Lectures 10 and 11: Linear Regression

Lecture 10: Linear Regression 1

Linear Regression – Problem 1

Suppose that:

- I want to relate two random scalar phenomena, X and Y, to identify the relationships existing between them,
- I can measure their values several times i, so I can have a set of pairs (x_i, y_i) with i spanning the interval of observation, say $i \in [0 \dots n-1]$

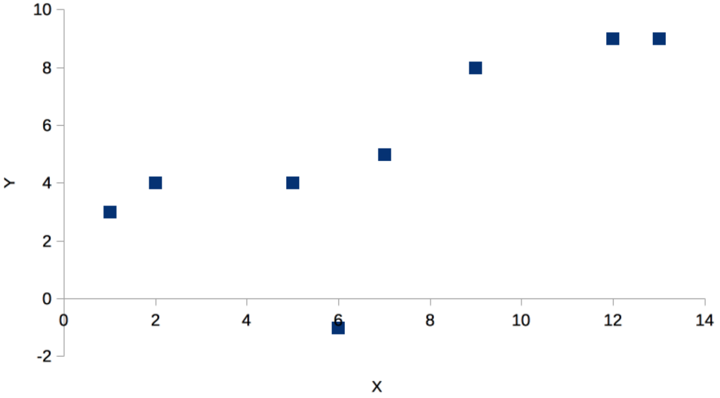
i	**X**	**Y**
0	1	3
1	2	4
2	5	4
3	6	-1
4	7	5
5	9	8
6	12	9
7	13	9

Linear Regression – Problem 2

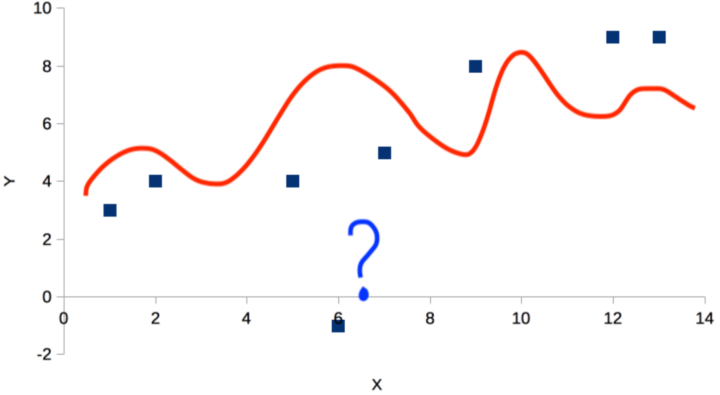
Using a simple and common approach, I may try to build a relationship between the two phenomena. However:

- What kind of relationships I am going to look for?
- How do I build it?

In other words, I have this set of points:



How can I build a line that represent the relationships between these two sets?



Linear Regression – Definition

We need to define:

- A mean function that represents the relationship that I hypothesize between the phenomena X and Y
- A cost-minimization function to define the parameters of the mean function

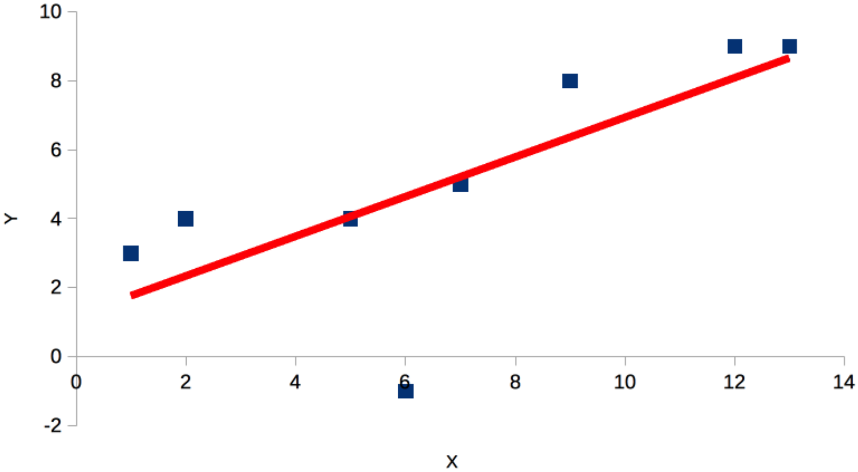
We will use initially:

- As mean function the simple line
- As cost function the square of the errors between the modeled values and the real values

We define Ordinary Least Squares (OLS) Linear Regression as a simple line that minimizes a square error between modelled values and real values.

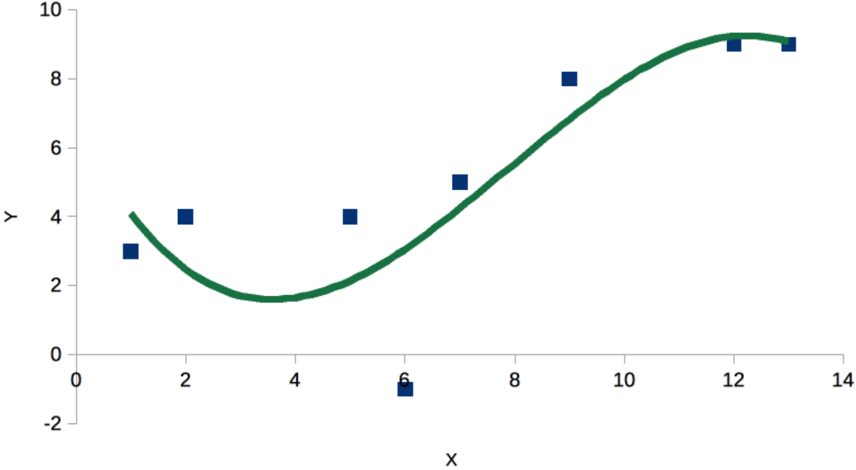
Linear Regression – Goal

This is what we would like to build:

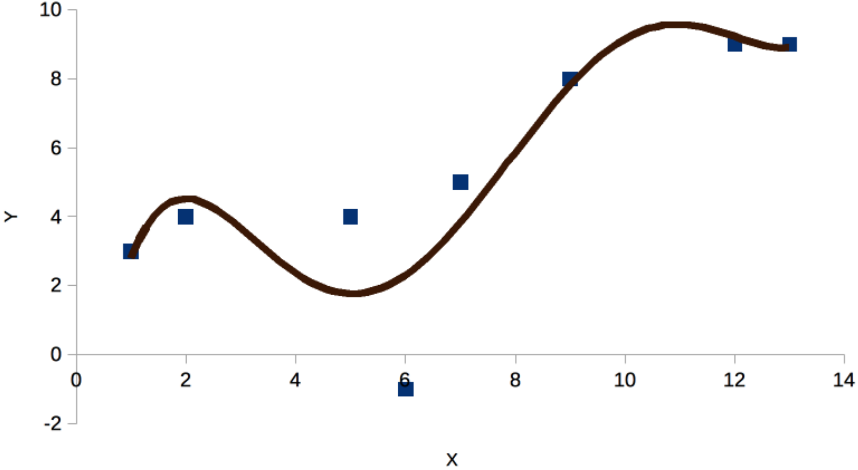


Linear Regression – Alternative Goal 1

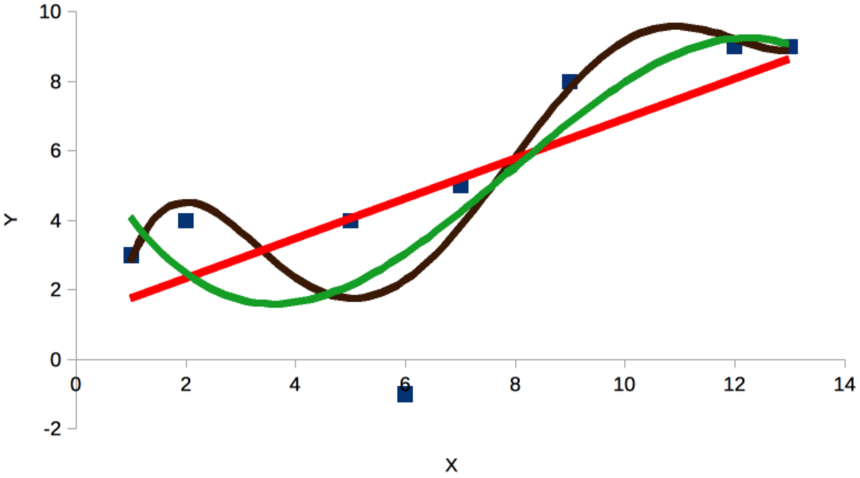
But we could have used as a mean function a cubic function:



But we could have used as a mean function a fifth order function:



What are the differences between all these 3?



I want to build a model of the kind:

$$Y = \theta_0 + \theta_1 X$$

Where X and Y are the phenomena that we are measuring.

Note:

- we know that there is no line passing for n arbitrary points with $n \leq 3$
- we need to introduce an approximation

$$\hat{Y} = \theta_0 + \theta_1 \hat{X} + \epsilon$$

- in our case ϵ is the error that is introduced by the approximation
- as we said, our cost function, our distance from the model, will be the square of the error ϵ^2
- θ_0 and θ_1 are called the regression coefficients

Altogether:

- we have a set of pairs (x_i,y_i) with $i \in [0 \dots n-1]$
- we want to build n linear equations of the kind (the mean function):

$$y_i = \theta_0 + \theta_1 x_i + \epsilon_i$$

- and we start with an approximation of the kind:

$$\hat{y}_i = \theta_0 + \theta_1 x_i$$

Linear Regression – Formula 3

Altogether:

- our goal is to compute θ_0 and θ_1 that minimize the quadratic error (the cost function)

$$\sum_{i=0}^{n-1} \epsilon_i^2$$

- notice that:
  - we will denote as (x_i, y_i) the original data
  - we will denote as $(\hat{x}_i, \hat{y}_i)$ the approximation that we obtain in the linear regression
  - x_i and $\hat{x}_i$ are the same
  - there could be errors in the slides and you get extra credits by finding them

Linear Regression – Computation

- Since

$$y_i = \theta_0 + \theta_1 x_i + \epsilon_i$$

- therefore

$$\epsilon_i = y_i - \theta_0 - \theta_1 x_i$$

- we need to minimize:

$$\sum_{i=0}^{n-1} \epsilon_i^2 = \sum_{i=0}^{n-1} (y_i - \theta_0 - \theta_1 x_i)^2$$

- we need to zero the two partial derivatives, for $j = 0, 1$:

$$\frac{\partial \sum_{i=0}^{n-1} (y_i - \theta_0 - \theta_1 x_i)^2}{\partial \theta_j}$$

- so we have to solve two simple equations and then to check the Hessian

Linear Regression – Computation for θ_0

$$\frac{\partial \sum_{i=0}^{n-1}(y_i - \theta_0 - \theta_1 x_i)^2}{\partial \theta_0} = 0 \Rightarrow$$

$$\frac{\partial \sum_{i=0}^{n-1}(y_i - \theta_0 - \theta_1 x_i)^2}{\partial \sum_{i=0}^{n-1}(y_i - \theta_0 - \theta_1 x_i)} \frac{\partial \sum_{i=0}^{n-1}(y_i - \theta_0 - \theta_1 x_i)}{\partial \theta_0} = 0 \Rightarrow$$

$$\sum_{i=0}^{n-1} 2(y_i - \theta_0 - \theta_1 x_i)(-1) = 0 \Rightarrow$$

$$2\sum_{i=0}^{n-1}(y_i - \theta_0 - \theta_1 x_i) = 0 \Rightarrow$$

$$\sum_{i=0}^{n-1}(y_i - \theta_0 - \theta_1 x_i) = 0$$

Linear Regression – Computation for θ_1

$$\frac{\partial \sum_{i=0}^{n-1}(y_i - \theta_0 - \theta_1 x_i)^2}{\partial \theta_1} = 0 \Rightarrow$$

$$\frac{\partial \sum_{i=0}^{n-1}(y_i - \theta_0 - \theta_1 x_i)^2}{\partial \sum_{i=0}^{n-1}(y_i - \theta_0 - \theta_1 x_i)} \frac{\partial \sum_{i=0}^{n-1}(y_i - \theta_0 - \theta_1 x_i)}{\partial \theta_1} = 0 \Rightarrow$$

$$\sum_{i=0}^{n-1} 2(y_i - \theta_0 - \theta_1 x_i)(-x_i) = 0 \Rightarrow$$

$$2\sum_{i=0}^{n-1} x_i(y_i - \theta_0 - \theta_1 x_i) = 0 \Rightarrow$$

$$\sum_{i=0}^{n-1} x_i(y_i - \theta_0 - \theta_1 x_i) = 0$$

From the first equation:

$$\sum_{i=0}^{n-1}(\theta_0) = \sum_{i=0}^{n-1}(y_i - \theta_1 x_i) \Rightarrow$$

$$\sum_{i=0}^{n-1}(\theta_0) = \sum_{i=0}^{n-1}(y_i) - \theta_1 \sum_{i=0}^{n-1}(x_i) \Rightarrow$$

$$n\theta_0 = n\bar{y} - n\theta_1\bar{x} \Rightarrow$$

$$\theta_0 = \bar{y} - \theta_1\bar{x}$$

$$\sum_{i=0}^{n-1} x_i(y_i - \theta_0 - \theta_1 x_i) = 0 \Rightarrow$$

$$\sum_{i=0}^{n-1} x_i y_i - \theta_0 \sum_{i=0}^{n-1} x_i - \theta_1 \sum_{i=0}^{n-1} x_i^2 = 0 \Rightarrow$$

$$\sum_{i=0}^{n-1} x_i y_i - n\theta_0 \bar{x} - n\theta_1 \bar{x^2} = 0 \Rightarrow$$

Linear Regression – Combining the result

Substituting $\theta_0 = \bar{y} - \theta_1\bar{x}$:

$$\sum_{i=0}^{n-1} x_i y_i - n(\bar{y} - \theta_1\bar{x}) - n\theta_1\overline{x^2} = 0 \Rightarrow$$

$$\sum_{i=0}^{n-1} x_i y_i - n\bar{y}\bar{x} + n\theta_1\bar{x}^2 - n\theta_1\overline{x^2} = 0$$

$$n\theta_1(\overline{x^2} - \bar{x}^2) = \sum_{i=0}^{n-1} x_i y_i - n\bar{y}\bar{x}$$

Linear Regression – Final step

$$\theta_1 = \frac{\sum_{i=0}^{n-1} x_i y_i - n\bar{y}\bar{x}}{n(\overline{x^2} - \bar{x}^2)}$$

$$\theta_1 = \frac{\frac{\sum_{i=0}^{n-1} x_i y_i}{n} - \bar{y}\bar{x}}{\overline{x^2} - \bar{x}^2}$$

$$\theta_1 = \frac{Cov(x, y)}{Var(x)}$$

Which we can also write as:

$$\theta_1 = \frac{\sum_{i=0}^{n-1}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=0}^{n-1}(x_i - \bar{x})^2}$$

Going back to our exercise...

Using the formula above we obtain that for the following dataset:

i	**X**	**Y**
0	1	3
1	2	4
2	5	4
3	6	-1
4	7	5
5	9	8
6	12	9
7	13	9

We have an equation:

$$\hat{Y} = \theta_0 + \theta_1 \hat{X}$$

with:

- $\theta_0 = 1.179$
- $\theta_1 = 0.574$

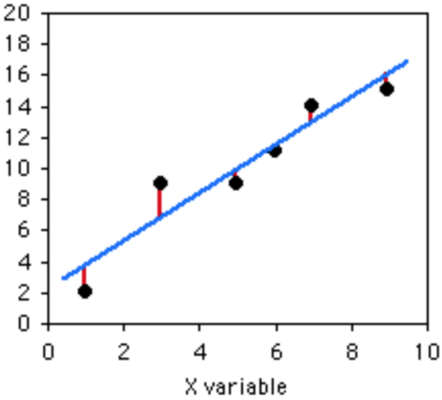
Our model

i	**X**	**Y**	$\hat{Y}$	ϵ
0	1	3	1.753	1.247
1	2	4	2.327	1.673
2	5	4	4.049	-0.049
3	6	-1	4.623	-5.623
4	7	5	5.197	-0.197
5	9	8	6.345	1.655
6	12	9	8.067	0.933
7	13	9	8.641	0.359

Build a linear regression for the following dataset:

X	Y
1	2
3	9
5	9
6	11
7	14
9	15

Linear Regression – Exercise



The regression equation for these numbers is $\hat{y} = 2.0286 + 1.5429x$. Now, fill the blanks using such equation and calculate the sum of squared deviations (last column).

x	y	Predicted y ($\hat{y}$)	Deviate from predicted (abs.)	Squared deviate
1	2			
3	9			
5	9			
6	11			
7	14			
9	15			

Results. The sum of squared deviations: 10.8

x	y	Predicted y ($\hat{y}$)	Deviate from predicted (abs.)	Squared deviate
1	2	3.57	1.57	2.46
3	9	6.66	2.34	5.48
5	9	9.74	0.74	0.55
6	11	11.29	0.29	0.08
7	14	12.83	1.17	1.37
9	15	15.91	0.91	0.83

Linear Regression – Modeling

In fact, we might think to use linear regression to model phenomena, assuming a linear dependence between input (the collected parameters) and output.

Here are some “real world” examples (w.r.t. certain assumptions):

- - Impact of SAT Score (or GPA) on College Admissions;
- - Impact of product price on number of sales;
- - Impact of rainfall amount on the number of fruits yielded;
- - Impact of blood alcohol content on coordination.

Linear Regression – Evaluation

We can evaluate the quality of linear regression, i.e. assess how good the model for the data that we have:

- \- by the sum of squares of residuals;
- \- by the coefficient of determination.

The sum of squared errors

The sum of squares of residuals, also called the residual sum of squares:

$$SS_{res} = \sum_i (y_i - \hat{y}_i)^2$$

In the case above SS_{res} is equal to 39.751672.

The coefficient of determination (R^2)

The coefficient of determination describes the proportion of variance of the dependent variable explained by the regression model. If the regression model is "perfect", SS_{res} is zero, and R^2 is 1.

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$

The total sum of squares:

$$SS_{tot} = \sum_i (y_i - \bar{y})^2$$

where

$$\bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i$$

In the example above

$$SS_{tot} = \sum_i (y_i - \bar{y})^2 = 82.875$$

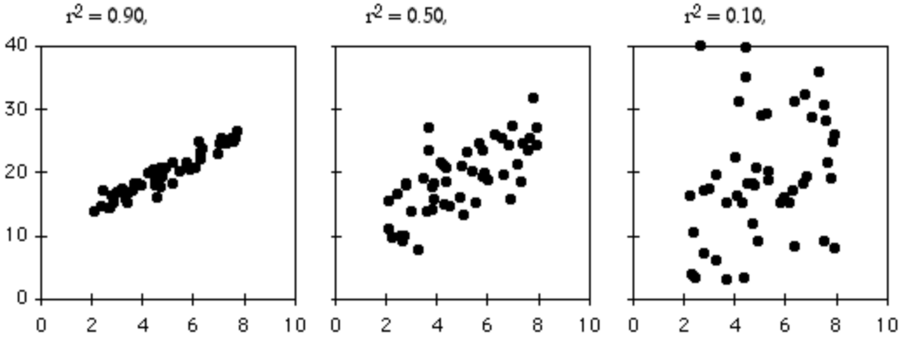
Remember that:

$$SS_{res} = \sum_i (y_i - \hat{y}_i)^2 = 39.751672$$

Therefore:

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}} = 1 - \frac{39.751672}{82.875} = 0.5203$$

Coefficient of determination (R^2)



- The "X" variable is often called "feature" in machine learning.
- Indeed, we could have multiple features, say, n.
- If we also have m observations, we could build a system of m equations of the kind:

$$y_i = \boldsymbol{\theta}^T \cdot \boldsymbol{x}_i + \epsilon_i, i = 1 \dots m$$

- and then we will build our linear regression (approximation) as:

$$\hat{y}_i = \boldsymbol{\theta}^T \cdot \boldsymbol{\hat{x}_i}, i = 1 \dots m$$

- where $\boldsymbol{x}_i$ and $\boldsymbol{\hat{x}_i}$– are vectors of $n+1$ features for the i-th observation

Question: Why here we use $n+1$?

A closed-form solution of Linear Regression

To find the value of $\boldsymbol{\theta}$, there is a closed-form solution, a mathematical equation that gives the result directly.
This is called the **Normal Equation**:

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

Derivation of the closed-form solution (1/4)

- We start considering a set of m equations of the form:

$$\hat{y}_i = \boldsymbol{\theta}^T \boldsymbol{x}_i, i = 1 \dots m$$

  where $\boldsymbol{x}_i$ has dimension $n+1$
- We move all the model in matrix format:

$$\hat{\boldsymbol{y}} = \boldsymbol{X} \cdot \boldsymbol{\theta}$$

  Notice that $\hat{\boldsymbol{y}}$ and $\boldsymbol{y}$ have dimension (m,1), $\boldsymbol{X}$ (m,n+1), and θ (n+1,1). $\boldsymbol{X} \cdot \boldsymbol{\theta}$ has therefore dimension (m,1) as it should be.
- The error vector $\boldsymbol{\epsilon}$ is defined for each pair as:

$$\boldsymbol{\epsilon} = \hat{\boldsymbol{y}} - \boldsymbol{y} = \boldsymbol{X} \cdot \boldsymbol{\theta} - \boldsymbol{y}$$

- And the square of the error is:

$$(\boldsymbol{X} \cdot \boldsymbol{\theta} - \boldsymbol{y})^T (\boldsymbol{X} \cdot \boldsymbol{\theta} - \boldsymbol{y})$$

Derivation of the closed-form solution (2/4)

- To determine the values of the parameters we take the partial derivatives and we null them:

$$\frac{\partial (\boldsymbol{X} \cdot \boldsymbol{\theta} - \boldsymbol{y})^T (\boldsymbol{X} \cdot \boldsymbol{\theta} - \boldsymbol{y})}{\partial \boldsymbol{\theta}} = 0$$

- Now we evaluate:

$$\frac{\partial (\boldsymbol{X} \cdot \boldsymbol{\theta} - \boldsymbol{y})^T (\boldsymbol{X} \cdot \boldsymbol{\theta} - \boldsymbol{y})}{\partial \boldsymbol{\theta}} =$$

$$= \frac{\partial ((\boldsymbol{X} \cdot \boldsymbol{\theta})^T (\boldsymbol{X} \cdot \boldsymbol{\theta}) - (\boldsymbol{X} \cdot \boldsymbol{\theta})^T \boldsymbol{y} - \boldsymbol{y}^T \boldsymbol{X} \cdot \boldsymbol{\theta} + \boldsymbol{y}^T \boldsymbol{y})}{\partial \boldsymbol{\theta}} =$$

$$= \frac{\partial ((\boldsymbol{X} \cdot \boldsymbol{\theta})^T (\boldsymbol{X} \cdot \boldsymbol{\theta}) - 2(\boldsymbol{X} \cdot \boldsymbol{\theta})^T \boldsymbol{y} + \boldsymbol{y}^T \boldsymbol{y})}{\partial \boldsymbol{\theta}}$$

Derivation of the closed-form solution (3/4)

- Now we can consider that:

$$\frac{\partial(\boldsymbol{y}^T\boldsymbol{y})}{\partial\boldsymbol{\theta}} = 0$$

- that:

$$\frac{\partial((\boldsymbol{X}\cdot\boldsymbol{\theta})^T\boldsymbol{y})}{\partial\boldsymbol{\theta}} = \boldsymbol{X}^T\boldsymbol{y}$$

- Notice that $\boldsymbol{X}^T\boldsymbol{y}$ has dimension (n+1,m) $\cdot$ (m,1), that is, (n+1,1).
- and finally that:

$$\frac{\partial((\boldsymbol{X}\cdot\boldsymbol{\theta})^T(\boldsymbol{X}\cdot\boldsymbol{\theta}))}{\partial\boldsymbol{\theta}} = 2\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{\theta}$$

- Notice that $\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{\theta}$ has dimension (n+1,m) $\cdot$ (m,n+1) $\cdot$ (n+1,1), that is, (n+1,1) as it should be.

Derivation of the closed-form solution (4/4)

- Substituting the results in the original formula:

$$2\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{\theta} - 2\boldsymbol{X}^T\boldsymbol{y} = 0 \Rightarrow$$

$$\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{\theta} = \boldsymbol{X}^T\boldsymbol{y} \Rightarrow$$

- Notice that $\boldsymbol{X}^T\boldsymbol{X}$ has dimension (n+1,m) $\cdot$ (m,n+1), that is, (n+1,n+1). Notice that m $\gg$ n, so we *hope* that $\boldsymbol{X}^T\boldsymbol{X}$ is invertible.

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

- QED.

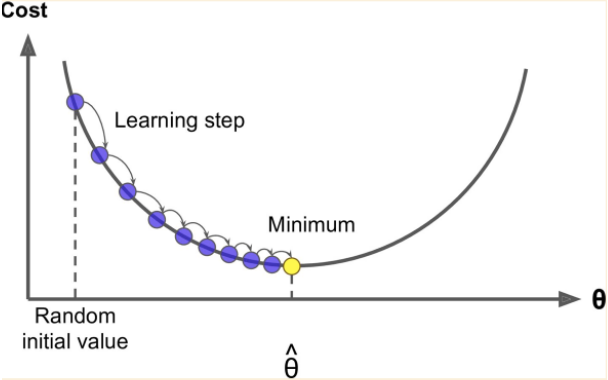
Computational complexity

The Normal Equation computes the inverse of $X^T \cdot X$, which is an n x n matrix (where n is the number of features).

The computational complexity of inverting such a matrix is typically about $O(n^{2.4})$ to $O(n^3)$ (depending on the implementation).

In other words, if you double the number of features, you multiply the computation time by roughly $2^{2.4} = 5.3$ to $2^3 = 8$.

Gradient Descent is a very generic optimization algorithm capable of finding optimal solutions to a wide range of problems. The general idea of Gradient Descent is to tweak parameters iteratively in order to minimize a cost function.



Gradient Descent - Computation

To implement Gradient Descent, you need to compute the gradient of the MSE cost function with regards to each model parameter θ_j.
Mean squared error (MSE) cost function for a Linear Regression model:

$$MSE(\theta) = \frac{1}{m}\sum_{k=1}^{m}(\boldsymbol{\theta}^T \cdot \boldsymbol{x}^{(k)} - \boldsymbol{y}^{(k)})^2$$

$x^{(k)}$ - k-th observation vector ($x^{(k)}$ is an n-dimensional vector)

Gradient Descent - Computation

To implement Gradient Descent, you need to compute the gradient of the MSE cost function with regards to each model parameter θ_j.

$$\frac{\partial}{\partial \theta_j} MSE(\theta) = \frac{2}{m} \sum_{i=1}^{m} (\theta^T \cdot \boldsymbol{x}^{(i)} - \boldsymbol{y}^{(i)}) x_j^{(i)}$$

Gradient Descent - Computation

In vector form:

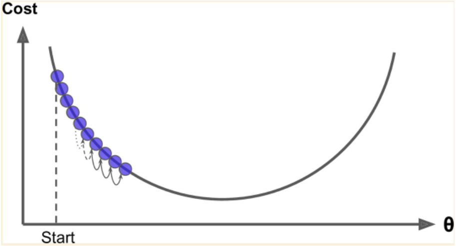
$$\nabla_\theta MSE(\theta) = \frac{2}{m}\boldsymbol{X}^T(\boldsymbol{X} \cdot \boldsymbol{\theta} - \boldsymbol{y})$$

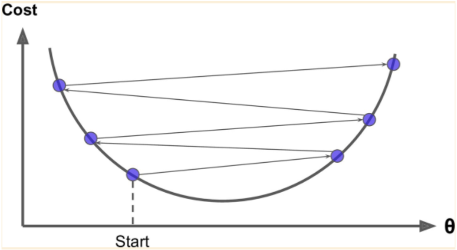
We update vector $\boldsymbol{\theta}$ step by step:

$$\boldsymbol{\theta}^{next} = \boldsymbol{\theta} - \eta \nabla_\theta MSE(\theta)$$

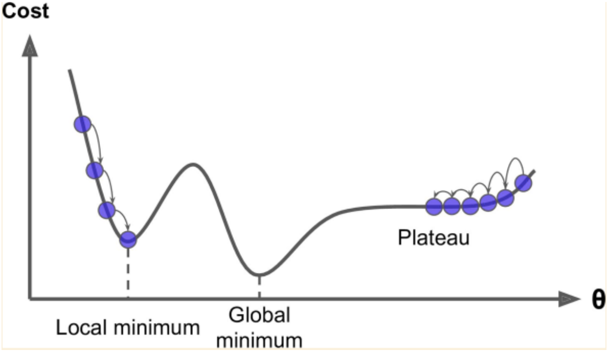
η – learning rate

Learning rate





Pitfalls of Gradient Descent



Linear Regression is a statistical model developed in the field of Regression Analysis.
Later it was borrowed for the use of Machine Learning field.

Terminology difference

Regression analysis	**Machine Learning**
estimation, fitting	training, learning
regressors	features
response	target

References

1) http://www.cs.umd.edu/~djacobs/CMSC426/Convolution.pdf

2) https://www.researchgate.net/post/Difference_between_convolution_and_correlation

3) https://www.tutorialspoint.com/signals_and_systems/convolution_and_correlation.htm