

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 i th 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 (θ_1 and θ_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 $[1 \times n+1]$ 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 $[n + 1 \times 1]$
- Now
 - θ^T is a matrix $[1 \times n+1]$
- Which means the inner dimensions of θ^T and X match, so they can be multiplied together as
 - $[1 \times n+1] * [n+1 \times 1]$
 - $= h_{\theta}(x)$
 - So, in other words, the transpose of our parameter vector * an input example X gives you a predicted hypothesis which is $[1 \times 1]$ 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

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

- Similarly, instead of thinking of J as a function of the $n+1$ numbers, $J()$ is just a function of the parameter vector
 - $J(\theta)$

Repeat {

- **Gradient descent** $\rightarrow \theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \dots, \theta_n)$
 } (simultaneously update for every $j = 0, \dots, n$)

- Once again, this is
 - $\theta_j = \theta_j$ - learning rate (α) times the partial derivative of $J(\theta)$ with respect to θ_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 $j = 0, \dots, n$) }

$\downarrow \frac{\partial}{\partial \theta_j} J(\theta)$

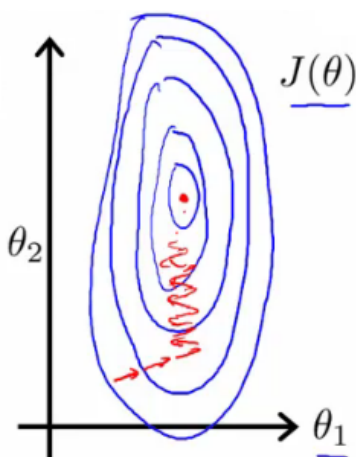
- What's going on here?
 - We're doing this for each j (0 until n) as a simultaneous update (like when $n = 1$)
 - So, we re-set θ_j to
 - θ_j minus the learning rate (α) times the partial derivative of the θ vector with respect to θ_j
 - In non-calculus words, this means that we do
 - Learning rate
 - 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.
 - x_1 = size (0 - 2000 feet)
 - x_2 = 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 x_1 and x_2 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 $(x_i - \text{mean})/\text{max}$
 - So your values all have an average of about 0

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

μ_1 ← avg value of x_1 in training set
 s_1 ← range (max-min) (or standard deviation)

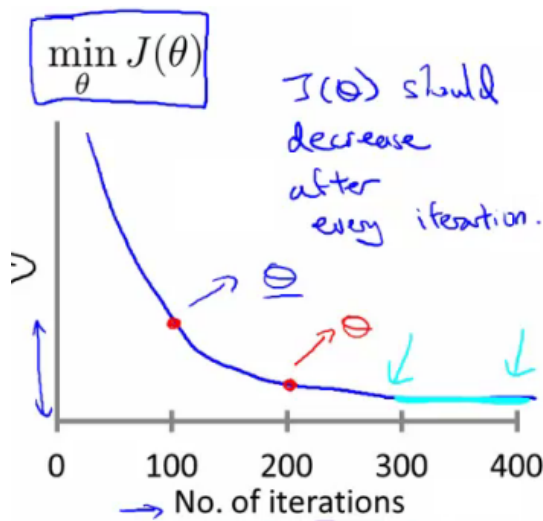
- Instead of max can also use standard deviation

Learning Rate α

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

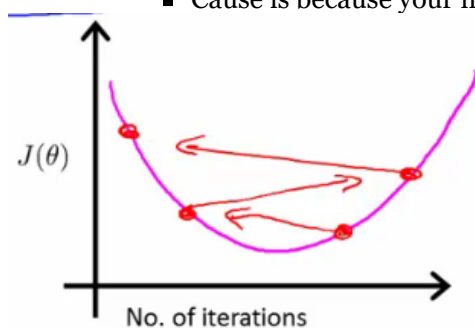
Make sure gradient descent is working

- Plot $\min J(\theta)$ vs. no of iterations
 - (i.e. plotting $J(\theta)$ over the course of gradient descent)
- If gradient descent is working then $J(\theta)$ 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 choose 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 there though!

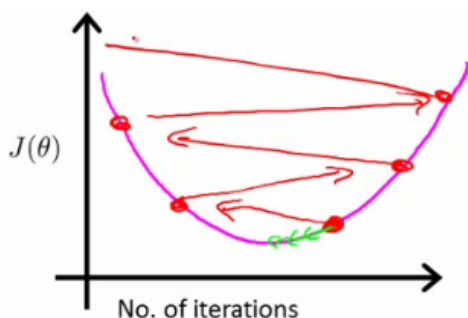


- Number of iterations varies a lot
 - 30 iterations
 - 3000 iterations
 - 3000 000 iterations
 - Very hard to tell in advance how many iterations will be needed
 - Can often make a guess based on a plot like this after the first 100 or so iterations
- Automatic convergence tests
 - Check if $J(\theta)$ 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 $J(\theta)$ 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)



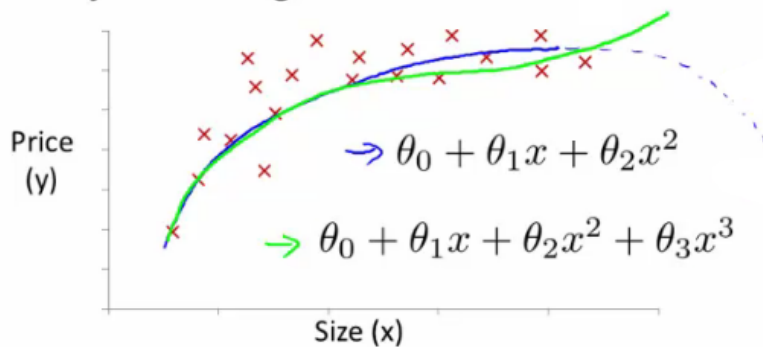
- So, use a smaller α
- Another problem might be if $J(\theta)$ looks like a series of waves
 - Here again, you need a smaller α
- However
 - If α is small enough, $J(\theta)$ will decrease on every iteration
 - BUT, if α is too small then rate is too slow
 - A less steep incline is indicative of a slow convergence, because we're decreasing by less on each iteration than a steeper slope
- Typically
 - Try a range of alpha values
 - Plot $J(\theta)$ 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

Polynomial regression



- 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 $^{1/\text{something}}$ - i.e. square root, cubed root etc
- Lots of features - later look at developing an algorithm to choose 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 converge
- Normal equation solves θ analytically
 - Solve for the optimum value of θ
- 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 $J(\theta)$ with respect to θ
 - Set that derivative equal to 0
 - Allows you to solve for the value of θ which minimizes $J(\theta)$
- 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 $J(\theta)$ 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 $J(\theta)$
 - 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 (feet ²)	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 $[m \times n+1]$ matrix
 - Do something similar for y
 - Construct a column vector y vector $[m \times 1]$ 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 $[m \times (n+1)]$ matrix

$$\underline{x^{(i)}} = \begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ x_2^{(i)} \\ \vdots \\ x_n^{(i)} \end{bmatrix} \in \mathbb{R}^{n+1} \quad \bigg| \quad \text{(design matrix)} \quad = \quad \begin{bmatrix} \text{---} (x^{(1)})^T \text{---} \\ \text{---} (x^{(2)})^T \text{---} \\ \vdots \\ \text{---} (x^{(m)})^T \text{---} \end{bmatrix}$$

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

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

- 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 choose 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 choose 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 $n \times n$ matrix
 - With most implementations computing a matrix inverse grows by $O(n^3)$
 - So not great
 - Slow if 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. $m \leq n$ (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