# ARTIFICIAL NEURAL NETWORKS

#### Pedro Larrañaga, Concha Bielza, Jose Luis Moreno

Computational Intelligence Group Artificial Intelligence Department Universidad Politécnica de Madrid







## Machine Learning Master in Data Science + Master in HMDA

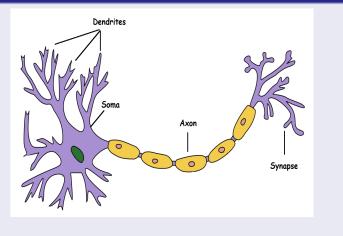
- Biological neuron
- 2 Multilayer perceptron
- 3 Deep neural network

- Biological neuron
- 2 Multilayer perceptron
- 3 Deep neural network

#### Soma, dendrites, axon, synapses

Artificial neural networks are computational models for information processing that attempt to mimic the learning of biological neural networks

#### Main elements

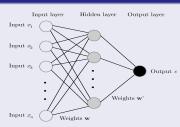


- 1 Biological neuron
- 2 Multilayer perceptron
- 3 Deep neural network

#### Input, hidden and output

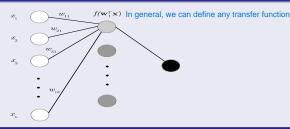
- MLP: An ANN arranged as (at least) three layers with input, hidden, and output neurons
- The edges connect nodes from one layer to the next one
- These connections consist of a set of adaptive weights, that is, numerical
  parameters that are tuned by the learning algorithm
- The inclusion of hidden nodes means that MLPs can approximate non-linear functions

#### MLP example of structure



#### MLP

#### Information processing of a single neuron



#### A three layer MLP

- $\bullet$  n input neurons,  $X_1, \ldots, X_n$ ; h hidden neurons,  $H_1, \ldots, H_h$ , and one output neuron, C
- $\mathbf{w}^T = (w_1, ..., w_h)$  denotes the vector of h weights connecting input and hidden neurons, where  $\mathbf{w}_j^T = (w_{1j}, w_{2j}, w_{3j}, ..., w_{nj})$  for j = 1, ..., h denotes the vector of weights for the j-th hidden neuron. The weights are n-dimensional vectors
- The result of applying the transfer function to this *j*-th hidden unit is denoted as  $f(\mathbf{w}_i^T \mathbf{x}) = f(\sum_{i=1}^n w_{ij} x_i)$
- The h outputs,  $f(\mathbf{w}_1^T\mathbf{x}), \dots, f(\mathbf{w}_h^T\mathbf{x})$ , provided by the h hidden units should be weighted with the vector  $\mathbf{w}'^T = (w_1', \dots, w_h')$ , resulting in the output of the MLP, that is,  $\hat{c} = \sum_{i=1}^h w_i' f(\mathbf{w}_i^T\mathbf{x}) = \sum_{i=1}^h w_i' f(\sum_{i=1}^n w_i' f(\sum_{i=1}^n w_i' x_i)$
- This output  $\hat{c}$  is compared with the real label c that is known
- lacktriangled MLP weights such that the N predictions,  $\hat{c}^1,\ldots,\hat{c}^N$ , are as close as possible to the true labels,  $c^1,\ldots,c^N$

#### **MLP** trainig process

#### A three step process

- The MLP is fed with training instances
- 2 The input values for each training instance are weighted and summed at each hidden layer neuron and the transfer function converts the weighted sum into the input of the output node layer. The MLP output values are calculated and compared to known labels to determine how closely the actual MLP matches the desired labels
- 3 The weights of the connections are changed so that the MLP can provide a better approximation of the desired labels

This process repeats many times until differences between MLP output values and the known labels for all training instances are as small as possible

## **Backpropagation** $E(\mathbf{w}, \mathbf{w}')$ Error function $\partial E$ $\partial E$ $\overline{\partial w_{ij}}$ $\frac{\mathbf{v}'}{(\mathbf{w},\mathbf{w}')^{(0)}}(\mathbf{w},\mathbf{w}')^*$ Gradient descent method for the minimization of $E(\mathbf{w}, \mathbf{w}')$

#### **MLP** trainig process

#### Minimization of $E(\mathbf{w}, \mathbf{w}')$

- The mean squared error,  $E(\mathbf{w}, \mathbf{w}') = \frac{1}{N} \sum_{k=1}^{N} (c^k \hat{c}^k)^2$ , is an example of an error measure often used as the objective function to be minimized
- The most important method to solve this unconstrained nonlinear optimization problem is the backpropagation algorithm
- This algorithm is a gradient descent method or method of steepest descent that finds the direction in which it is best to change the weights in the error space to reduce the error measure most
- This requires partial derivatives of the error function E with respect to each weight w<sub>ii</sub> to be calculated
- The weight updating from  $w_{ij}^{old}$  to  $w_{ij}^{new}$ :  $w_{ij}^{new} = w_{ij}^{old} \eta \frac{\partial E}{\partial w_{ij}}$ .  $\frac{\partial E}{\partial w_{ij}}$  is the gradient of the error function E with respect to  $w_{ij}$  and  $\eta$  is called the learning rate and controls the size of the gradient descent step
- The backpropagation algorithm requires an iterative process, and there are two versions of weight updating schemes: batch mode and on-line mode
- Batch mode: weights are updated after all training instances are evaluated
- On-line mode, the weights are updated after each instance evaluation
- Each pass of all instances is called an epoch

#### MLP. Advantages and disadvantages

#### **Advantages**

- They do not require a priori assumptions about the underlying data generating process
- The modeling process is highly adaptive
- Well-established mathematical properties for accurately approximating functions
- Nonlinear and nonparametric models
- They are fault tolerant, able to model incomplete and noisy information

#### **Disadvantages**

- High computational burden
- Overfitting
- Black box systems

- Biological neuron
- 2 Multilayer perceptron
- 3 Deep neural network

#### Deep neural network

#### Deep neural network

More than one hidden layer -> more hyperparameters to tune

