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
    - $h_\theta(x) = 80 + 0.1 x_1 + 0.01 x_2 + 3 x_3 - 2 x_4$
      - 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 $j = 0, \ldots, n$) $\}$

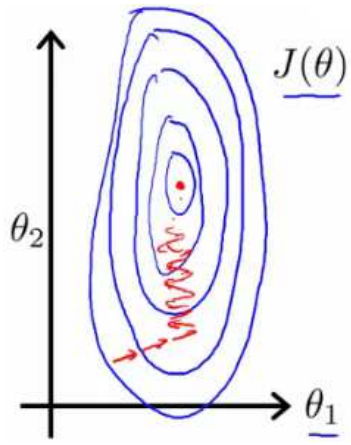
- What's going on here?
  - We're doing this for each j (0 until n) as a simultaneous update (like when n = 1)
  - So, we re-set θ_j to
    - θ_j minus the learning rate (α) times the partial derivative of of the θ vector with respect to θ_j
    - In non-calculus words, this means that we do
      - 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

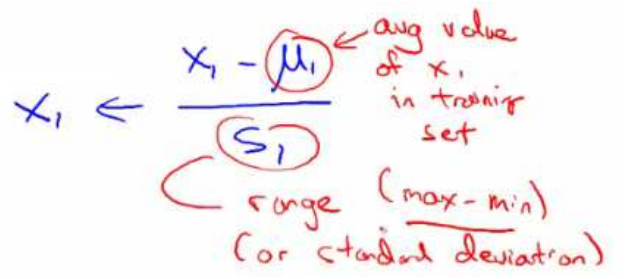
Gradient Decent in practice: 1 Feature Scaling

- 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



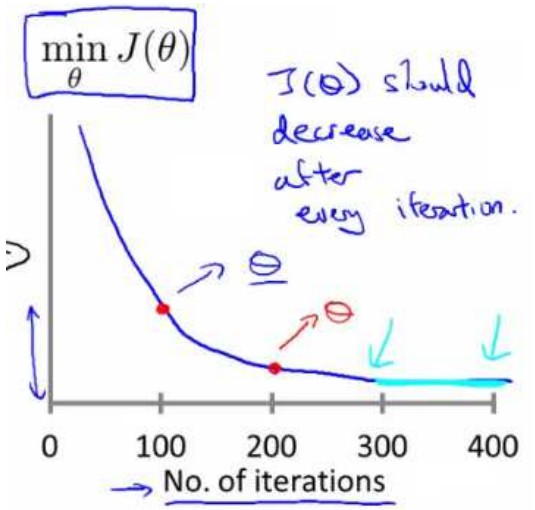
- Instead of max can also use standard deviation

Learning Rate α

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

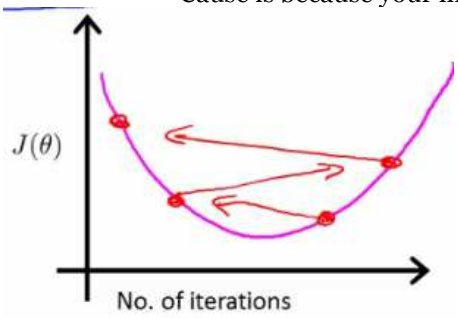
Make sure gradient descent is working

- 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!

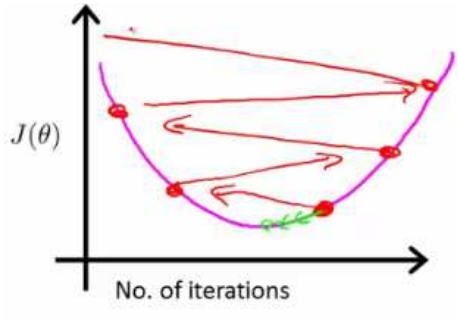


    - Number of iterations varies a lot
        - 30 iterations
        - 3000 iterations
        - 3000 000 iterations
        - Very hard to tel in advance how many iterations will be needed
        - Can often make a guess based a plot like this after the first 100 or so iterations
    - Automatic convergence 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)



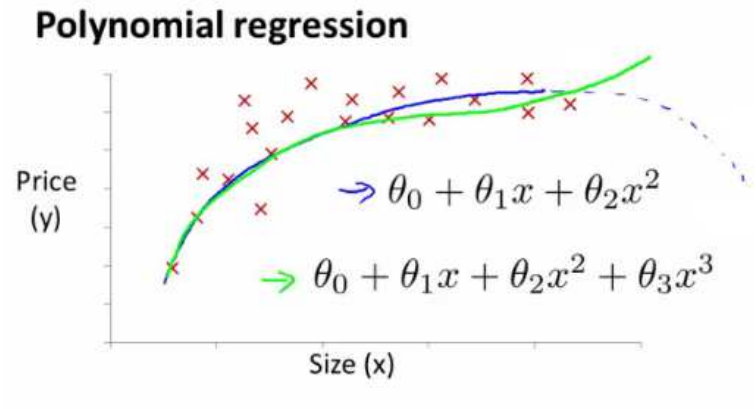
    - So, use a smaller α
- Another problem might be if J(θ) looks like a series of waves
    - Here again, you need a smaller α
- However
    - If α is small enough, J(θ) will decrease on every iteration
    - BUT, if α is too small then rate is too slow
        - A less steep incline is indicative of a 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
        - $\frac{d}{d\theta} J(\theta) =$
            - 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) x_1	Number of bedrooms x_2	Number of floors x_3	Age of home (years) x_4	Price ($1000) y
2104	5	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178

- 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

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

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

- 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

$$x^{(i)} = \begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ x_2^{(i)} \\ \vdots \\ x_n^{(i)} \end{bmatrix} \in \mathbb{R}^{n+1} \qquad \left(\text{design matrix} \right) = \begin{bmatrix} — (x^{(1)})^T — \\ — (x^{(2)})^T — \\ \vdots \\ — (x^{(m)})^T — \end{bmatrix}$$

  - **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