

# 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  $i^{\text{th}}$  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 ( $\theta_1$  and  $\theta_0$ ) 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  $\theta$
      - 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
    - $h_\theta(x) = \theta^T x$ 
      - $\theta^T$  is an  $[1 \times n+1]$  matrix
      - In other words, because  $\theta$  is a column vector, the transposition operation transforms it into a row

- vector
- So before
  - $\theta$  was a matrix  $[n + 1 \times 1]$
- Now
  - $\theta^T$  is a matrix  $[1 \times n+1]$
- Which means the inner dimensions of  $\theta^T$  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  $\theta_0$  to  $\theta_n$
  - Instead of thinking about this as  $n$  separate values, think about the parameters as a single vector ( $\theta$ )
    - Where  $\theta$  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 ( $\alpha$ ) times the partial derivative of  $J(\theta)$  with respect to  $\theta_j$
  - We do this through a **simultaneous update** of every  $\theta_j$  value
- Implementing this algorithm
  - When  $n = 1$

Repeat {

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

$\underbrace{\hspace{10em}}_{\frac{\partial}{\partial \theta_0} J(\theta)}$

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

(simultaneously update  $\theta_0, \theta_1$ ) }

- Above, we have slightly different update rules for  $\theta_0$  and  $\theta_1$ 
  - 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  $\theta_j$  for  $j = 0, \dots, n$ ) }

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

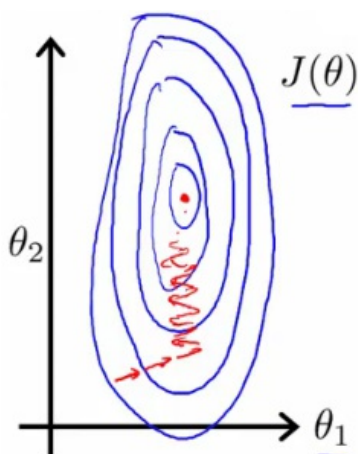
- What's going on here?
  - We're doing this for each  $j$  (0 until  $n$ ) as a simultaneous update (like when  $n = 1$ )
  - So, we re-set  $\theta_j$  to
    - $\theta_j$  minus the learning rate ( $\alpha$ ) times the partial derivative of of the  $\theta$  vector with respect to  $\theta_j$
    - 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  $\theta_1$  vs.  $\theta_2$  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

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

$\mu_1$  ← avg value of  $x_1$  in training set  
 $s_1$  ← range (max-min) (or standard deviation)

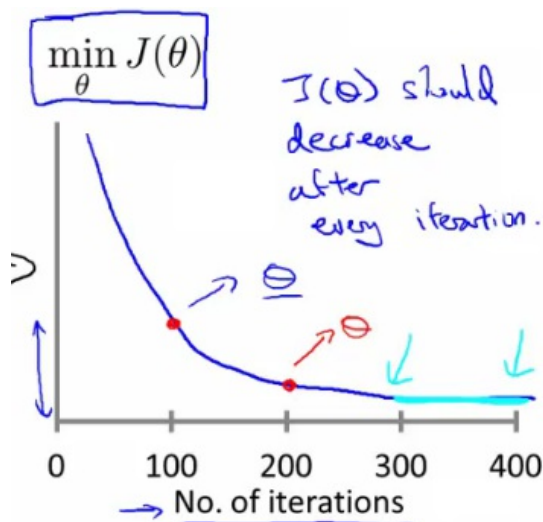
- Instead of max can also use standard deviation

## Learning Rate $\alpha$

- Focus on the learning rate ( $\alpha$ )
- Topics
  - Update rule
  - Debugging
  - How to choose  $\alpha$

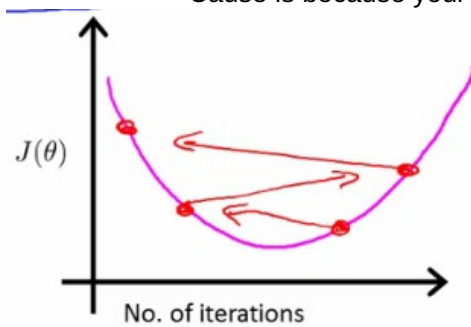
### **Make sure gradient descent is working**

- 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!

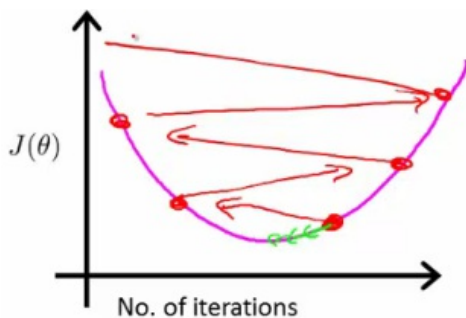


- Number of iterations varies a lot
  - 30 iterations
  - 3000 iterations
  - 3000 000 iterations
  - Very hard to tell in advance how many iterations will be needed
  - Can often make a guess based on a plot like this after the first 100 or so iterations
- Automatic convergence tests
  - Check if  $J(\theta)$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



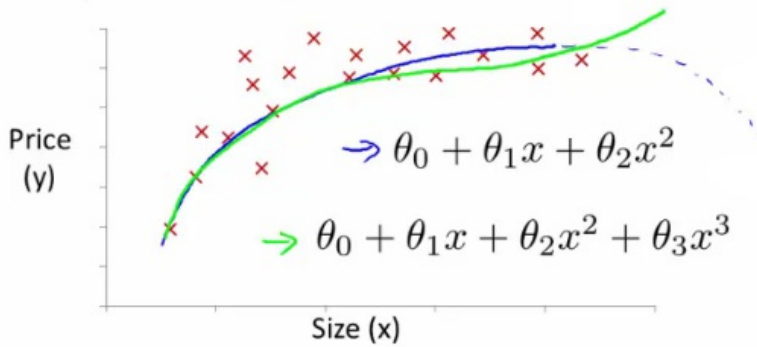
- So, use a smaller  $\alpha$
- Another problem might be if  $J(\theta)$  looks like a series of waves
  - Here again, you need a smaller  $\alpha$
- However
  - If  $\alpha$  is small enough,  $J(\theta)$  will decrease on every iteration
  - BUT, if  $\alpha$  is too small then rate is too slow
    - 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  $\theta$  analytically
  - Solve for the optimum value of theta
- Has some advantages and disadvantages

### How does it work?

- Simplified cost function
  - $J(\theta) = a\theta^2 + b\theta + c$ 
    - $\theta$  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  $\theta$
        - Set that derivative equal to 0
        - Allows you to solve for the value of  $\theta$  which minimizes  $J(\theta)$
- In our more complex problems;
  - Here  $\theta$  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  $\theta_j$  and set to 0 for every  $j$
      - Do that and solve for  $\theta_0$  to  $\theta_n$
      - This would give the values of  $\theta$  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 <sup>2</sup> )	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 ( $X^T X$  inverse times  $X^T y$ )
 
$$\theta = (X^T X)^{-1} X^T y$$

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

- 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  $\rightarrow$  row) and using it for a row in the design  $A$
    - This creates an  $[m \times (n+1)]$  matrix

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

- **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 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  $n \times n$  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