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)
  - $\mathbf{x^i}$
    - 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
  - $\mathbf{x_j^i}$
    - 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

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

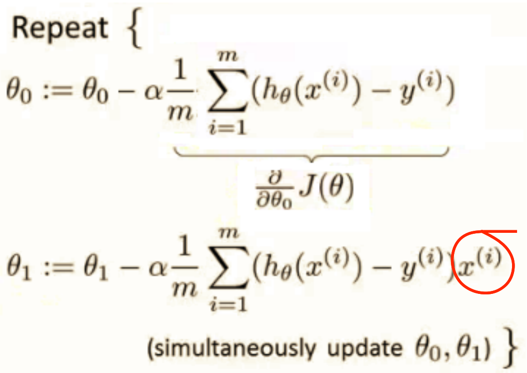
basically yhr avg. of the distance between your validation data points and the n-dimensional prediction contour hø(x) (thus reducing J(Ø) implies a better fitting prediction contour)

- 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** →

$$\begin{aligned}&\text{Repeat } \{\\ &\quad \theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \ldots, \theta_n)\\ &\} \qquad \text{(simultaneously update for every } j = 0, \ldots, n)\end{aligned}$$

ie. if the gradient along the param. feature-j is sloping upwards, weight lower, sloping downwards (towards min.) weight more

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



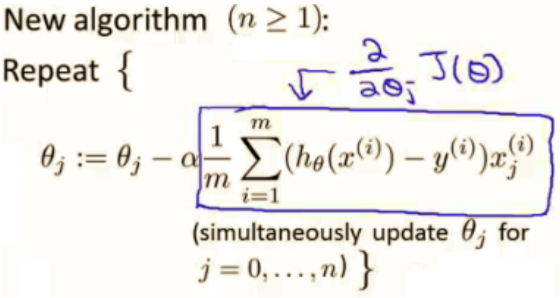
Repeat {

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

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

(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 $(n \geq 1)$:

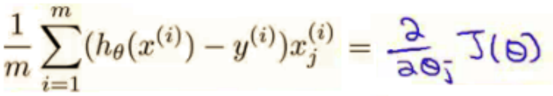
Repeat {

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

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

when slope is neg. (towards minimum), we step towards it (+) in param. Øj

- 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



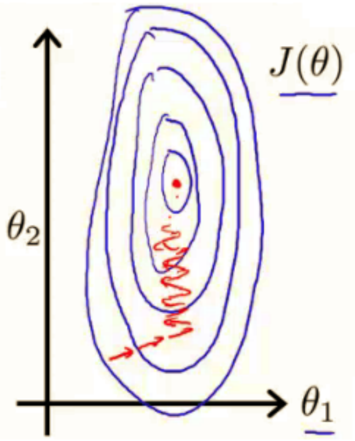
$$\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)} = \frac{\partial}{\partial\theta_j}J(\theta)$$

= slope of the cost function

- 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 —> more chance of overshooting as we step down the contour
  - Running gradient descent on this kind of cost function can take a long time to find the global minimum



REMEBER: the cost function J(Ø) for linear regression has NO LOCAL optima (so can't get stuck at some local optima rather than the true global optimum)

- 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

$$x_1 \leftarrow \frac{x_1 - \mu_1}{s_1}$$

avg value of x_1 in training set

range (max - min)

(or standard deviation)

avg. value of feature n over the entire training set

range of value of feature n over entire training set

- Instead of max can also use standard deviation

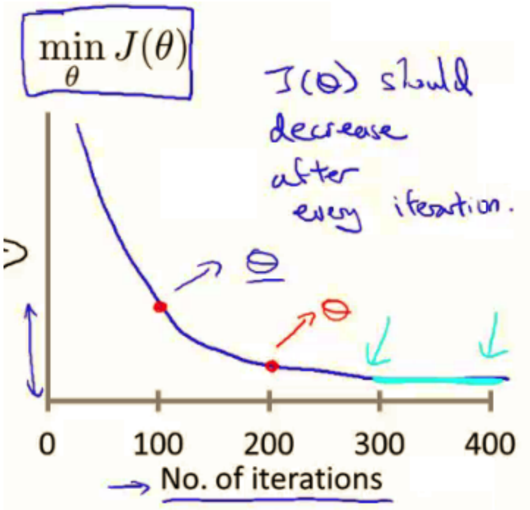
Learning Rate α

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

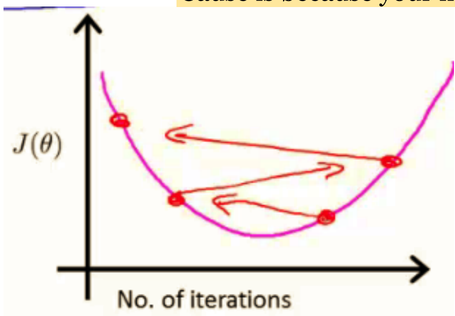
Make sure gradient descent is working

- 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

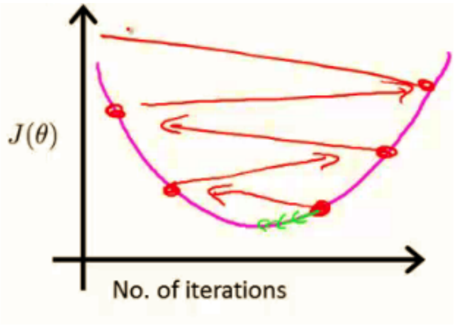
- If, for example, after 1000 iterations you reduce the parameters by nearly nothing you could chose to only run 1000 iterations in the future
- Make sure you don't accidentally hard-code thresholds like this in and then forget about why they're their though!



- 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



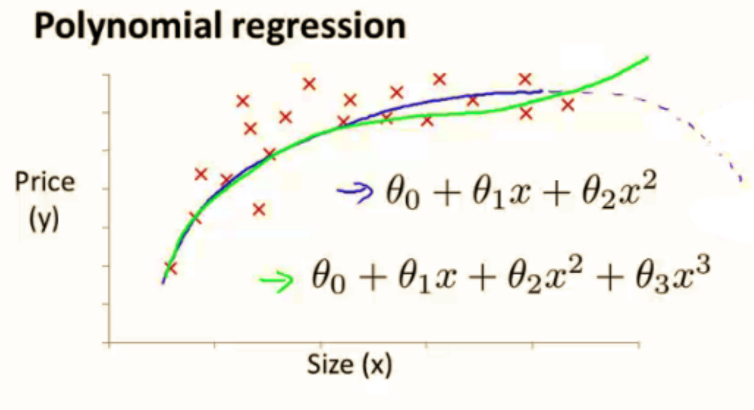
- But you overshoot, so reduce learning rate so you actually reach the minimum (green line)



    - 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



We can change the behavior or curve of our hypothesis function by making it a quadratic, cubic or square root function (or any other form).

For example, if our hypothesis function is hθ(x)=θ0+θ1x1 then we can create additional features based on x1, to get the quadratic function hθ(x)=θ0 + θ1*x1 + θ2*x1^2 or the cubic function hθ(x)=θ0 + θ1*x1 + θ2*x1^2 + θ3*x1^3

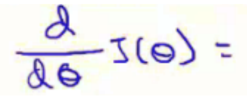
- How do we fit the model to this data
    - To map our old linear hypothesis and cost functions to these polynomial descriptions the easy thing to do is

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

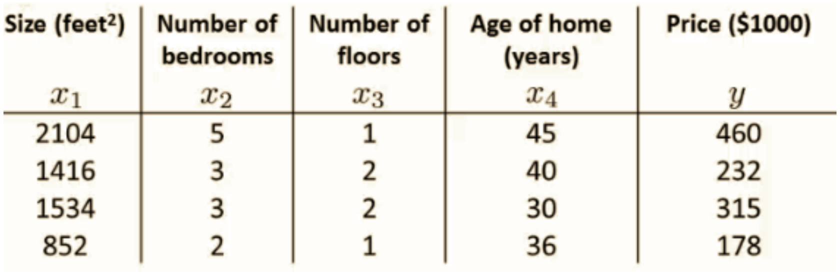
- For some linear regression problems the normal equation provides a better solution
- So far we've been using gradient descent
    - Iterative algorithm which takes steps to converse
- Normal equation solves θ analytically
    - Solve for the optimum value of theta
- Has some advantages and disadvantages

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)	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

      $\theta = (X^TX)^{-1}X^Ty$

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

- 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

$$\underline{x^{(i)}} = \boxed{\begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ x_2^{(i)} \\ \vdots \\ x_n^{(i)} \end{bmatrix}} \in \mathbb{R}^{n+1} \qquad \underset{\text{(design Matrix)}}{X} = \begin{bmatrix} \text{---} \; (x^{(1)})^T \; \text{---} \\ \text{---} \; (x^{(2)})^T \; \text{---} \\ \vdots \\ \text{---} \; (x^{(m)})^T \; \text{---} \end{bmatrix}$$

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

$$\boxed{\theta = (X^TX)^{-1}X^Ty}$$

the normal eq. formula to get values for all ø0, ..., øn

- 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

for many learning algs. we will see later, the normal eq. does not apply and does not work, but for linear regression it can be more efficient

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 as opposed to octave's inv() function
                - 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 ie. certain features are linearly related to each other
                    - 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