### Aprendizagem Aplicada à Segurança

(Mestrado em Cibersegurança-DETI-UA)





LECTURE 1 ML MODULE
Supervised learning –
Linear Regression

Petia Georgieva (petia@ua.pt)

DETI/IEETA – UA

#### LINEAR REGRESSION - Outline

#### 1. Univariate linear regression

- Cost (loss) function Mean Squared Error (MSE)
- Cost function convergence
- Gradient descent algorithm

#### 2. Multivariate linear regression

-Overfitting problem

**3. Regularization =>** way to deal with overfitting



# Supervised Learning - CLASSIFICATION vs REGRESSION

**Classification**- the label is an integer number.

(e.g. 0, 1 for binary classification)

Ex. CPU load, Network traffic, memory use => anomaly detection (yes/no)

**Regression** - the label is a real number.

#### **Examples of regression problems:**

- Weather forecast
- Predicting wind velocity from temperature, humidity, air pressure
- Time series prediction of stock market indices

Ex. Network traffic at times k, k-1, k-p =>

Predict Network traffic at time k+1



### Standard Notations & Data shape

x – input vector of features, attributes

y – output vector of labels, ground truth, target

m - number of training examples

n - number of features

 $h_{\theta}(x)$  - model (hypothesis)

 $\boldsymbol{\theta}$  - vector of model parameters

Training set: data matrix X (m rows, n columns)

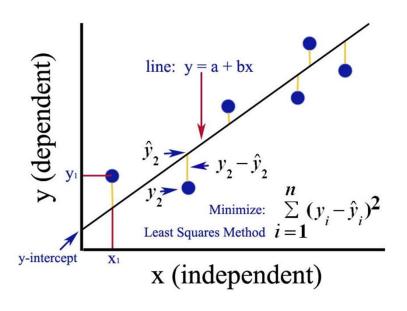
	feature x <sub>1</sub>	feature x <sub>2</sub>	 feature x <sub>n</sub>	output(label) y
Example 1	X1 <sup>(1)</sup>		X <sub>n</sub> <sup>(1)</sup>	y <sup>(1)</sup>
Example 2	X <sub>1</sub> <sup>(2)</sup>		x <sub>n</sub> <sup>(2)</sup>	y <sup>(2)</sup>
Example i	X1 <sup>(i)</sup>		x <sub>n</sub> <sup>(i)</sup>	y <sup>(i)</sup>
Example m	X <sub>1</sub> <sup>(m)</sup>		x <sub>n</sub> <sup>(m)</sup>	y <sup>(m)</sup>



# Supervised Learning – univariate regression

Problem: Learning to predict the housing prices (output) as a function of the living area (input/feature)

Living area (feet <sup>2</sup> )	Price (1000\$s)
2104	400
1600	330
2400	369
1416	232
3000	540
:	:





# Supervised Learning – univariate linear regression

$$h_{\theta}(x) = \theta_{0} + \theta_{1}x_{1} = \begin{bmatrix} 1 & x_{1} \begin{bmatrix} \theta_{0} \\ \theta_{1} \end{bmatrix} = \vec{x}^{T}\vec{\theta}$$

$$\vec{x} = \begin{bmatrix} x_{0} = 1 \\ x_{1} \end{bmatrix}$$
 => in Python => np.dot(X, Theta)

	X <sub>0</sub>	feature x <sub>1</sub>	output(label) y
	(extra column)	(living area)	(price)
Example 1=>	1	x <sup>(1)</sup>	y <sup>(1)</sup>
Example 2=>	1	x <sup>(2)</sup>	y <sup>(2)</sup>
	1		
Example m=>	1	x <sup>(m)</sup>	y <sup>(m)</sup>



### Mean Square Error (MSE)

Linear Model (hypothesis) =>

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

**Cost (loss) function** (Mean Square Error)

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

**m** – number of training examples

$$\min_{\theta} J(\theta)$$

Gradient descent algorithm => iterative algorithm; at each iteration all parameters (theta) are updated simultaneously

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

alpha – learning rate > 0



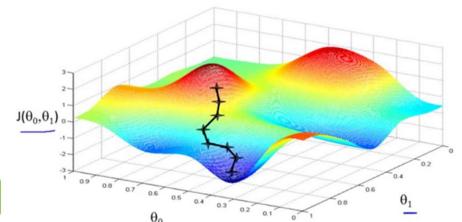
### Linear Regression – iterative gradient descent algorithm (summary)

Inicialize model parameters (e.a.  $\theta = 0$ ) Repeat until J converge {

Compute Linear Regression Model =>

Compute cost function =>

Compute cost function gradients =>



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

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} \left( h_{\theta}(x^{(i)}) - y^{(i)} \right)^{2}$$

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

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

## Batch/mini batch/stochastic gradient descent for parameter update

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

**Batch learning** (classical approach):

update parameters after all training examples have been processed, repeat several iterations until convergence

**Mini batch learning** (if big training data):

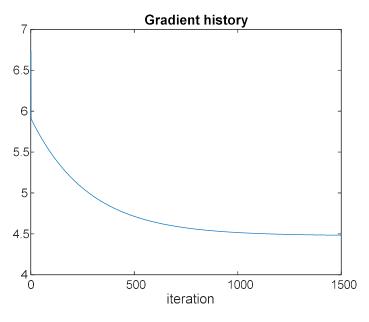
devide training data into small batches update parameters after each mini batch has been processed, repeat until convergence

**Stochastic (incremental) learning (**large-scale ML problems): update parameters after every single training example has been processed.

**Stochastic Gradient Descent (SGD):** the true gradient is approximated by a gradient at a single example. Adaptive learning rate.

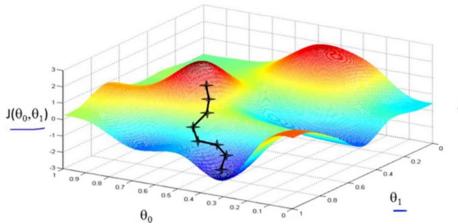
### Cost function convergence

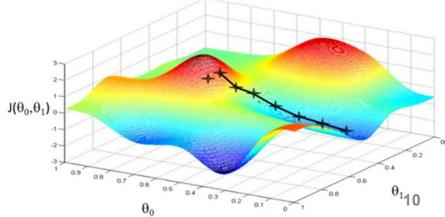
$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^{2}$$



#### Linear Regression (LR):

starting from different initial values of the parameters the cost function J should always converge (<u>maybe to a local</u> <u>minimum !!!</u>) if LR works properly.



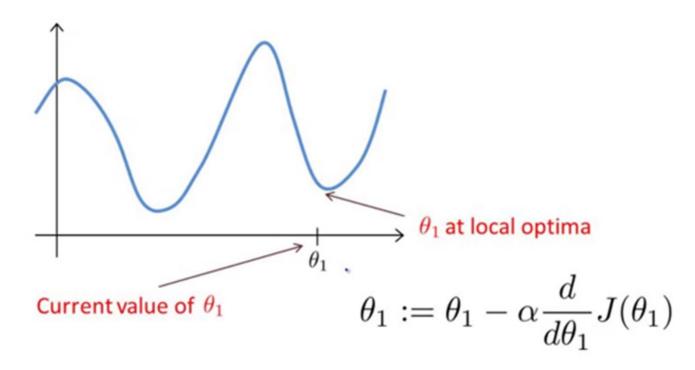


#### Lin Reg Cost function – local minimum

Suppose  $\theta_1$  is at a local optima as shown in the figure.

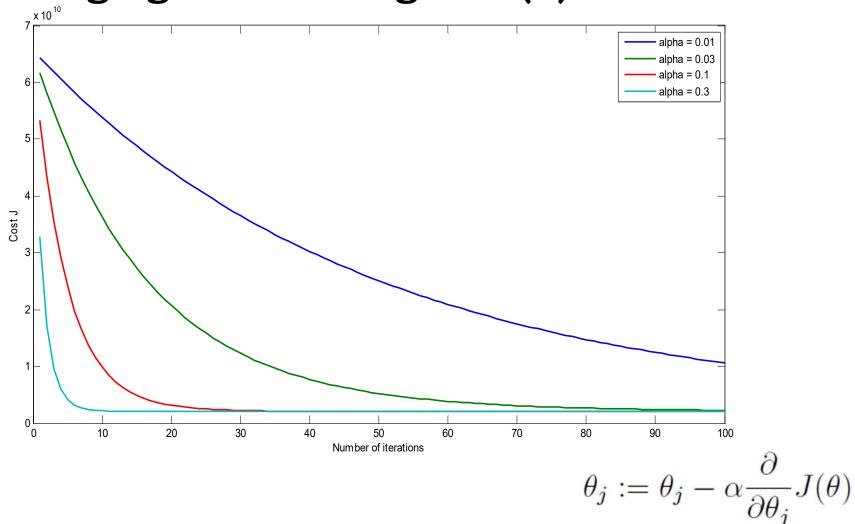
#### What will one step of Gradient Descent do?

- 1) Leave  $\theta_1$  unchanged
- 2) Change  $\theta_1$  in a random direction
- 3) Decrease  $\theta_1$
- 4) Move  $\theta_1$  in direction to the global minimum of J



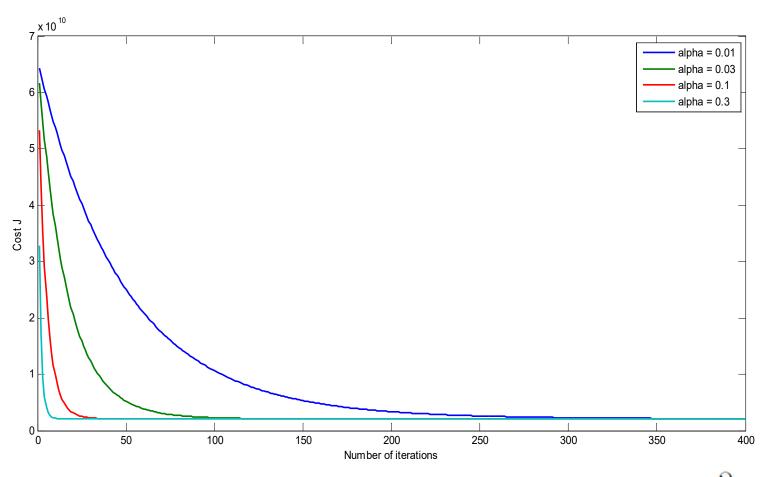


## Cost function convergence changing the learning rate ( $\alpha$ ) -100 iter.



If  $\alpha$  too small: slow convergence of the cost function J (the Gradient Descent optimization can be slow)

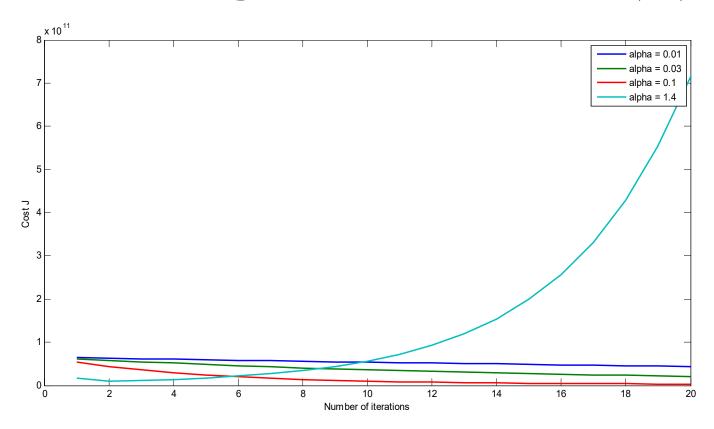
## Cost function convergence changing the learning rate ( $\alpha$ ) -400 iter.





$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

### LinReg Cost function convergence learning rate variation ( $\alpha$ )

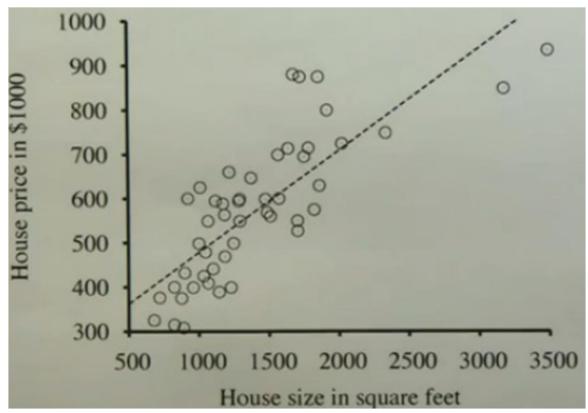


If  $\alpha$  too large: the cost function J may no converge (decrease at each iteration). It may diverge!  $\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$ 



### Univariate Regression

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



Given the house area, what is the most likely house price? If univariate linear regression model is not sufficiently good model, add more data (ex. # bedrooms).

### Multivariate Regression

Problem: Learning to predict the housing price as a function of living area & number of bedrooms.

Living area (feet <sup>2</sup> )	#bedrooms	Price (1000\$s)
2104	3	400
1600	3	330
2400	3	369
1416	2	232
3000	4	540
:	:	:

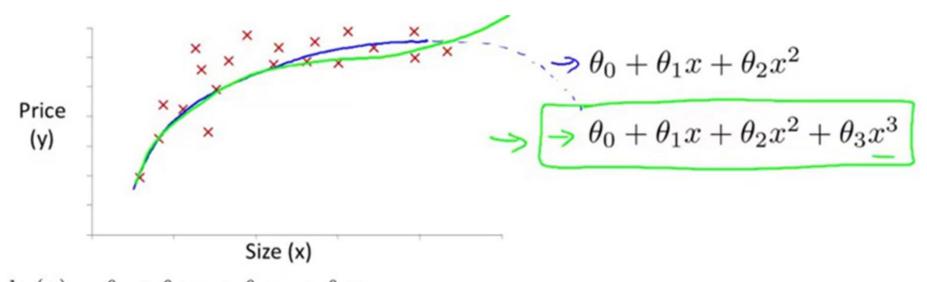
$$h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 = \begin{bmatrix} \theta_0 & \theta_1 & \theta_2 \end{bmatrix} \begin{bmatrix} x_0 = 1 \\ x_1 \\ x_2 \end{bmatrix} = \vec{\theta}^T \vec{x}$$



### **Polynomial Regression**

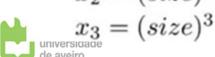
If univariate linear regression model is not a good model, try polynomial model.

Univariate (x1=size) housing price problem transformed into multivariate (still linear !!!) regression model x=[ x1=size, x2=size^2, x3=size^3 ]



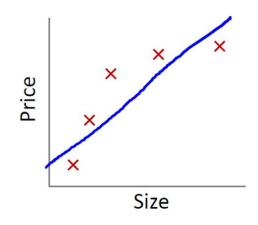
$$h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3$$
  
=  $\theta_0 + \theta_1 (size) + \theta_2 (size)^2 + \theta_3 (size)^3$   
$$x_1 = (size)$$

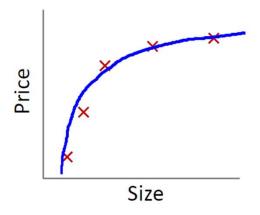
$$x_2 = (size)^2$$

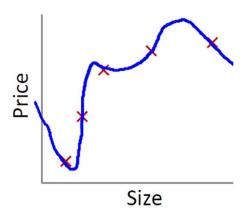


### Overfitting problem

Overfitting: If we have too many features (e.g. high order polynomial model), the learned hypothesis may fit the training set very well but fail to generalize to new examples (predict prices on new examples).







#### underfit

(1st order polin. model)

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

#### just right

(3rd order polinom. model)

#### overfit

(higher ord. polinom. Model)

$$h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 \quad h_{\theta}(x)$$

$$h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3$$
  $h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \dots + \theta_{16} x^n$ 



### Overfitting problem

Overfitting: If we have too many features (x1,...x100) the learned model may fit the training data very well but fails to generalize to new examples.

 $x_1 =$  size of house

 $x_2 = \text{ no. of bedrooms}$ 

 $x_3 = \text{ no. of floors}$ 

 $x_4 = age of house$ 

 $x_5$  = average income in neighborhood

 $x_6 =$ kitchen size

:

 $x_{100}$ 

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



### How to deal with overfitting problem?

#### 1. Reduce number of features.

- Manually select which features to keep.
- Algorithm to select the best model complexity.
- **2. Regularization** (add extra term in cost function) Regularization methods shrink model parameters  $\theta$  towards zero to prevent overfitting by reducing the variance of the model.

#### 2.1 Ridge Regression (L2 norm)

- Reduce magnitude of  $\theta$  (but never make them =0) => keep all features
- Works well when all features contributes a bit to the output y.

#### 2.2 Lasso Regression (L1 norm)

- May shrink some of the elements of vector  $\theta$  to become 0.
- Eliminate some of the features => Serve as feature selection



# Regularized Linear Regression (cost function)

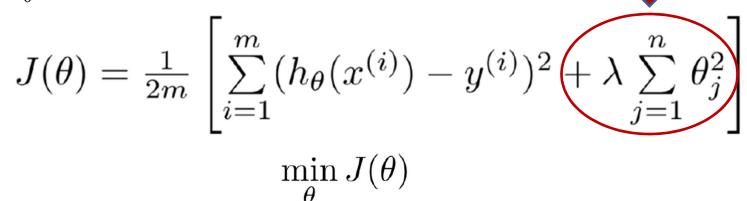
**Unregularized cost function =>** 

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} \left( h_{\theta}(x^{(i)}) - y^{(i)} \right)^{2}$$

#### Regularized cost function

(add extra regularization term don't regularize  $\theta_0$ 

#### **Ridge Regression**





### Regularized Linear Regression

What if lambda is set to an extremely large value?

- Algorithm fails to eliminate overfitting.
- Algorithm results in under-fitting. (Fails to fit even training data well).
- Gradient descent will fail to converge.





### Regularization: Lasso Regression

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \left[ -y^{(i)} \log(h_{\theta}(x^{(i)})) - (1 - y^{(i)}) \log(1 - h_{\theta}(x^{(i)})) \right] + \frac{\lambda}{2m} \sum_{j=1}^{n} |\theta_{j}|$$

Ridge Regression shrinks  $\theta$  towards zero, but never equal to zero => all features are included in the model no matter how small are the coefficients.

Lasso Regression is able to shrink coefficients to exactly zero => reduces the number of features. This makes Lasso Regression useful in cases with high dimension.

Lasso Regression involves absolute values (not differentiable)=> computing is difficult => relevant algorithms available in sklearn Python library.



#### JUPYTER NOTEBOOK

Project Jupyter - 2014 by <u>Fernando Pérez</u> Reference to the 3 core programming languages supported <u>Julia</u>, <u>Python</u>, <u>R</u>

<u>open-source software</u>, open-standards, language agnostic <u>web-based interactive</u> computational environment for creating notebook documents.

Ordered list of input/output cells which can contain code, text (using Markup language – html, latex, ), maths, plots

MATLAB-BASED IPYTHON NOTEBOOKS:

https://anneurai.net/2015/11/12/matlab-based-ipython-notebooks/.

