

Artificial Neural Networks

Inteligencia Artificial en los Sistemas de Control Autónomo
Máster en Ciencia y Tecnología desde el Espacio

Departamento de Automática

Objectives

1. Describe biological neurons and networks
2. Basics of artificial neurons and networks
3. Understand the role of training in ANNs
4. Strengths and weaknesses of ANNs

Bibliography

- A. Tettamanzi, M. Tomassini. Soft Computing. Integrating Evolutionary, Neural, and Fuzzy Systems. Springer-Verlag. 2001
- McCulloch, W. and Pitts, W. (1943). A logical calculus of the ideas immanent in nervous activity. Bulletin of Mathematical Biophysics, 7:115 - 133.
- Rosenblatt, Frank. (1958). The Perceptron: A Probabilistic Model for Information Storage and Organization in the Brain. Psychological Review, 65:386-408

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- Bias in a MLP

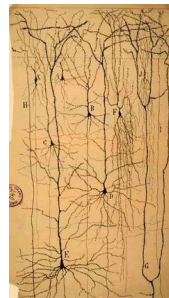
5. Training algorithms

- Problem statement
- Gradient descent algorithm
- Stochastic Gradient Descent
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Introduction

History

- 1888 Ramón y Cajal. Discovery of biological neurons
- 1943 McCulloch & Pitts. First neural network designers
- 1949 Hebb. First learning rule
- 1958 Rosenblatt. Perceptron
- 1969 Minsky & Papert. Perceptron limitation - Death of ANN
- 1986 Rumelhart et al. Re-emergence of ANN: Backpropagation
- 201X Convolutional Neural Networks (CNNs) - Deep learning
- 2014 Goodfellow et al. Generative Adversarial Networks (GANs)



Introduction

Structure of neurons (I)

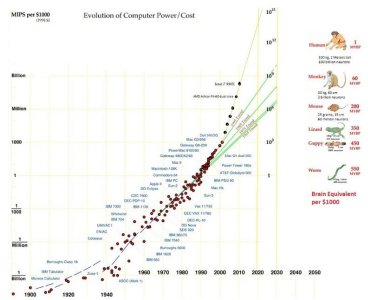
ANIMAL	NEURONS
Sponge	0
Roundworm	302
Jellyfish	800
Ant	250,000
Cockroach	1,000,000
Frog	16,000,000
Mouse	71,000,000
Cat	760,000,000
Macaque	6,376,000,000
Human	86,000,000,000
Elephant	267,000,000,000

Human brain

Neuron switching time: 0.001 s

Synapsis: 10-100 thousand

Scene recognition time: 0.1 s



(Source)

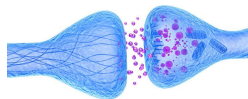
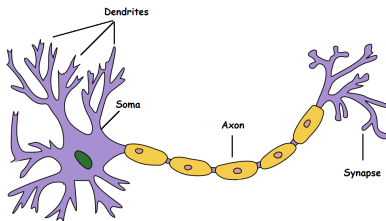
Introduction

Structure of neurons (II)

A neuron has a cell body ...

- ... a branching input structure (dendrite) and
- ... a branching output structure (axon)

Axons connect to dendrites via **synapses**



Introduction

Structure of neurons (III)

A neuron only fires if its input signal exceeds a threshold

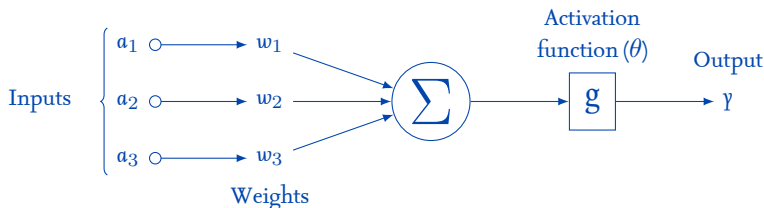
- Good connections allowing a large signal
- Slight connections allowing a weak signal
- Synapses may be either excitatory or inhibitory

Synapses vary in strength

- Biological learning involves setting that strength

Artificial neurons

Definition (I)



a_i Normalized input ($0 \leq a_i \leq 1$)

w_i Weight of input j

θ Threshold

g Activation function

Neuron model
(perceptron)

$$\gamma = g \left(\sum_{i=1}^n w_i a_i \right)$$

Artificial neurons

Definition (II)

- Each neuron has a threshold value
- Each neuron has weighted inputs
- The input signals form a weighted sum
- If the activation level exceeds the threshold, the neuron activates

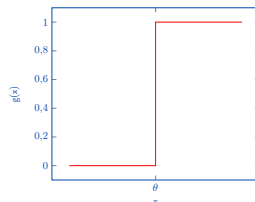
Artificial neurons

Definition (III)

The idealized activation function is a step function

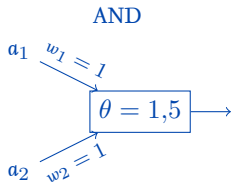
$$g(x) = \begin{cases} 1 & \text{if } \sum_{i=1}^N w_i x_i > \theta \\ 0 & \text{otherwise} \end{cases}$$

The step function is rarely used in practice

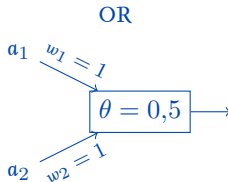


Artificial neurons

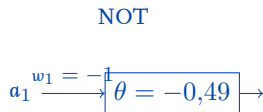
Logical gates with a neuron



a_1	a_2	γ
0	0	0
0	1	0
1	0	0
1	1	1



a_1	a_2	γ
0	0	0
0	1	1
1	0	0
1	1	1

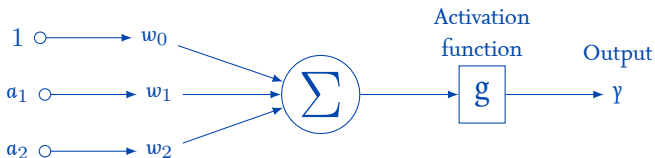


a_1	γ
0	1
1	0

(A neuron in Excel)

Artificial neurons

Definition of neuron (alternative version)



a_i Normalized input ($0 \leq a_i \leq 1$)

w_i Weight of input j

w_0 Bias

g Activation function

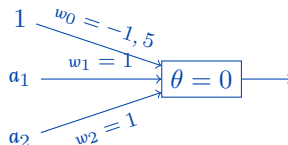
Neuron model

$$\gamma = g \left(\sum_{i=0}^n w_i a_i \right)$$

Artificial neurons

Example of biased neuron

AND logical gate with a biased input

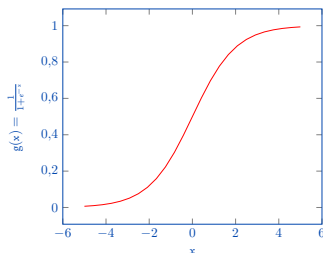


a_0	a_1	a_2	Output
I	O	O	O
I	O	I	O
I	I	O	O
I	I	I	I

Artificial neurons

Activation functions: Sigmoid function

- Biological motivation
- S-shaped, continuous and everywhere differentiable
- Asymptotically approach saturation points
- Derivative fast computation
- Range $\in [0, 1]$



Sigmoid function

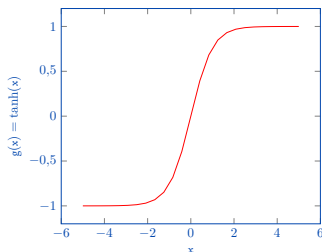
$$g(x) = \frac{1}{1 + e^{-x}}$$

$$g'(x) = g(x)(1 - g(x))$$

Artificial neurons

Activation functions: Tanh function

- Asymptotically approach saturation points
- Range $\in [-1, 1]$
- Bigger derivative than sigmoid (faster training)



Tanh function

$$g(x) = \tanh(x) = \frac{2}{1 + e^{-2x}} - 1$$

$$g'(x) = 1 - g(x)^2$$

Artificial neurons

Activation functions: Softmax function

- Generalization of the logistic function
- Usually used in the output layer in classification problems
- Asymptotically approach saturation points

Softmax function

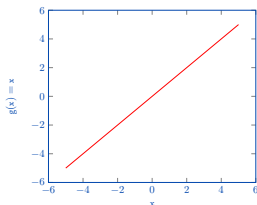
$$g(\mathbf{z})_j = \frac{e^{z_j}}{\sum_{k=1}^K e^{z_k}} \text{ for } j = 1, \dots, K$$

with \mathbf{z} a K-dimensional vector

Artificial neurons

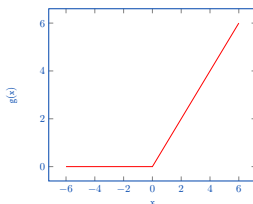
Other activation functions

Linear function



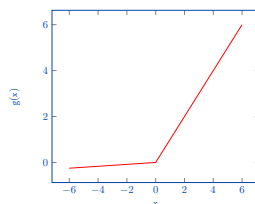
- Used in regression

Rectified Linear (ReLU)



- Faster derivate
- Popular in DL

Leaky ReLU

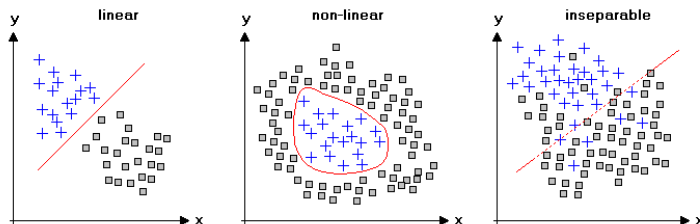


- More informative derivate
- Popular in DL

The lack of non-linear activation function makes a network a simple linear regression

Artificial neurons

Learning limits (I)

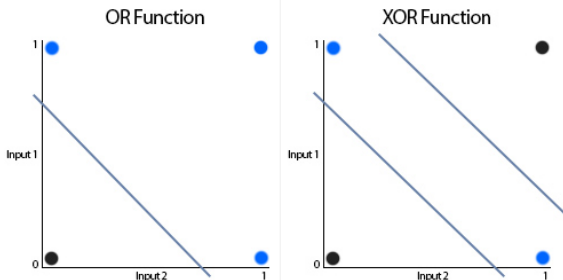


Problem: A single neuron only can solve linearly separable problems

Artificial neurons

Learning limits (II)

XOR cannot be implemented with a neuron



Solution: Neuronal networks

Artificial Neural Networks

Definition (II)

ANN properties

- Noise tolerance
- General function approximator

Machine Learning tasks

- Supervised learning (classification and regression)
- Unsupervised learning (known as **self-organizing maps** in ANN terminology)

Many topologies

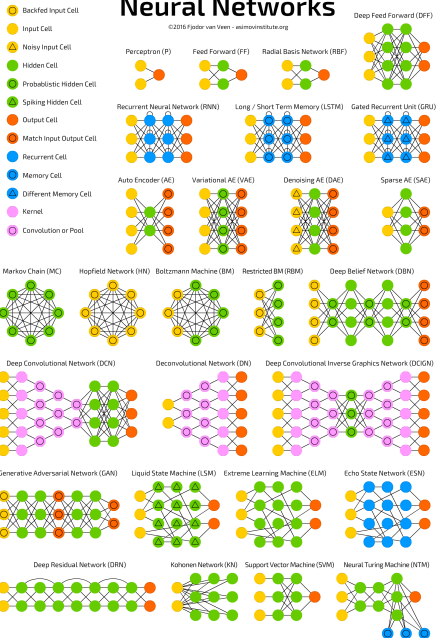
- Acyclic, recurrent (cyclic), modular, etc
- Feed Forward networks (MLPs)

Human readability less important than performance

A mostly complete chart of

Neural Networks

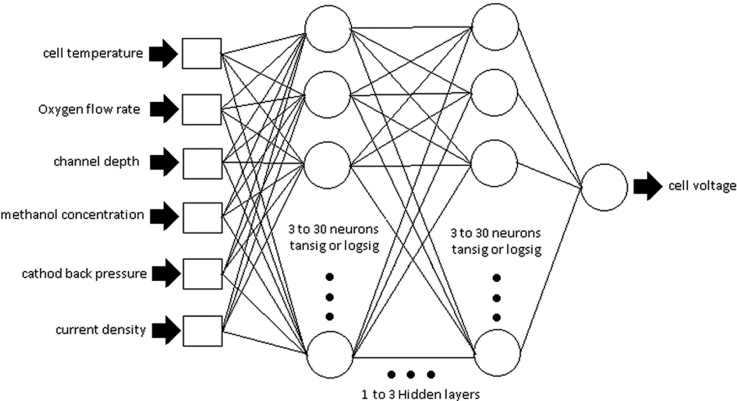
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(More info)

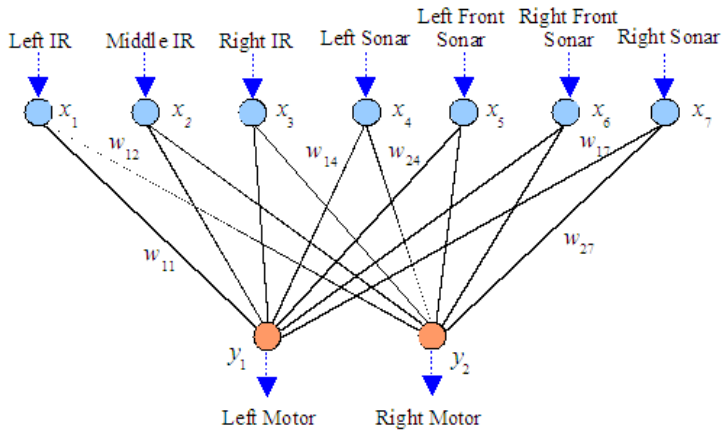
Artificial Neural Networks

Application examples (I)



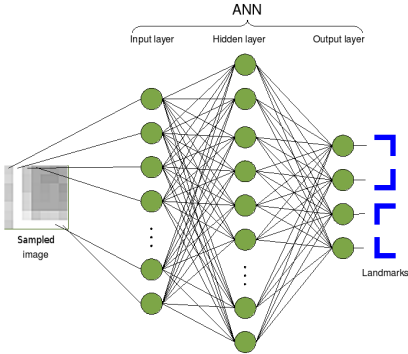
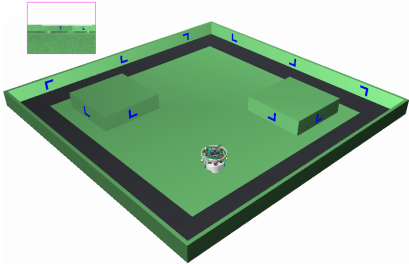
Artificial Neural Networks

Application examples (II)



Artificial Neural Networks

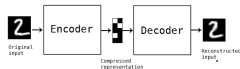
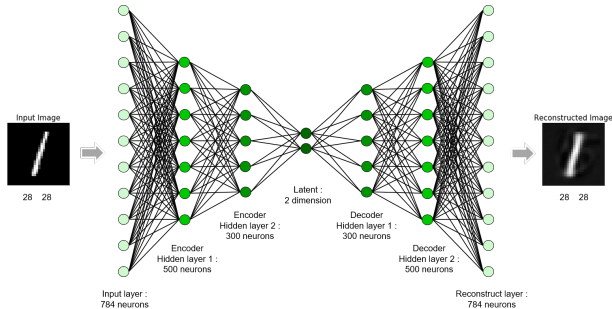
Application examples (III)



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Artificial Neural Networks

Application examples (IV)



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Feedforward networks

Definition (I)

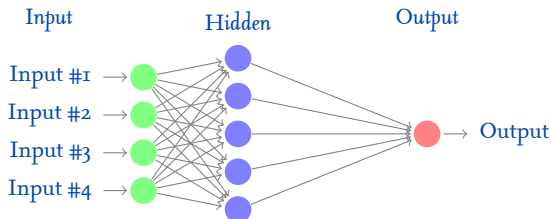
Neurons are arranged in **layers**

Input Which consists of any normalized data

Output Which are the net outcome

Hidden (Optional) No direct interaction

Also known as **multilayer perceptron (MLP)**



Feedforward networks

Definition (II)

The input layer

- Introduces input values into the network
- No activation function or other processing

The hidden layer(s)

- Perform classification of features
- Two hidden layers are sufficient to solve any problem
- Features imply more layers may be better

The output layer

- Functionally just like the hidden layers
- Outputs are passed on to the world outside the neural network


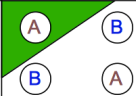
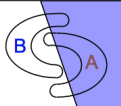


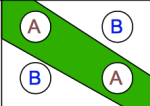
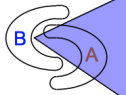
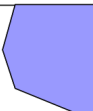
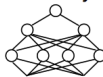
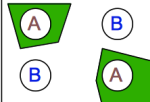

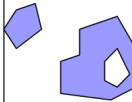
Feedforward Networks

Demo

(Online demo)

Feedforward Networks

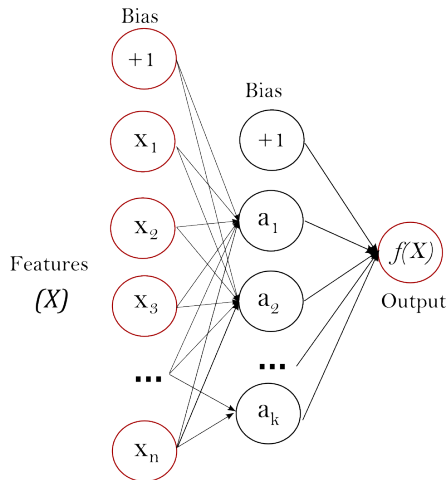
Separability

Structure	Types of Decision Regions	Exclusive-OR Problem	Classes with Meshed regions	Most General Region Shapes
Single-Layer 	Half Plane Bounded By Hyperplane			
Two-Layer 	Convex Open Or Closed Regions			
Three-Layer 	Arbitrary (Complexity Limited by No. of Nodes)			

(A MLP in Excel)

Feedforward Networks

Bias in a MLP



(Source)

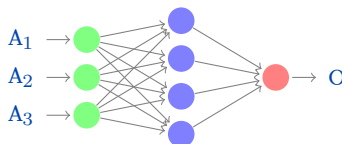
Training algorithms

Problem statement (I)

ANNs can perform different tasks

- Classification, regression, others

Classification (or supervised learning) uses a training set



A ₁	A ₂	A ₃	O	Y
1,1	2,5	4,5	0,2	-0,1
0,9	2,4	1,2	0,5	0,4
1,0	2,0	9,9	0,4	1,2

Toss function: Measure of the error

- Y and O are the desired and observed outputs
- Usually mean squared error (MSE): $f(w) = E = \frac{1}{2}(\gamma - o)^2$

Training algorithms

Problem statement (II)

Problem: Determine \vec{w} that minimize $f(\vec{w})$

- Remember, \vec{w} is our network
- This is a classical optimization problem
- Any optimization algorithm can be used
- ... in AI, optimization means search

We do know analytically $f(\vec{w}) \Rightarrow$ Optimization based on gradients

Training algorithms

Gradient Descent (I)

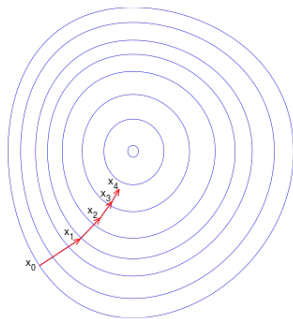
Calculate the gradient of the loss function with respect weights

- Adjust weights along gradient direction
- Gradient provides the direction
- α is the **learning rate** ($|\alpha| < 1$)

Gradient descent

```

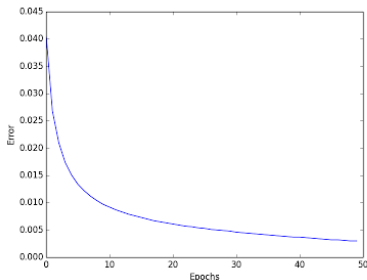
1:  $\vec{w} \leftarrow \text{random}()$ 
2: while Not converged do
3:   for all  $w_i \in \vec{w}$  do
4:      $w_i \leftarrow w_i - \alpha \frac{\partial}{\partial w_i} f(\vec{w})$ 
5:   end for
6: end while
  
```



Training algorithms

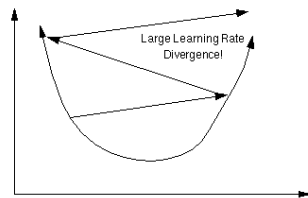
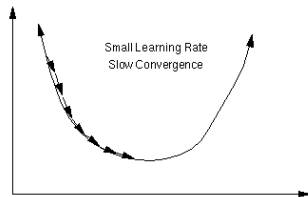
Gradient Descent (II)

Each iteration is named **epoch**



(Source)

Learning rate



(Source)

Training algorithms

Stochastic Gradient Descent (I)

SDG approximates the gradient sampling the dataset

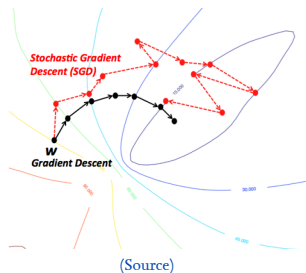
On-line One sample

Mini-batch Several samples

Batch All the samples (Gradient Descent)

Computations are faster ...

- ... but gradient estimation looses accuracy



Training algorithms

Stochastic Gradient Descent (II)

Usually, a **momentum** is introduced as

$$w^{k+1} = w^k - \alpha z^{k+1}$$

with

$$z^{k+1} = \beta z^k + \nabla g(\text{in})$$

where ...

- α is the learning rate
- β is the momentum strength
- If $\beta = 0$ then gradient descent

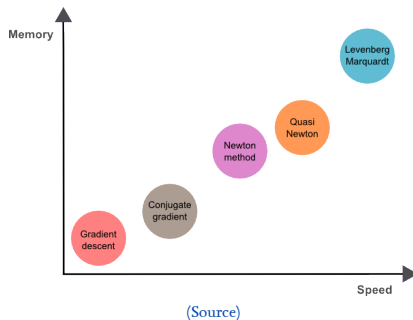
(On-line demo)

Training algorithms

Other optimization algorithms (I)

Other second derivative-based optimization algorithms

- Newton's method
- Quasi-Newton's method
- Levenberg-Marquardt method
- Conjugate Gradient



Training algorithms

Other optimization algorithms (II)

Learning reate / momentum adaptative methods

- AdaGrad - Adaptive Gradient Algorithm
- RMSProp - Root Mean Square Propagation
- Adam - Adaptive Moment Estimation

Training algorithms

Backpropagation

Backpropagation is an efficient algorithm to compute gradients

- It applies the chain rule to propagate errors
- Implicit in optimization algorithms

Backpropagation algorithm

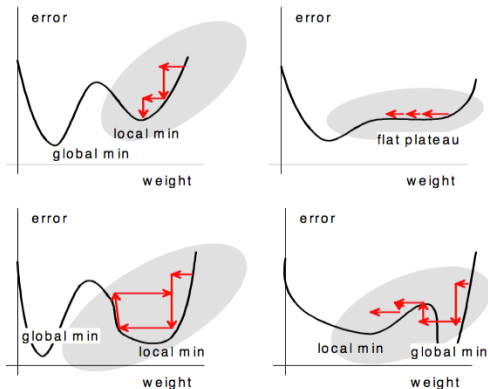
1. Compute output
2. Compute error
3. For each layer, repeat the following steps
 - 3.1 Propagate errors backwards
 - 3.2 Update weights between two layers

Training algorithms

Learning problems

Potential problems

- Local minima
- Flat plateau
- Oscillation
- Missing good minima



Training algorithms

Learning problems: Under and overfitting (I)

Underfitting: Does not learn

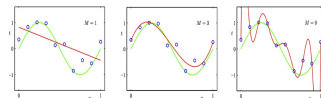
- Topology too simple

Overfitting: Memorizes samples

- Topology too complex
- Perhaps, the most serious concern in ML
- The net fails when exposed to new data

Under- and Over-fitting examples

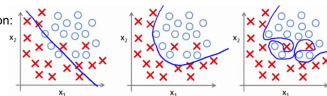
Regression:



predictor too inflexible:
cannot capture pattern

predictor too flexible:
fits noise in the data

Classification:



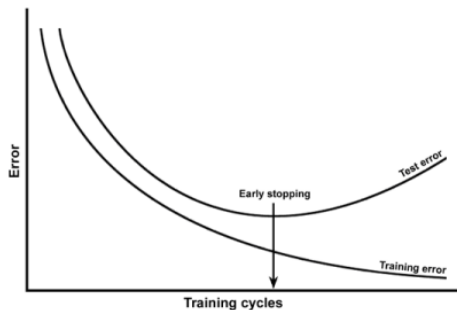
(Source)

Training algorithms

Learning problems: Under and overfitting (II)

Solution: Evaluate generalization capabilities

- Split training and validation sets and measure errors



(Source)

Acknowledgements

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- Daniel Rodríguez, Universidad de Alcalá, Alcalá de Henares, Spain