

# CS395: Selected CS1 (Introduction to Machine Learning)

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#### References:

https://www.coursera.org/learn/machine-learning (Andrew Ng)
Machine learning A to Z: Kirill Eremenko ©superdatascience

# Linear Algebra review: Matrices and vectors

(Self review)

#### Vector: Special case of the matrix

#### n x 1 matrix

$$y = \begin{bmatrix} 4 \\ 50 \\ 3 \\ 25 \end{bmatrix} 4 - dimentional vector n = 4$$

$$y_i = i^{th} \text{ element.}$$

$$y_2 = 50$$

1-indexed vs 0-indexed:

$$y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} \qquad y = \begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

#### **Matrix Addition**

$$\begin{bmatrix} 1 & 5 & 9 \\ 2 & 6 & 11 \\ 3 & 7 & 12 \end{bmatrix} + \begin{bmatrix} 10 & 0 & 5 \\ 2 & 4 & 3 \\ 5 & 2 & 2 \end{bmatrix} = \begin{bmatrix} 11 & 5 & 14 \\ 4 & 10 & 14 \\ 8 & 9 & 14 \end{bmatrix}$$
3 x 3

We can add only two matrices that are of **the same dimensions**. So this example is a 3 x 3 matrix, the result in same dimension 3x3.

Addition and subtraction are **element-wise**, so you simply add or subtract each corresponding element

#### Scalar Multiplication

$$3 \times \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} = \begin{bmatrix} 3 & 6 \\ 9 & 12 \end{bmatrix} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \times 3$$

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} / 4 = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \times \frac{1}{4} = \begin{bmatrix} 1/4 & 1/2 \\ 3/4 & 1 \end{bmatrix}$$

**Combination of Operands** 

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

Scaler Multiplication

$$\begin{bmatrix} 3 \\ 12 \\ 6 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 5 \end{bmatrix} - \begin{bmatrix} 1 \\ 0 \\ \frac{2}{3} \end{bmatrix} =$$

$$\begin{bmatrix} 2 \\ 12 \\ 10\frac{1}{3} \end{bmatrix}$$

#### Matrix Vector Multiplication

$$\begin{bmatrix} 5 & 1 \\ 2 & 6 \\ 3 & 4 \end{bmatrix} = \begin{bmatrix} 15 \\ 34 \\ 26 \end{bmatrix}$$

$$A \times x = y$$

$$\begin{bmatrix} 5 & 1 \\ 2 & 6 \\ 3 & 4 \end{bmatrix} \begin{bmatrix} 2 \\ 5 \end{bmatrix} = \begin{bmatrix} 15 \\ 34 \\ 26 \end{bmatrix}$$

$$3 \times 2 \qquad 2 \times 1 \qquad 3 \times 1 \text{ matrix} \rightarrow 3 \text{ dim vector}$$

To get

 $y_i$ , multiply A's  $i^{th}$  row with elements of vector x, and add them up.

$$5 \times 2 + 1 \times 5 = 15$$

$$2 \times 2 + 6 \times 5 = 34$$

$$3 \times 2 + 4 \times 5 = 26$$

An m x n matrix multiplied by an n x 1 vector results in an m x 1 vector.

#### **Matrix Multiplication**

$$C_{11}=1+0+6=7$$
 $C_{21}=4+0+12=16$ 
 $C_{12}=2+10+3=15$ 
 $C_{22}=8+25+6=39$ 

An **m x n matrix** multiplied by an **n x o matrix** results in an **m x o** matrix. In the above example, a 2 x 3 matrix times a 3 x 2 matrix resulted in a 2 x 2 matrix.

#### Matrix Multiplication Properties

- •Matrices are **not commutative**:  $A \times B \neq B \times A$
- •Matrices are **associative**:  $(A \times B) \times C = A \times (B \times C)$
- •Identity Matrix I, or  $I_{n\times n}$  for any A, A, I=I, A=A

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

#### Inverse and Transpose

- The **inverse** of a matrix A ( $m \times m$ ) is denoted $A^{-1}$ . Multiplying by the inverse results in the identity matrix.  $A \times A^{-1} = 1$
- A non square matrix does not have an inverse matrix.

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

#### Transpose

- The **transposition**  $B_{ij} = A_{ji}$  of a matrix is like rotating the matrix 90° in clockwise direction and then reversing it.
- $\bullet \quad A_{ij} = A_{ij}^T$

# Numerical Example on Linear Regression with one variable

# Recap:

Hypothesis: 
$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

Parameters: 
$$\theta_0, \theta_1$$

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

Goal: 
$$\min_{\theta_0, \theta_1} \text{minimize } J(\theta_0, \theta_1)$$

### **Gradient Descent**

- We make steps down the cost function in the direction with the steepest descent, and the size of each step is determined by the parameter  $\alpha$ , which is called the **learning rate**.
- The gradient descent algorithm is:

Repeat until **convergence** {

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)$$
 (for  $j = 0$  and  $j = 1$ )

**Learning rate (step size)** 

# **Gradient Descent for Linear Regression**

• When specifically applied to the case of **linear regression**, a new form of the gradient descent equation can be derived. We can substitute our actual cost function and our actual hypothesis function and modify the equation to:

Start by initializing the parameters  $heta_0, heta_1$  randomly

$$\text{Should be done simultaneously} \begin{cases} \theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m \left(h_\theta(x^{(i)}) - y^{(i)}\right) & \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) \\ \theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^m \left(h_\theta(x^{(i)}) - y^{(i)}\right) \cdot x^{(i)} & \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) \\ \end{cases}$$

# Hypothesis using Matrix Product

$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

$$x = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} \in \mathbb{R}^2 \qquad \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} \in \mathbb{R}^2$$

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} \in \mathbb{R}^2$$

For convenience of notation, define  $x_0 = 1$ 

$$h_{\theta}(x) = \theta_0 x_0 + \theta_1 x_1 = \begin{bmatrix} \theta_0 \theta_1 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \theta^T x$$

# Linear Regression with one variable Example:

 Suppose we are given a dataset, and we need to find the hypothesis of linear regression:

Experience (X)	Salary (y) (in lakhs)	
2	3	
6	10	
5	4	
7	13	

Experience (X)	Salary (y) (in lakhs)		
2	3		
6	10		
5	4		
7	13		

- a) In the start,  $\theta_0$  and  $\theta_1$  values are randomly chosen.
  - Let us suppose,  $\theta_0 = 0$  and  $\theta_1 = 0$ .
- b) Predicted values after iteration 1 with Linear regression hypothesis.

$$h_{\theta} = \theta_0 x_0 + \theta_1 x_1 = \begin{bmatrix} \theta_0 \theta_1 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix}$$

$$h_{\theta} = \left[ \begin{array}{ccc} \theta_0 & \theta_1 \end{array} \right] \left[ \begin{array}{cccc} x_0 & x_0 & x_0 \\ x_1 & x_2 & x_3 & x_4 \end{array} \right]$$
 One training example 
$$= \left[ \begin{array}{cccc} 0 & 0 \end{array} \right] \cdot \left[ \begin{array}{cccc} 1 & 1 & 1 & 1 \\ 2 & 6 & 5 & 7 \end{array} \right] = \left[ \begin{array}{ccccc} 0 & 0 & 0 & 0 \end{array} \right]$$

#### c) Cost function Error

= 36.75

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} [h_{\theta}(x_i) - y_i]^2$$

$$= \frac{1}{2*4} [(0-3)^2 + (0-10)^2 + (0-4)^2 + (0-13)^2]$$

$$= \frac{1}{8} [9 + 100 + 16 + 169]$$

#### d) Gradient Descent – Updating $\theta_0$ value

Here, j=0

$$\theta_0 = \theta_0 - \frac{\alpha}{m} \sum_{i=1}^{m} (h_{\theta}(x_i) - y_i)$$

$$= 0 - \frac{0.001}{4} [(0 - 3) + (0 - 10) + (0 - 4) + (0 - 13)]$$

$$= -\frac{0.001}{4} [(-3) + (-10) + (-4) + (-13)]$$

$$= -\frac{0.001}{4} [-30]$$

$$= 0.0075$$
Algorithm repeated to the property of the

# Experience (X) Salary (y) (in lakhs) 2 3 6 10 5 4 7 13

#### **Algorithm GD for linear regression:**

repeat until convergence {

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

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

#### e) Gradient Descent – Updating $\theta_1$ value

Here, j=1

 $=-\frac{0.001}{4}[-177]$ 

= 0.04425

$$\theta_1 = \theta_1 - \frac{\alpha}{m} \sum_{i=1}^m (h_\theta(x_i) - y_i) \cdot x_i$$

$$= 0 - \frac{0.001}{4} [(0 - 3)2 + (0 - 10)6 + (0 - 4)5 + (0 - 13)7]$$

$$= -\frac{0.001}{4} [(-6) + (-60) + (-20) + (-91)]$$

#### **Algorithm GD for linear regression:**

repeat until convergence {

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

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

Experience (X)

2

6

5

Salary (y) (in lakhs)

3

10

4

13

**Iteration 2 – \theta\_0 = 0.0075 and \theta\_1 = 0.04425** Predicting values after iteration 1 with linear regression hypothesis

$$h_{\theta} = \begin{bmatrix} \theta_0 & \theta_1 \end{bmatrix} \begin{bmatrix} x_0 & x_0 & x_0 & x_0 \\ x_1 & x_2 & x_3 & x_4 \end{bmatrix}$$

$$= \begin{bmatrix} 0.0075 & 0.04425 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 6 & 5 & 7 \end{bmatrix}$$

$$= \begin{bmatrix} 0.096 & 0.273 & 0.22875 & 0.31725 \end{bmatrix}$$

- Similar to iteration no. 1 performed above
  - we will again calculate Cost function and update  $\theta_j$  values using Gradient Descent.
  - We will keep on iterating until Cost function doesn't reduce further (converge). At that point, model achieves best θ values.
  - Using these θ values in the model hypothesis will give the best prediction results.

#### **Testing:**

If we have the house sizes and the hypotheses  $(h_{\theta})$ , and you need to predict the prices of these houses

#### house sizes:

$$h_{\theta}(x) = -40 + 0.25 x$$

#### Matrix 4x2:

#### Prediction 4x1 matrix:

 $h_{\theta}(2100)$ 

$$\begin{bmatrix}
 -40 \times 1 + 0.25 \times 2100 \\
 -40 \times 1 + 0.25 \times 3150 \\
 -40 \times 1 + 0.25 \times 4152 \\
 -40 \times 1 + 0.25 \times 1108
 \end{bmatrix}$$

#### **Testing:**

If we have the house sizes and more than one hypotheses  $(h_{\theta})$ :

#### house sizes: 2100 3150 4152 1108 $m \times n$ matrix Matrix 4x2:

$$h_{\theta}(x) = -40 + 0.25 x$$
 $h_{\theta}(x) = 200 + 0.1 x$ 
 $h_{\theta}(x) = -150 + 0.4 x$ 

$$\times \begin{bmatrix} -40 \\ 0.25 \end{bmatrix} \begin{bmatrix} 200 \\ 0.1 \end{bmatrix} = 0.4$$

Prediction 4x3 matrix:



**m x o** matrix

2x3

n x o matrix

# Linear regression with multiple variables

#### **Multiple variables (Features)**

Linear regression with multiple variables is also known as "multivariate linear regression".

$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

Size $(feet)^2$ $x$	Price (\$1000) y	
2104	460	
1416	232	
1534	315	
852	178	

Could the prediction be more accurate if we add #of rooms?



#### **Multiple variables (Features)**

Siz	$ze(feet)^2$	Number of bedrooms	Number of floors	Age of home (years)	<i>Price</i> (\$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
				···	•••

**m**, number of training examples

**n**, number of features

 $x^{(i)}$ , the input (features) of the  $i^{th}$  training example

 $x_j^{(i)}$ , value of feature j in the  $i^{th}$  training example

$$x^{(2)} = \begin{bmatrix} 1416 \\ 3 \\ 2 \\ 40 \end{bmatrix}$$

$$x_4^{(3)} = 30$$

#### Hypothesis

$$h_{\theta}(x) = \theta_0 + \theta_1 x \times$$

Size (feet) <sup>2</sup>	Number of bedrooms	Number of floors	Age of home (years)	<i>Price</i> (\$1000)
$\uparrow x_1$	$\uparrow x_2$	$\uparrow x_3$		y
2104	<b>5</b>	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178

$$h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \theta_4 x_4$$

$$h_{\theta}(x) = 80 \quad 0.1x_1 \quad 0.01x_2 \quad 3x_3 \quad 2x_4$$

$$h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n$$

$$h_{\theta}(x) = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n$$

For convenience of notation, define 
$$x_0 = 1$$
 
$$h_{\theta}(x) = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n$$
 
$$x = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^{n+1}$$
 
$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \\ \vdots \\ \theta_n \end{bmatrix} \in \mathbb{R}^{n+1}$$

#### Hypothesis for Multiple Features

$$x = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^{n+1} \qquad \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \\ \vdots \\ \theta_n \end{bmatrix} \in \mathbb{R}^{n+1}$$

$$h_{\theta}(x) = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n$$

$$h_{\theta} = \theta^T x = \begin{bmatrix} \theta_0 & \theta_1 & \dots & \theta_n \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix}$$

$$\begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$$

#### GD. for Multiple Variables

$$x_0 = 1$$

Hypothesis: 
$$h_{\theta}(x) = \theta^T x = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n$$

Parameters: 
$$\theta_0$$
,  $\theta_1$ , ....,  $\theta_n$ 

$$\theta$$
 is  $n+1$  dimension vector

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

$$= \frac{1}{2m} \sum_{i=1}^{m} (\theta^T x^{(i)} - y^{(i)})^2$$

$$= \frac{1}{2m} \sum_{i=1}^{m} (\left( \sum_{j=0}^{n} \theta_{j} x_{j}^{(i)} \right) - y^{(i)})^{2}$$

#### **GD** for Multiple Variables

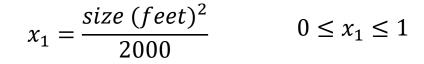
# The gradient descent equation itself is generally the same form; we just have to repeat it for our n features

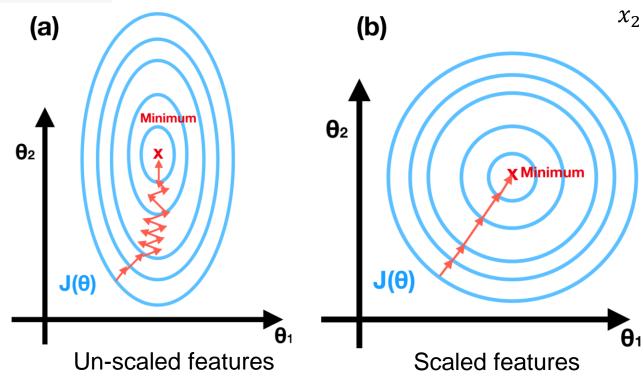
```
repeat until convergence : {
                \theta_0 \coloneqq \theta_0 - \alpha \frac{\partial}{\partial \theta_i} J(\theta), simultaneously updates for every j = 0,1,2,...,n
     Previously (n=1):
                                                                                           For (n>1):
     Repeat {
                                                                                           repeat until convergence : {
        \theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)})
\underbrace{\frac{\partial}{\partial \theta_0} J(\theta)}
                                                                                                           \theta_i := \theta_i - \alpha \frac{1}{m} \sum_{i=1}^m \left( h_{\theta}(x^{(i)}) - y^{(i)} \right) x_i^{(i)}
                                                                                                                     , simultaneously updates \theta_i
         \theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) x^{(i)}
                                                                                                                      for every j = 0,1,2,...,n
                           (simultaneously update \theta_0, \theta_1)
```

- We can speed up gradient descent by having each of our input values in roughly the same range.
- Because  $\theta$  will:
  - descend quickly on small ranges
  - descend slowly on large ranges, and
  - oscillate inefficiently down to the optimum when the variables are very uneven.
- The way to prevent this is to modify the ranges of our input variables so that they are all roughly the same.

#### Make sure features are on same scale.

Example: 
$$x_1 = size(0 - 2000 feet^2)$$
  
 $x_2 = number of bedrooms (1 - 5)$ 





$$x_2 = \frac{No\ of\ bedrooms}{5} \qquad 0 \le x_2 \le 1$$

Get every feature into approximately  $-1 \le x_j \le 1$  range

(Do not apply to  $x_0 = 1$ )

#### 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

#### Mean Normalization

• Replace  $x_i$  with  $\mu_i$  to make features have approximately zero mean (**Do not apply to**  $x_0 = 1$ )

$$x_i = \frac{x_i - \mu_i}{S_i}, \qquad x_1 = \frac{size - 1000}{2000}$$

 $\mu_i$ , is the average value of x in the training dataset  $s_i$ , is the range of values (max - min) or the standard deviation.

$$\sigma = \sqrt{rac{\sum (x_i - \mu)^2}{N}}$$

 $\sigma$  = population standard deviation

 $oldsymbol{N}$  = the size of the population

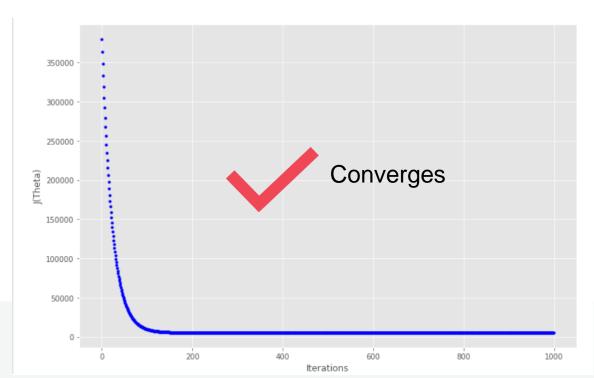
 $oldsymbol{x_i}$  = each value from the population

 $\mu$  = the population mean

#### Gradient Descent in Practice II - Learning Rate

- Debugging gradient descent.
- Make a plot with <u>number of iterations</u> of gradient descent on the x axis and the cost function  $J(\theta)$  on the y axis.
- $J(\theta)$  should decrease after each iteration else decrease  $\alpha$

**Automatic convergence test.** Declare convergence if  $J(\theta)$  decreases by less than  $\varepsilon$  in one iteration, where  $\varepsilon$  is some small value such as  $10^{-3}$ . However in practice it's difficult to choose this threshold value.



#### Gradient Descent in Practice II - Learning Rate

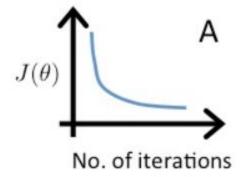
It has been proven that if learning rate  $\alpha$  is sufficiently small, then  $J(\theta)$  will decrease on every iteration. When Gradient Descent can't decrease the cost-function anymore and remains more or less on the same level, we say it has **converged**.

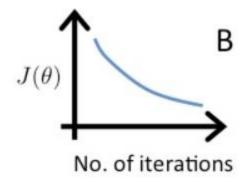
#### Note:

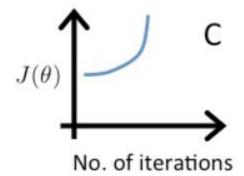
If you see in the plot that your learning curve is just going up and down, without really reaching a lower point, you also should try to decrease the learning rate.

If  $\alpha$  is too small: slow convergence.

If  $\alpha$  is too high: the cost function is increasing







#### Features and Polynomial Regression / choice of features

- We can improve our features and the form of our hypothesis function.
- We can combine multiple features into one. For example, we can combine  $x_1$  and  $x_2$  into a new

feature  $x_3$  by taking  $x_1$ .  $x_2$ 

Hypothesis:  $h_{\theta}(x) = \theta_0 + \theta_1 x_1$  $h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2(x_1)^2 + \theta_3(x_1)^3$  $h_{\theta}(x) = \theta_0 + \theta_1(x_1) + \theta_2 \sqrt{x_1}$ 

square root function 200000 feature scaling becomes very important.

## Thanks