

# Classical Data Analysis



**Master in Big Data Solutions 2020-2021** 

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# **Today's Objective**

- Review concepts from previous sessions
- Artificial Neural Networks
  - Theory
  - Artificial Neural Networks with Python



#### **Contents**

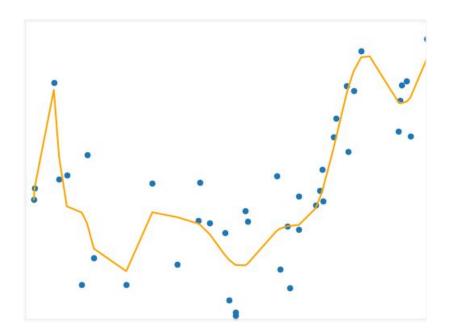
- Introduction to data analysis
- Linear Regression
- Logistic Regression
- Regression analysis (Polynomial, Ridge, Lasso, etc.)
- Neural Networks
- Support Vector Machines (SVM)
- Decision Trees
- Ensemble Methods
- Other Classifier (KNN, Naïve Bayes)
- K-Means
- PCA
- Hierarchical Clustering
- Recommender Systems

# Previous session: Polynomial Regression



Limitation of linear Regression

 Linear regression requires the relation between the dependent variable and the independent variable to be linear.

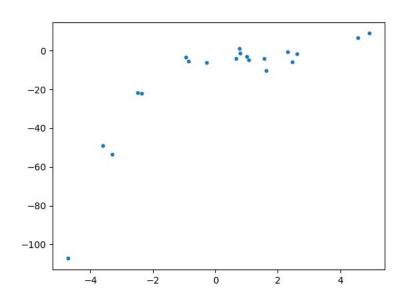


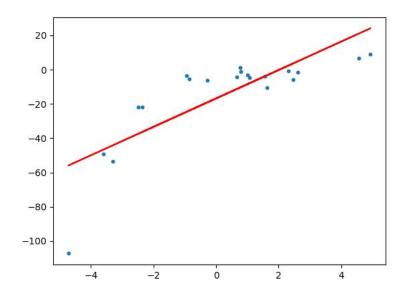
Can linear models be used to fit non-linear data?



#### Why Polynomial Regression?

#### Linear regression model



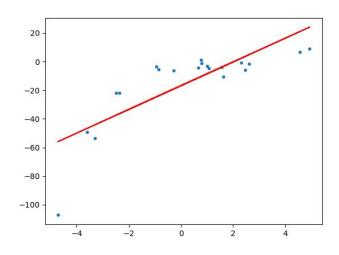


The model is unable to capture the patterns in the data. This is an example of **under-fitting**.



#### Why Polynomial Regression?

#### Linear regression model



How to overcome under-fitting?



Increase the complexity of the model. We need to add more features to the data

$$Y = \theta_0 + \theta_1 x$$



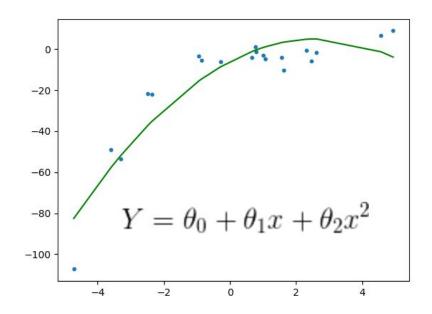
$$Y = \theta_0 + \theta_1 x$$
  $\longrightarrow$   $Y = \theta_0 + \theta_1 x + \theta_2 x^2$ 

This is still considered to be a linear model as the coefficients/weights associated with the features are still linear. x<sup>2</sup> is only a new feature.



Why Polynomial Regression?

Linear regression model 2nd degree polynomial

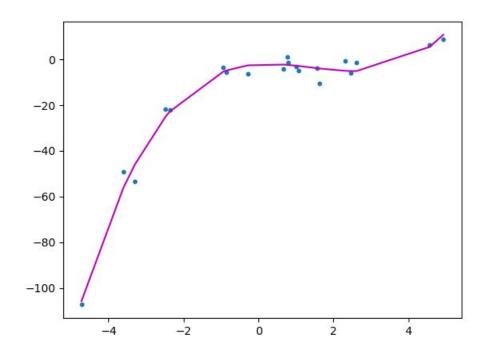


It is clear from the plot that the quadratic curve (2nd degree polynomial) is able to fit the data better than the linear line.



Why Polynomial Regression?

Linear regression model polynomial of degree 3

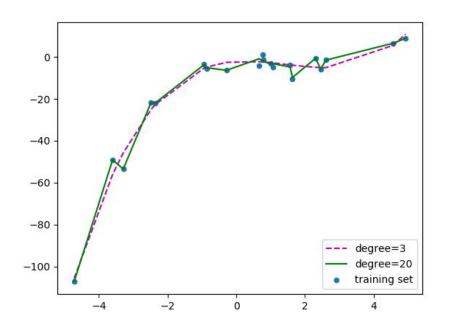


It passes through more data points than the quadratic and the linear plots.



Why Polynomial Regression?

Linear regression model polynomial of degree 20

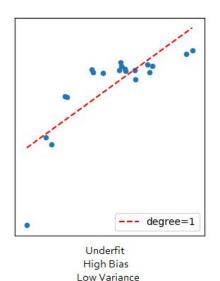


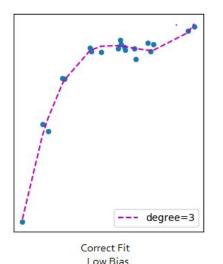
It passes through more data points but here we have a problem: **Overfitting**, i.e., the model is also capturing the noise in the data and even if it works well on the training set it will fail to generalize (the performance in the test set will be poor).



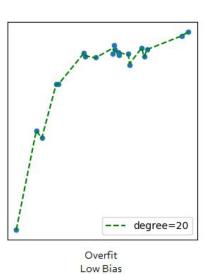
#### Bias vs Variance trade-off

- Bias: error due to the model's simplistic assumptions in fitting the data. A high bias means that the model is unable to capture the patterns in the data and this results in underfitting.
- Variance: error due to the complex model trying to fit the data. High variance results in over-fitting the data. Variance refers to how much the model is dependent on the training data.





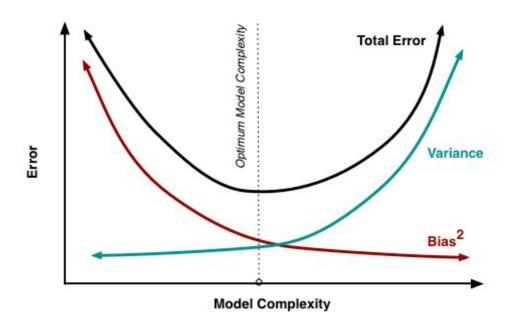
Low Variance



High Variance



#### Bias vs Variance trade-off



# Regularizatioin: Ridge, Lasse and Elastic Net

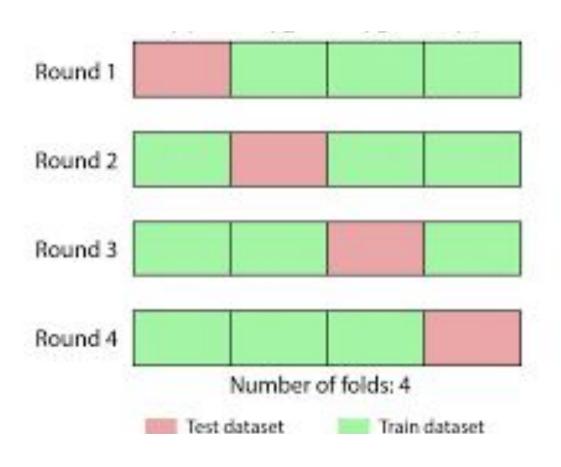


#### How to address overfitting

- In classical linear regression if the model feels like one particular feature is particularly important, the model may place a large weight to the feature. This might lead to overfitting in small datasets.
- Reduce Number of feature (Manually or Model selection algorithm)
- Regularization
- Collect More data
- Cross Validation
- Ensembling (Combine prediction from multiple separate models)



#### **Cross Validation**





#### How to address overfitting

- In classical linear regression if the model feels like one particular feature is particularly important, the model may place a large weight to the feature. This might lead to overfitting in small datasets.
- Regularization techniques consist of modifying the cost function, adding a penalty term, to restrict the values of our coefficients.
- Regularization techniques:
  - Lasso, also called L1-Norm
  - Ridge, also called L2-Norm
  - Elastic Net: is a combination of Lasso and Ridge



#### LASSO

 Adds an additional term to the cost function, adding the sum of the coefficient values (the L-1 norm) multiplied by a constant lambda.

$$\min_{eta \in \mathbb{R}^p} \left\{ rac{1}{N} \|y - Xeta\|_2^2 + \lambda \|eta\|_1 
ight\}.$$

- Lambda set the coefficients of the bad predictors mentioned above 0 (feature selection).
- If lambda=0, we effectively have no regularization.
- Large lambda leads coefficients to 0.



#### **RIDGE**

 Sums the squares of coefficient values (the L-2 norm) and multiplies it by some constant lambda.

$$\hat{eta}^{ridge} = \mathop{argmin}_{eta \in \mathbb{R}} \lVert y - XB 
Vert_2^2 + \lambda \lVert B 
Vert_2^2$$

- will decrease the values of coefficients, but is unable to force a coefficient to exactly 0 (No feature selection).
- If lambda=0, we effectively have no regularization
- It will also select groups of colinear features (grouping effect)

Analysis of both Lasso and Ridge regression has shown that neither technique is consistently better than the other; try both methods to determine which to use!



#### **Elastic Net**

Includes both L-1 and L-2 norm regularization terms.

$$\hat{eta} \equiv \operatorname*{argmin}_{eta} (\|y - Xeta\|^2 + \lambda_2 \|eta\|^2 + \lambda_1 \|eta\|_1).$$

It seems to have the predictive power better than Lasso, while still performing feature selection. We therefore get the best of both worlds, performing feature selection of Lasso with the feature-group selection of Ridge.

# "Artificial" Neural Networks



Why do we need another learning algorithm?

- Linear Regression
- Logistic regression

 Example of machine learning problem where ne need complex non-linear hypotheses

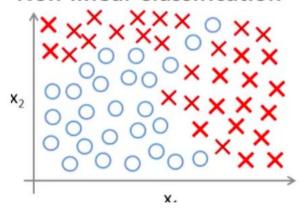
Non-linear Classification



Why do we need another learning algorithm?

Example of machine learning problem where ne need complex non-linear hypotheses

#### Non-linear Classification



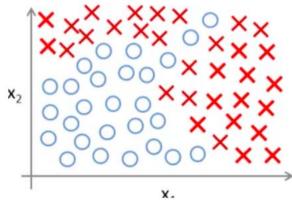
To apply logistic regression to this problem we have to use a lot of non linear features like the following sigmoid function

$$g(\Theta_0 + \Theta_1 x_1 + \Theta_2 x_2 + \Theta_3 x_1 x_2 + \Theta_4 x_1^2 x_2 + \dots)$$



Why do we need another learning algorithm?

#### Non-linear Classification



To apply logistic regression to this problem we have to use a lot of non linear features

$$g(\Theta_0 + \Theta_1 x_1 + \Theta_2 x_2 + \Theta_3 x_1 x_2 + \Theta_4 x_1^2 x_2 + \dots)$$

Logistic regression method tends to work well when we have only few features, because in that case we can add all polynomial terms.

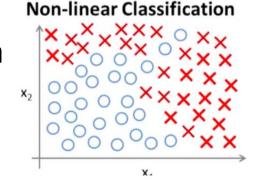
In many machine learning problems we will have a lot more feature than just two.



Why do we need another learning algorithm?

To apply logistic regression to this problem we have to use a lot of non linear features

$$g(\Theta_0 + \Theta_1 x_1 + \Theta_2 x_2 + \Theta_3 x_1 x_2 + \Theta_4 x_1^2 x_2 + \dots)$$





Many features -> Complex Model

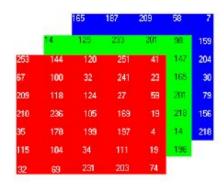


- High Risk of overfitting
- Computation would be too expensive



# Example of ML problem with many examples: Computer Vision

 We want to train a classifier able to examine an image and tell us if the image is a car or not



An image is a matrix of pixels



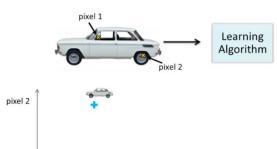
pixel 2

Imagine to plot a object of the dataset using a couple of pixel locations (pixel 1 and pixel 2)



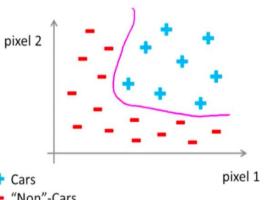
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Imagine to plot a object of the dataset using a couple of pixel locations (pixel 1 and pixel 2)

#### Plot all objects

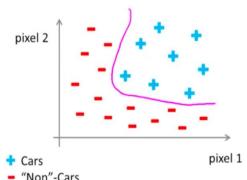


if we use a 50 × 50 pixel we have a vector of 2500 pixel intensities. If we try to learn a non-linear hypothesis by including all the quadratic terms, we obtain about 3 million features and it would be too large.



Example of ML problem with many examples: Computer Vision

#### Plot all objects



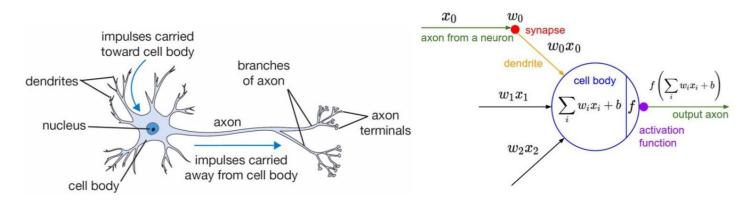
if we use a 50 × 50 pixel we have a vector of 2500 pixel intensities. If we try to learn a non-linear hypothesis by including all the quadratic terms, we obtain about 3 million features and it would be too large.

Logistic regression with the addition of quadratic (or cubic) features is not a good idea to learn a complex non-linear hypothesis when the number of features is large because we end up with too many features.



#### **Artificial Neural Network**

 Neural Network is a learning algorithm inspired on how human brain works and it is very useful to approach different machine learning problems.



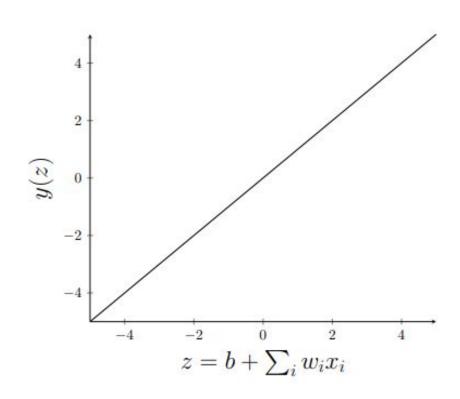
- Neurons pass information through the synapses
- Synapses between neurons adapt
- Clusters of neurons learn to perform computations.



$$y = b + \sum_{i} w_i x_i$$

#### **Linear Neuron**

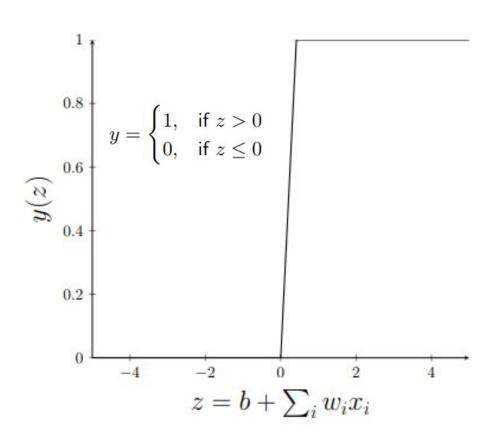
- Simplest model.
- Equivalent to weighted sum of the inputs.
- Useful for regression.





#### **Binary Neuron**

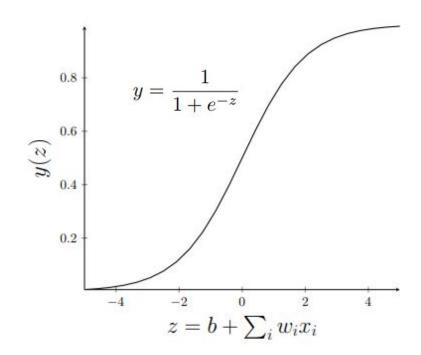
- Thought for classification.
- Simplified version of sigmoid.
- Not used in practice.(Impossible to train with gradient descent).





#### **Sigmoid Neuron**

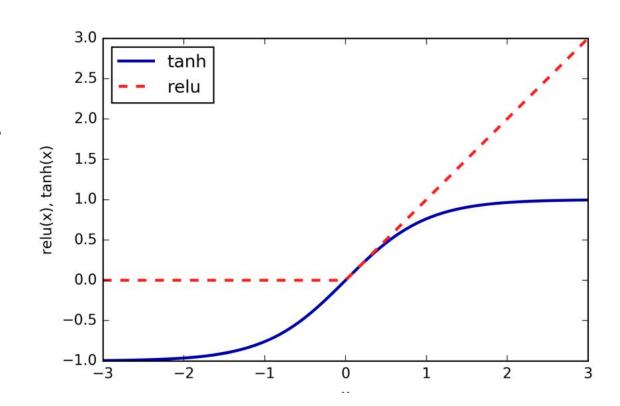
- Thought for classification.
- Equivalent to logistic regression.
- Has problems with vanishing gradients. (Saturates very quickly).





#### Popular neurons for ML

- **tanh** is very similar to logistic regression.
- relu is an adaptation
   of the linear unit in
   order to avoid vanishing
   gradients.

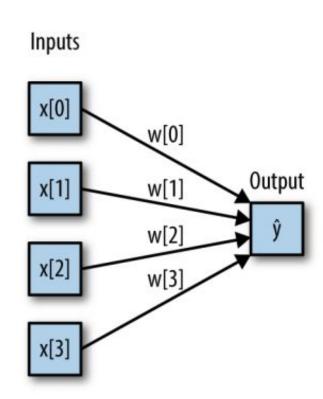




# Perceptron

- It is the simplest network with only one "processing" neuron.
- The first layer corresponds to the input.

  Each "neuron" in that layer has an activation equal to the input vector.
- We usually add one more input whose activation is always set to 1. The weight corresponding to that neuron will be the bias.
- With a logistic activation function this is logistic regression.

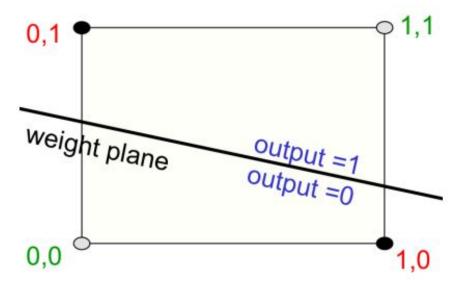


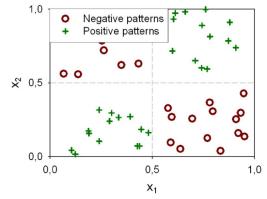


# The XOR problem

- The XOr, or "exclusive or", problem is a classic problem in ANN research.
- It is the problem of using a neural network to predict the outputs of XOr logic gates given two binary inputs.
- An XOr function should return a true value if the two inputs are not equal and a false value if they are equal.

Input 1	Input 2	Output
0	0	0
0	1	1
1	1	0
1	0	1



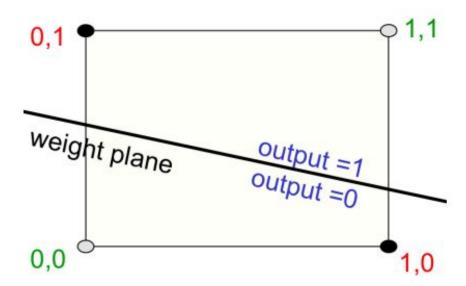


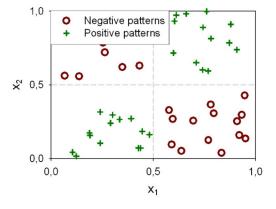


# The XOR problem

- Linear classifiers have strong limitations.
- To overcome this, we can stack more layers in the architecture and add non-linear activation functions.
- This more layers, the more complex the model
- These architectures are commonly known as Multi-layer perceptrons.

Input 1	Input 2	Output
0	0	0
0	1	1
1	1	0
1	0	1

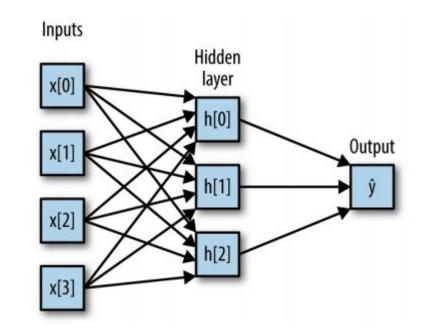






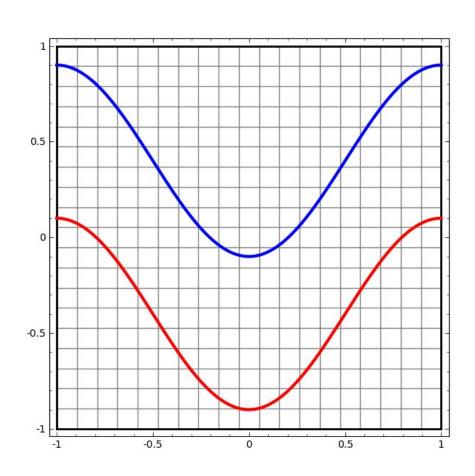
# Multi Layer Perceptron or MLP

- Also known as feedforward networks.
- Information can only flow forward.
- At each layer you obtain a new representation of the input.
- The output is the representation of the last layer.
- Intermediate layers are called hidden layers, because you do not see their values.



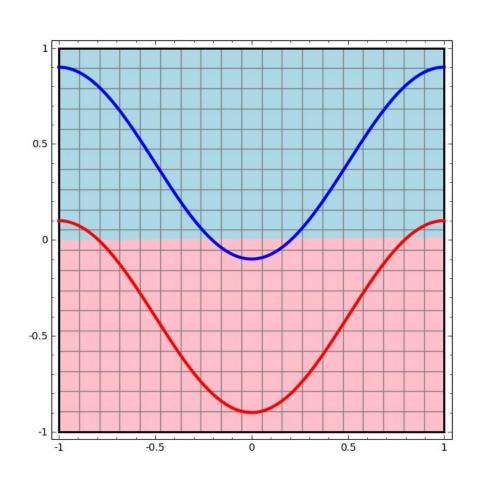


The idea of the hidden layers, is to introduce (nonlinear) transformations that eventually will make your data linearly separable.



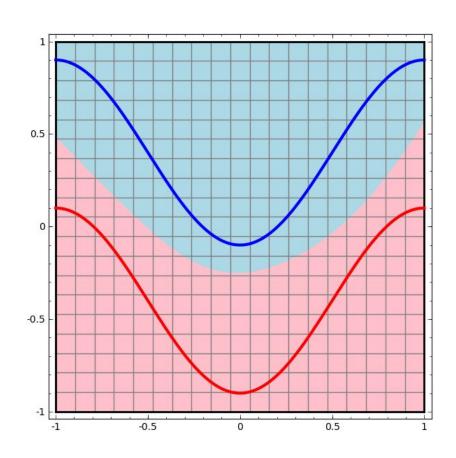


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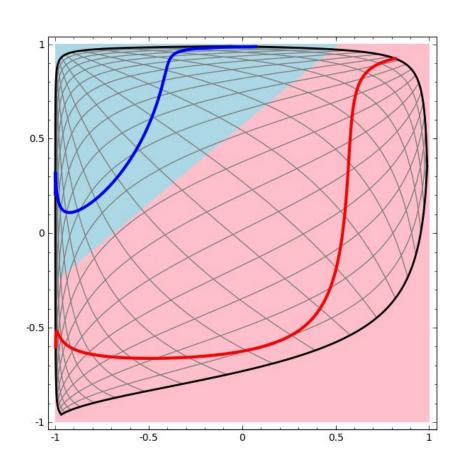


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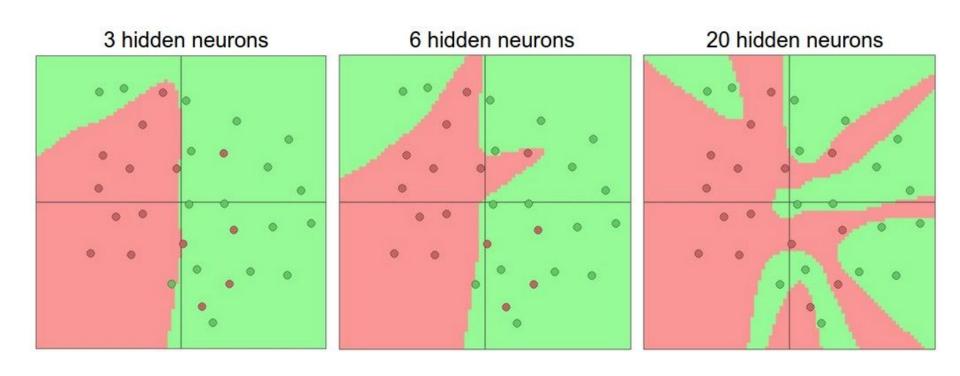


The idea of the hidden layers, is to introduce (nonlinear) transformations that eventually will make your data linearly separable.



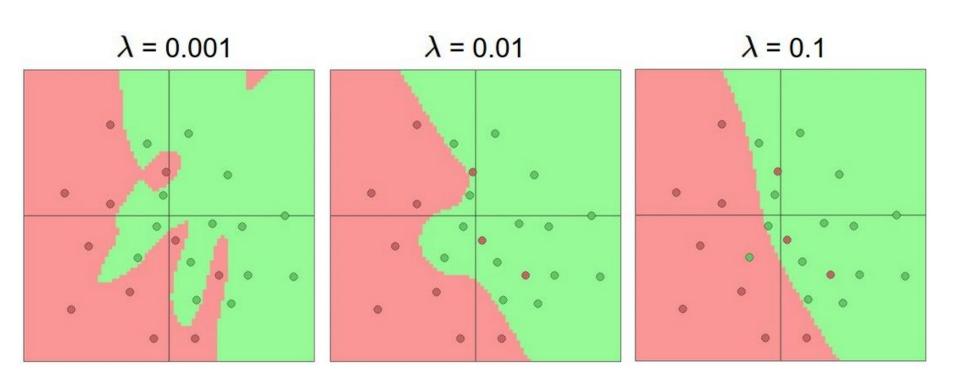


The more hidden units, the more complex the model becomes and it is more prone to overfitting.





It is common to add an L2 regularization term to the loss function of a neural network. The hyper-parameter multiplying the regularization term is adjusted to prevent overfitting.

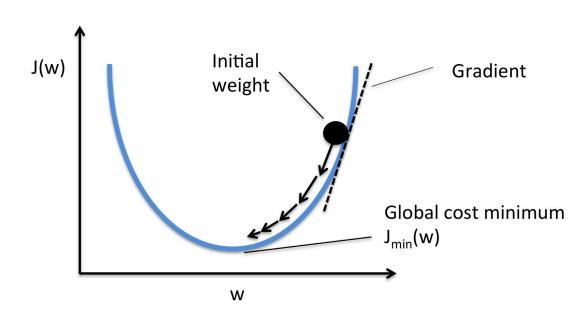




# **Gradient Descent**

The multi-layer perceptron is trained with gradient descent.

The gradient at each step is computed with a method called back-propagation.



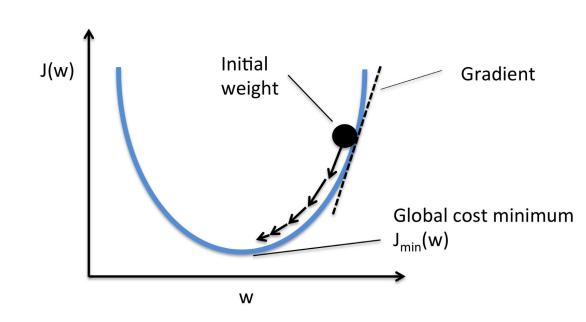


# **Gradient Descent**

$$Wj,i \leftarrow Wj,i + \alpha \times \Delta i$$

 $\alpha$  is the learning rate

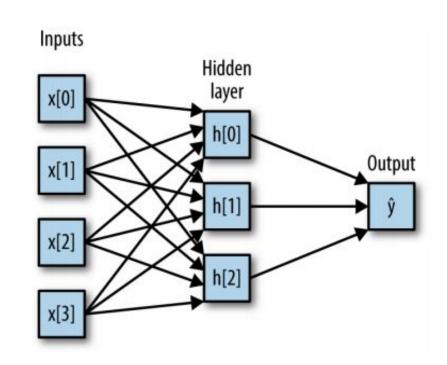
 $\Delta i$  is the gradient of the weights





# **Backpropagation - intuition**

The error of the output units is straight-forward to compute (by comparing to the desired output). The error of the weights in the hidden units is derived based on their contribution to the output.

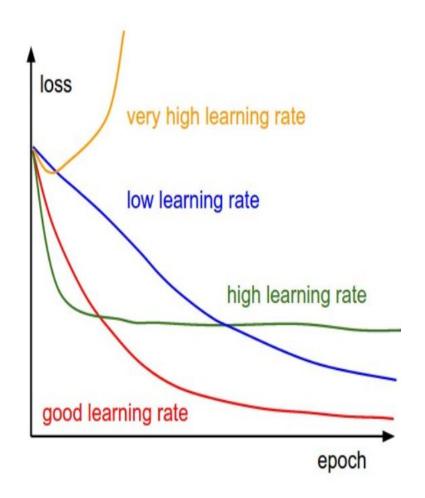




# **Gradient Descent properties**

Finding a good learning rate will be fundamental for the convergence of gradient descent.

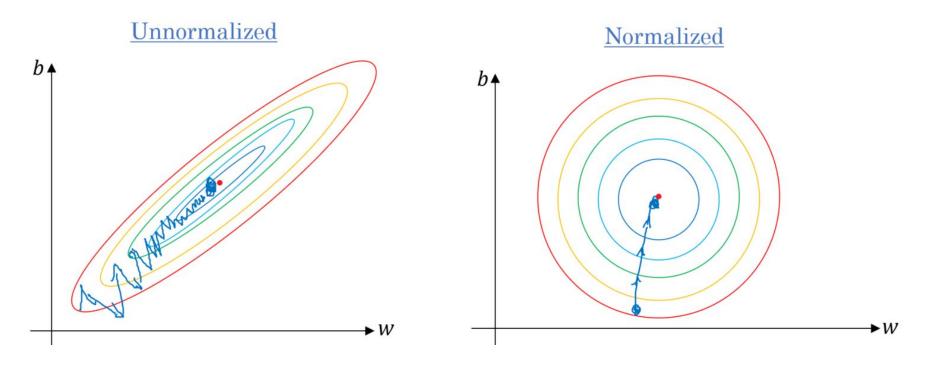
An extended practice consists in decreasing the learning rate as every few iterations.





# **Gradient Descent properties**

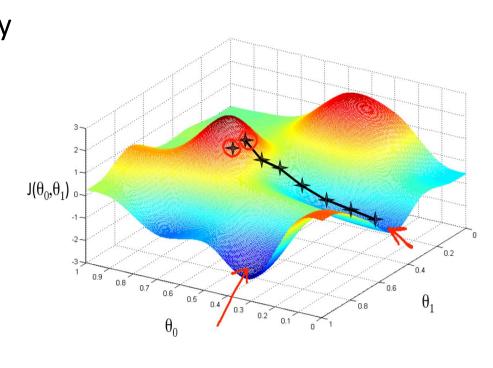
Normalization matters. If the data is not normalized the algorithm will take longer to converge to the minima.





# **Gradient Descent properties**

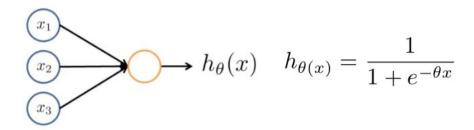
This method is very sensitive to global minima, therefore it is very sensitive to the starting point. It is common practice to train several networks with different initializations of weights. There are methods to improve the gradient descent (Adam, RMSprop, Momentum...) and it is currently an active





Model Representation: Logistic Unit

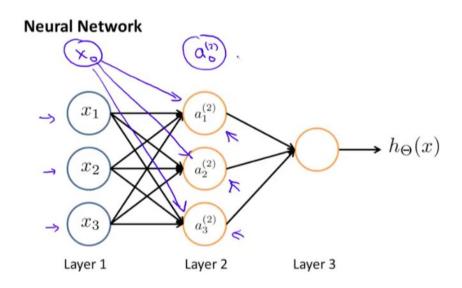
We model a neuron as a simple logistic unit



• In neural networks the sigmoid function ( or logistic function) is also called **Activation function** and the parameters θ are called weights of the model.



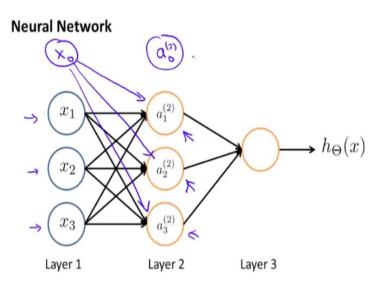
Model Representation :Logistic Unit



 a neural network is a proof of different neurons models that interact each other



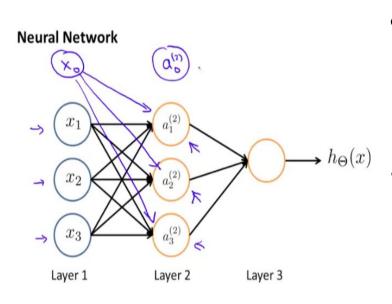
Model Representation :Logistic Unit



- 3 neurons a<sup>2</sup><sub>1</sub>, a<sup>2</sup><sub>2</sub>, a<sup>2</sup><sub>3</sub> more the bias unit a<sup>2</sup><sub>0</sub>;
- input layer (layer 1): in this layer we input the features x<sub>1</sub>, x<sub>2</sub> and x<sub>3</sub> (of our training set);
- hidden layer (layer 2): it contains values that we don't observe in the training set;
- output layer (layer 3): it has a neuron / units (it can have more units) that output the final value computed by the hypothesis.

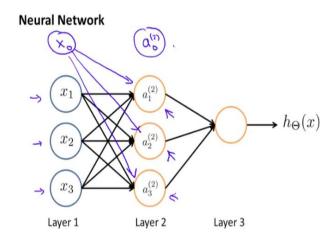


Model Representation :Logistic Unit



- a<sub>i</sub><sup>(j)</sup>: Activation of unit i in layer j (i.e., the value that is computed by and that is the output of a specify unit);
- Θ<sup>(j)</sup>: matrix of weights that controls the function mapping from layer j to layer j + 1.

#### Model Representation: Computation



$$a_{1}^{(2)} = g(\Theta_{10}^{(1)}x_{0} + \Theta_{11}^{(1)}x_{1} + \Theta_{12}^{(1)}x_{2} + \Theta_{13}^{(1)}x_{3})$$

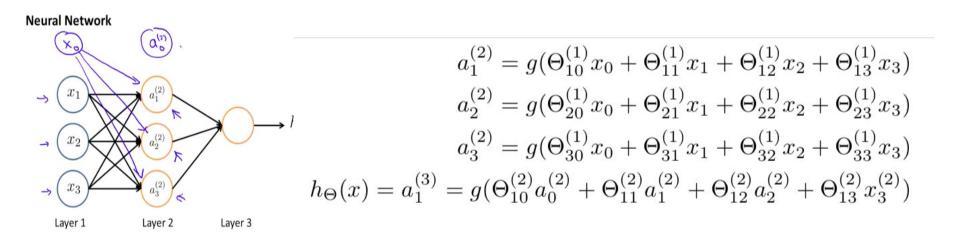
$$a_{2}^{(2)} = g(\Theta_{20}^{(1)}x_{0} + \Theta_{21}^{(1)}x_{1} + \Theta_{22}^{(1)}x_{2} + \Theta_{23}^{(1)}x_{3})$$

$$a_{3}^{(2)} = g(\Theta_{30}^{(1)}x_{0} + \Theta_{31}^{(1)}x_{1} + \Theta_{32}^{(1)}x_{2} + \Theta_{33}^{(1)}x_{3})$$

$$h_{\Theta}(x) = a_{1}^{(3)} = g(\Theta_{10}^{(2)}a_{0}^{(2)} + \Theta_{11}^{(2)}a_{1}^{(2)} + \Theta_{12}^{(2)}a_{2}^{(2)} + \Theta_{13}^{(2)}x_{3}^{(2)})$$



Model Representation: Computation



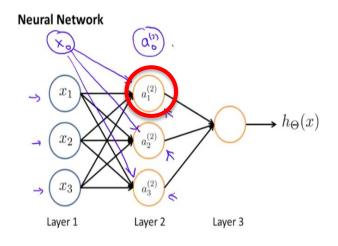
If a network has  $S_j$  units in layer j,  $S_{j+1}$  units in layer j + 1, then  $\Theta^{(j)}$  is a  $S_j+1\times S_j+1$  matrix:

$$\Theta^{(j)} \in \mathbb{R}^{S_{j+1} \times S_j + 1}$$

 $\Theta^{(1)}$  is 3 × 4 matrix, so  $\Theta^{(1)} \in \mathbb{R}^{3\times4}$ .



Model Representation: Computation



$$\Theta^{(j)} \in \mathbb{R}^{S_{j+1} \times S_j + 1}$$

- S<sub>j+1</sub> = S<sub>2</sub> = 3
   S<sub>j</sub> = S<sub>1</sub> = 4 (we are considering also  $x_0$
- $\Theta^{(1)}$  is  $3 \times 4$  matrix. so  $\Theta^{(1)} \in \mathbb{R}^{3\times 4}$

$$a_{1}^{(2)} = g(\Theta_{10}^{(1)}x_{0} + \Theta_{11}^{(1)}x_{1} + \Theta_{12}^{(1)}x_{2} + \Theta_{13}^{(1)}x_{3})$$

$$a_{2}^{(2)} = g(\Theta_{20}^{(1)}x_{0} + \Theta_{21}^{(1)}x_{1} + \Theta_{22}^{(1)}x_{2} + \Theta_{23}^{(1)}x_{3})$$

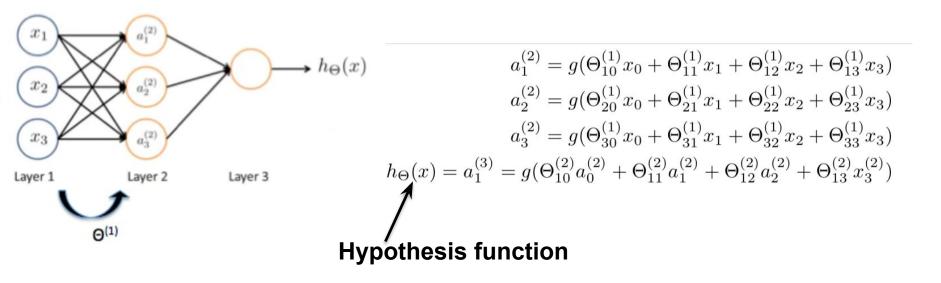
$$a_{3}^{(2)} = g(\Theta_{30}^{(1)}x_{0} + \Theta_{31}^{(1)}x_{1} + \Theta_{32}^{(1)}x_{2} + \Theta_{33}^{(1)}x_{3})$$

$$h_{\Theta}(x) = a_{1}^{(3)} = g(\Theta_{10}^{(2)}a_{0}^{(2)} + \Theta_{11}^{(2)}a_{1}^{(2)} + \Theta_{12}^{(2)}a_{2}^{(2)} + \Theta_{13}^{(2)}x_{3}^{(2)})$$

To compute the activation function of a neuron a<sub>1</sub><sup>(2)</sup> we need a 1x4 vector. Since in the layer 2 there are 3 neurons we need 3 1x4 vectors, i.e., a 3x4 matrix



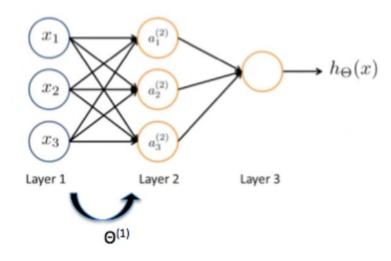
Model Representation: Computation



The computation of  $h_{\Theta}(x)$  is called **forward propagation** because it starts with the activation of the input units, it propagates that to the hidden layer computing the activation function of this layer and the propagation follows with the activation of the output layer.



### Model Representation



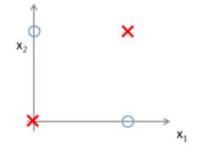
Architecture of a Neural Network: how the different neurons of a network are connected each others.

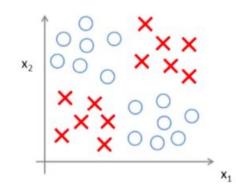


#### **Example and Intuition**

#### Non-linear classification example: XOR/XNOR







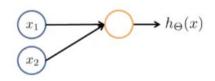
- Positive (y=1)
- Negative (y=0)

- Input features x1 and x2 that are binary values
- On the left we have a simplified version of a more complex (on the right) learning problem.
- We would like to learn a non-linear function (decision boundary) to separate positive and negative examples.



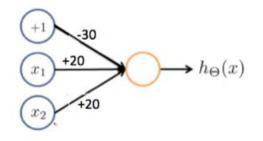
### **Example and Intuition**

Let's start building a neural network that fits the **AND logic** function at first and then some other logic functions



- $x_1, x_2 \in \{0, 1\}$
- $y = x_1 \wedge x_2$

Let's add the bias unit and assign some values to the weights (parameters) of the network



- $\Theta_{10}^{(1)} = -30$
- $\Theta_{11}^{(1)} = +20$
- $\Theta_{12}^{(1)} = +20$

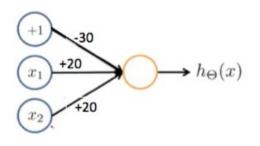
AND Hypothesis function

$$h_{\Theta}(x) = g(-30 + 20x_1 + 20x_2)$$



### **Example and Intuition**

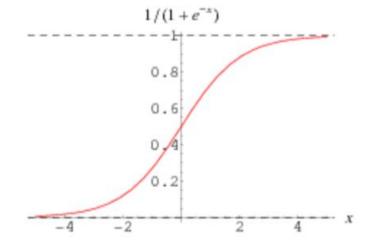
## **AND logic function**



- $\Theta_{10}^{(1)} = -30$
- $\Theta_{11}^{(1)} = +20$
- $\Theta_{12}^{(1)} = +20$

AND Hypothesis function

$$h_{\Theta}(x) = g(-30 + 20x_1 + 20x_2)$$

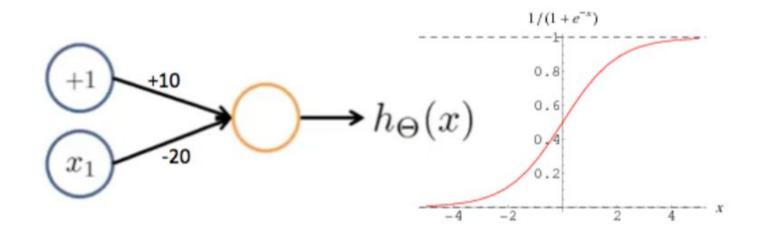


$x_1$	$x_2$	$h_{\Theta}(x) = g(-30 + 20x_1 + 20x_2)$
0	0	$g(-30) \approx 0$
0	1	$g(-30+20)\approx 0$
1	0	$g(-30+20)\approx 0$
1	1	$g(-30 + 20 + 20) \approx 1$



#### **Example and Intuition**

### **NOT logic function**

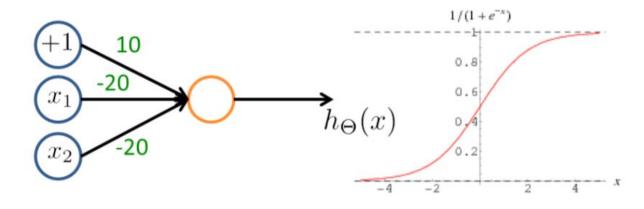


$$x_1$$
  $h_{\Theta}(x) = g(10 - 20x_1)$   
 $0$   $g(10) \approx 1$   
 $1$   $g(+10 - 20) \approx 0$ 



# **Example and Intuition**

# (NOT) AND (NOT) logic function

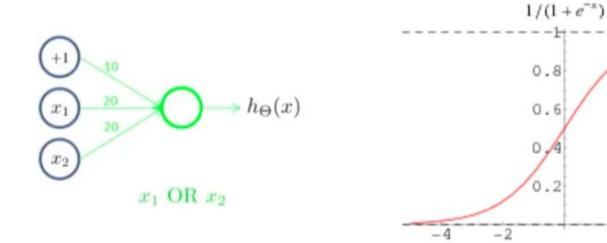


$x_1$	$x_2$	$h_{\Theta}(x) = g(10 - 20x_1 - 20x_2)$
0	0	$g(10) \approx 1$
0	1	$g(+10 - 20) \approx 0$
1	0	$g(+10-20) \approx 0$
1	1	$g(+10 - 20 - 20) \approx 0$



## **Example and Intuition**

## **OR logic function**



$x_1$	$x_2$	$h_{\Theta}(x) = g(-10 + 20x_1 + 20x_2)$
0	0	$g(-10) \approx 0$
0	1	$g(-10+20)\approx 1$
1	0	$g(-10 + 20) \approx 1$
1	1	$g(-10 + 20 + 20) \approx 1$



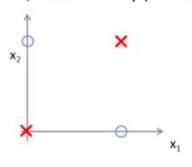
### **Example and Intuition**

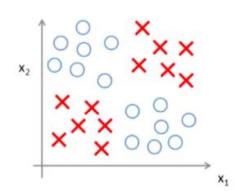
# **XNOR logic function**

we want to put together the neural networks we have seen previously in order to compute x1 XNOR x2.

#### Non-linear classification example: XOR/XNOR

 $x_1$ ,  $x_2$  are binary (0 or 1).



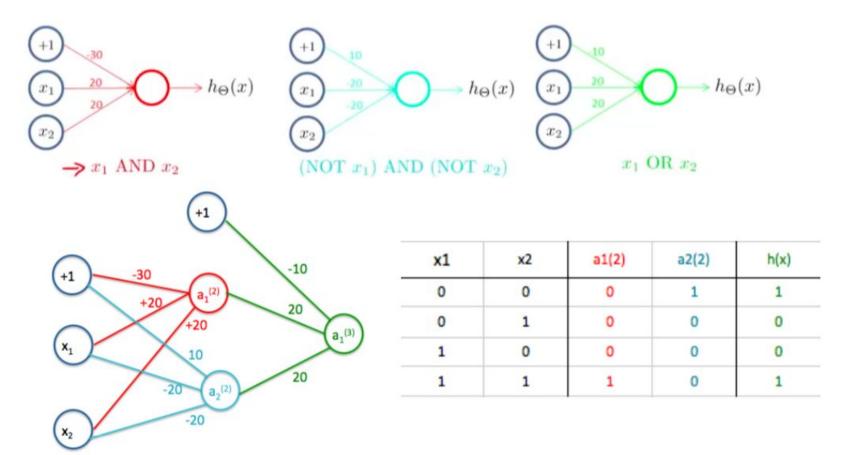


- Positive (y=1)
- Negative (y=0)



### **XNOR logic function**

we want to put together the neural networks we have seen previously in order to compute x1 XNOR x2.

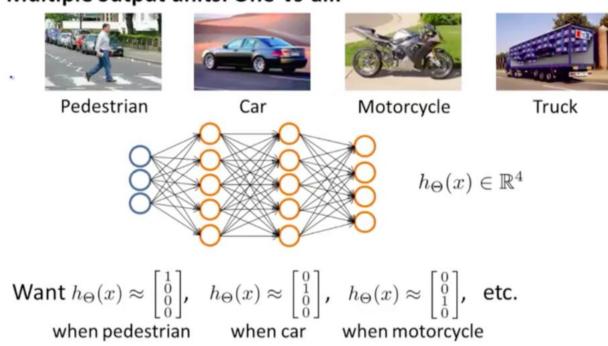




#### **Multiclass Classification**

- We want to recognize four categories of objects (given an image): pedestrian, car, motorcycle, truck.
- Network with four output units







Neural Networks: learning Cost function

The cost function for a neural network can be defined as a generalization of the logistic regression cost function:

$$J(\Theta) = -\frac{1}{m} \left[ \sum_{i=1}^{m} \sum_{k=1}^{K} y_k^{(i)} \log(h_{\Theta}(x^{(i)}))_k + (1 - y_k^{(i)}) \log(1 - (h_{\Theta}(x^{(i)}))_k) \right] + \frac{\lambda}{2m} \sum_{l=1}^{L} \sum_{i=1}^{S_l} \sum_{j=1}^{S_{l+1}} (\Theta_{ij}^{(l)})^2$$

- L is the total number of layer in the considered network
- S<sub>1</sub> is the number of units in layer I.



Neural Networks: learning Cost function

$$J(\Theta) = -\frac{1}{m} \left[ \sum_{i=1}^{m} \sum_{k=1}^{K} y_k^{(i)} \log(h_{\Theta}(x^{(i)}))_k + (1 - y_k^{(i)}) \log(1 - (h_{\Theta}(x^{(i)}))_k) \right] + \frac{\lambda}{2m} \sum_{l=1}^{L} \sum_{i=1}^{S_l} \sum_{j=1}^{S_{l+1}} (\Theta_{ij}^{(l)})^2$$

- As in the case of logistic regression we need to minimize the cost function in order to find the parameters (weights) that are the best decision boundary for our data.
- We use backpropagation algorithm and gradient descent.



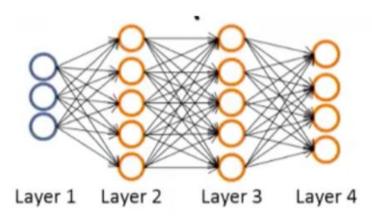
Neural Networks: learning Cost function

- $\boldsymbol{\delta}^{(l)}_{j}$ : Error of node j in layer I (it can be defined as the difference between the hypothesis output  $h_{\Theta}(x)$  and the real output value y)
- The backpropagation algorithm is based on the intuition that for each node j of the neural network, the value  $\delta^{(l)}_{j}$ , that represents the error of the node j in layer I is computed.



Neural Networks: learning Cost function

δ<sup>(l)</sup><sub>j</sub>: Error of node j in layer



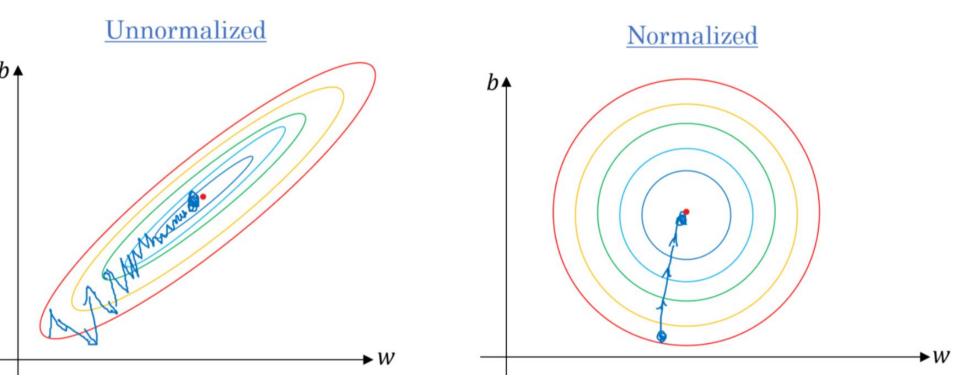
$$\begin{split} \delta^{(4)} &= a^{(4)} - y \\ \delta^{(3)} &= (\Theta^{(3)})^T \delta^{(4)} \cdot * g'(z^{(3)}) \\ \delta^{(2)} &= (\Theta^{(2)})^T \delta^{(3)} \cdot * g'(z^{(2)}) \end{split}$$

The error of the output units is straightforward to compute (by comparing to the desired output). The error of the weights in the hidden units is derived based on their contribution to the output.



#### **Gradient Descent**

If the data is not normalized the algorithm will take longer to converge to the minima.



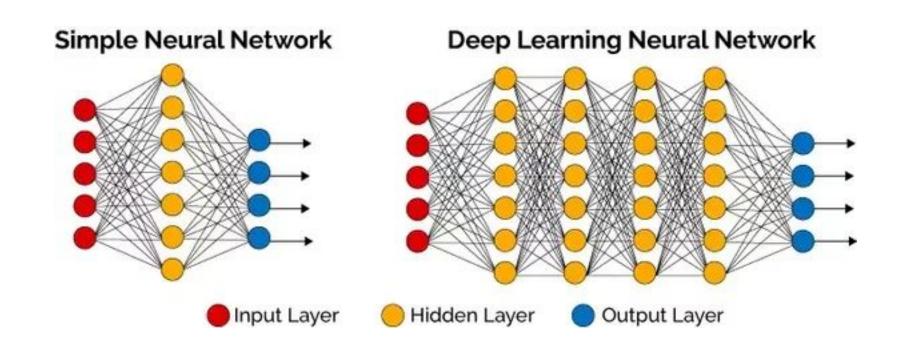


#### **Activation Functions**

- So far we are using sigmoid, but in some cases other functions can be a lot better.
- Tanh activation function (usually works better than sigmoid activation function for hidden units)
- Relu: generally used in the hidden layers (much faster when compared to sigmoid or tanh)



### Neural Networks VS Deep Learning





#### Resources

- Tan, Pang-Ning. Introduction to data mining. Pearson Education India, 2006.
- Friedman, Jerome, Trevor Hastie, and Robert Tibshirani. The elements of statistical learning. Vol. 1. New York: Springer series in statistics, 2001.
- Introduction to Machine Learning with python. Andreas C.
   Müller & Sarah Guido.
- Andrew Ng lectures: <a href="https://www.youtube.com/playlist?list=PLLssT5z\_Ds">https://www.youtube.com/playlist?list=PLLssT5z\_Ds</a>
   K-h9vYZkQkYNWcItqhlRJLN
- http://cs231n.github.io/



