$

- So update each j in θ sequentially
- So, we must;
  - Supply code to compute J(θ) and the derivatives
  - Then plug these values into gradient descent
- Alternatively, instead of gradient descent to minimize the cost function we could use
  - **Conjugate gradient**
  - **BFGS** (Broyden-Fletcher-Goldfarb-Shanno)
  - **L-BFGS** (Limited memory - BFGS)
- These are more optimized algorithms which take that same input and minimize the cost function
- These are *very* complicated algorithms
- Some properties
  - **Advantages**
    - No need to manually pick alpha (learning rate)
      - Have a clever inner loop (line search algorithm) which tries a bunch of alpha values and picks a good one
    - Often faster than gradient descent
      - Do more than just pick a good learning rate
    - Can be used successfully without understanding their complexity
  - **Disadvantages**
    - Could make debugging more difficult
    - Should not be implemented themselves
    - Different libraries may use different implementations - may hit performance

Using advanced cost minimization algorithms

- How to use algorithms
  - Say we have the following example

Example:

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

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

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

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

- Example above
  - θ_1 and θ_2 (two parameters)

  - Cost function here is $J(\theta) = (\theta_1 - 5)^2 + (\theta_2 - 5)^2$
  - The derivatives of the $J(\theta)$ with respect to either θ_1 and θ_2 turns out to be the $2(\theta_i - 5)$
- First we need to define our cost function, which should have the following signature

```
function [jval, gradent] = costFunction(THETA)
```

- Input for the cost function is `THETA`, which is a vector of the θ parameters
- Two return values from `costFunction` are
  - `jval`
    - How we compute the cost function θ (the underived cost function)
      - In this case = $(\theta_1 - 5)^2 + (\theta_2 - 5)^2$
  - **gradient**
    - 2 by 1 vector
    - 2 elements are the two partial derivative terms
    - i.e. this is an n-dimensional vector
      - Each indexed value gives the partial derivatives for the partial derivative of $J(\theta)$ with respect to θ_i
      - Where i is the index position in the **gradient** vector
- With the cost function implemented, we can call the advanced algorithm using

```
options= optimset('GradObj', 'on', 'MaxIter', '100'); % define the
options data structure
initialTheta= zeros(2,1); # set the initial dimensions for theta %
initialize the theta values
[optTheta, funtionVal, exitFlag]= fminunc(@costFunction,
initialTheta, options); % run the algorithm
```

- Here
  - `options` is a data structure giving options for the algorithm
  - `fminunc`
    - function minimize the cost function (**f**ind **min**imum of **unc**onstrained multivariable function)
  - `@costFunction` is a pointer to the costFunction function to be used
- For the octave implementation
  - `initialTheta` must be a matrix of at least two dimensions

- How do we apply this to logistic regression?
  - Here we have a vector

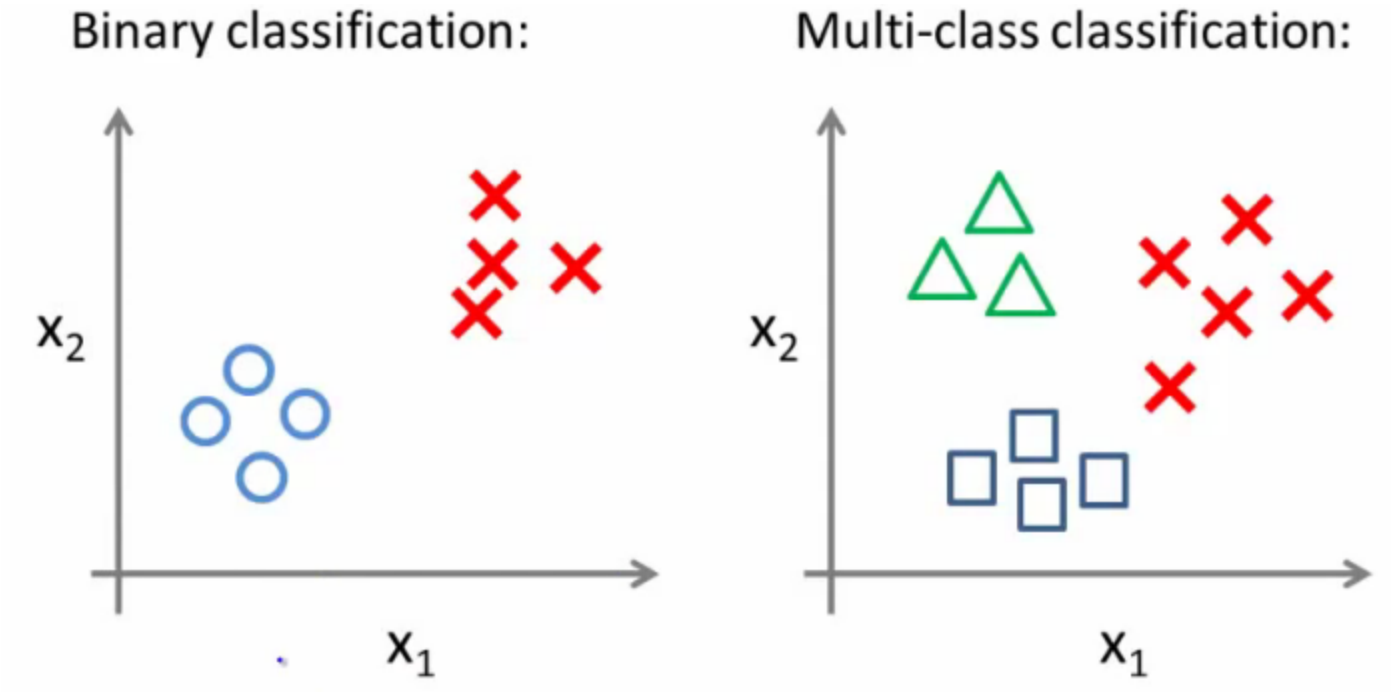
$$\text{theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix}$$

```
function [jVal, gradient] = costFunction(theta)
      jVal = [ code to compute J(θ)];
      gradient(1) = [code to compute ∂/∂θ0 J(θ)];
      gradient(2) = [code to compute ∂/∂θ1 J(θ)];
        :
      gradient(n+1) = [code to compute ∂/∂θn J(θ)  ];
```

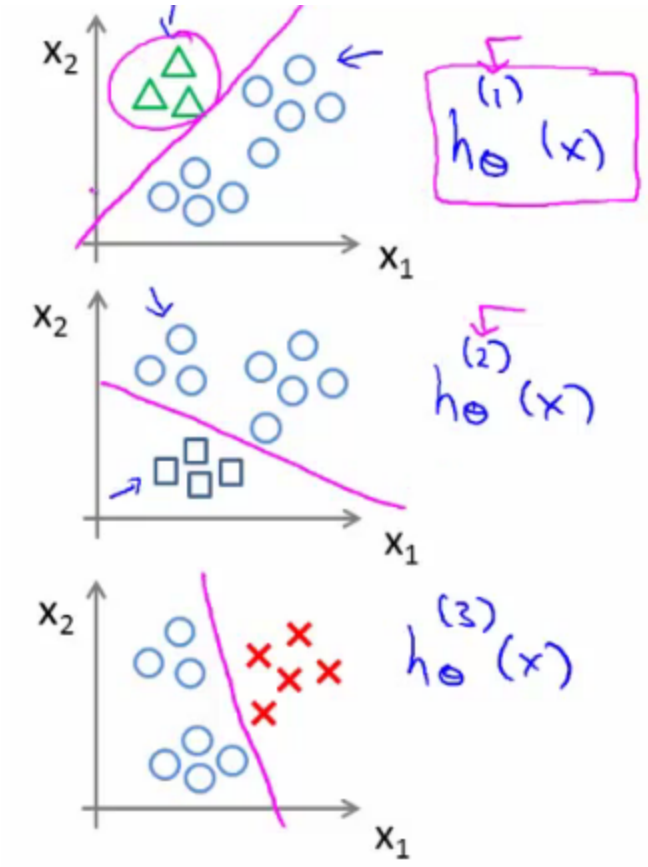
- Here
  - theta is a n+1 dimensional column vector
  - Octave indexes from 1, not 0
- Write a cost function which captures the cost function for logistic regression

Multiclass classification problems

- Getting logistic regression for multiclass classification using **one vs. all**
- Multiclass - more than yes or no (1 or 0)
  - Classification with multiple classes for assignment



- Given a dataset with three classes, how do we get a learning algorithm to work?
  - Use one vs. all classification make binary classification work for multiclass classification
- **One vs. all classification**
  - Split the training set into three separate binary classification problems
    - i.e. create a new fake training set
      - Triangle (1) vs crosses and squares (0) $h_\theta^1(x)$
        - $P(y=1 \mid x_1; \theta)$
      - Crosses (1) vs triangle and square (0) $h_\theta^2(x)$
        - $P(y=1 \mid x_2; \theta)$
      - Square (1) vs crosses and square (0) $h_\theta^3(x)$
        - $P(y=1 \mid x_3; \theta)$



- **Overall**
  - 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 the probability that $h_\theta^{(i)}(x) = 1$