

AI for Astrophysics: Simple Neural Networks

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The brain as model

« *There is a fantastic existence proof that learning is possible, which is the bag of water and electricity (together with a few trace chemicals) sitting between your ears [...] which is the squishy thing that your skull protects* »

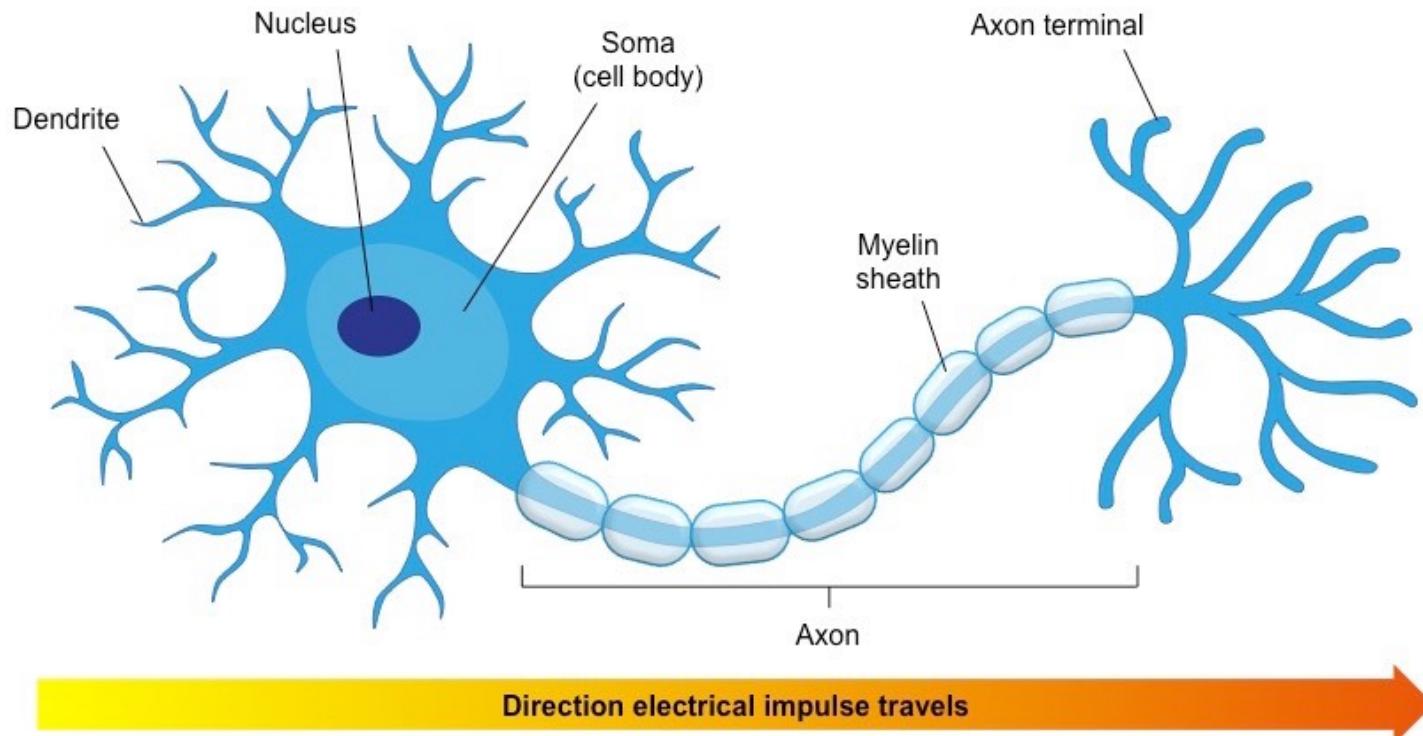
*Stephen Marsland

The brain does exactly what we want for data analysis:

- Extract complex information in a compressed form
- Deal with noisy and/or inconsistent data
- Work in highly-dimensional spaces
- Give the appropriate answer most of the time
- Provide results very quickly
- Remain robust through aging (neuron loss)

The biological neuron

Elementary brick of a biological brain (10^{11} in the human brain).
The idea will be to use it as a model to emulate learning capabilities.



Perform the **sum** of various electrochemical **input signals**. If this total signal is sufficient, it sends a **new signal** through its axon to **transfer information** (toward other neurons).

Biological Neural Networks

A connection between two neurons is called **a synapse** (10^{14} in the human brain).

A neuron is a binary compute unit that either “fire” or “not-fire” in response to a signal.

→ In this view, a brain is a **massively parallel super-computer of 10^{11} processing units**.

A simplified view of how it learns

The synapses represent the “strength” of the connection between two neurons.

Learning = modifying this connection (either positive or negative and changing its intensity)

→ This is called **plasticity**

The **Hebb law** defines a simplified rule for learning:

If two neurons “fire” **at the same time**, there must be some **correlation** between them, and their connection must be strengthened.

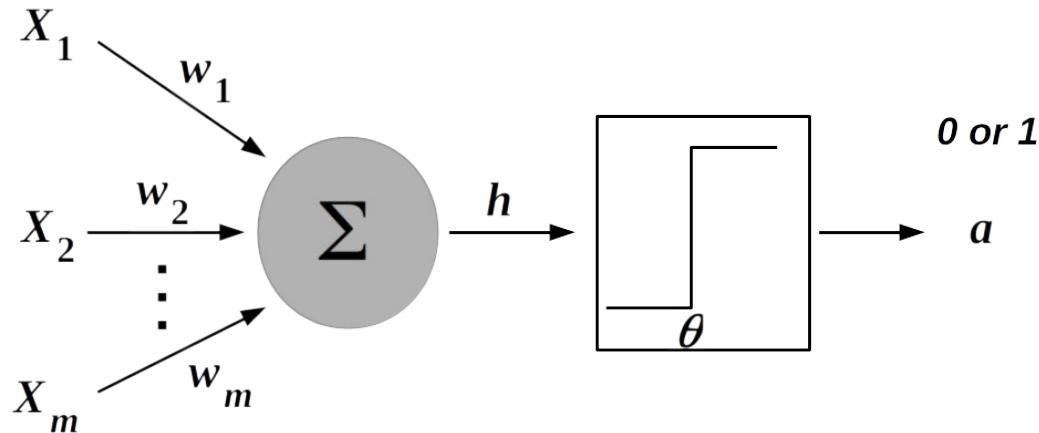
→ This is called **conditioning**

*These rules are not enough to train a neural system but illustrate the processes that occur in the biological brain.

To create an algorithm from these biological concepts, one first need to create a **mathematical model**.

Model of a Neuron

Mathematical model from **McCulloch and Pitts**, inspired by the biological neuron.

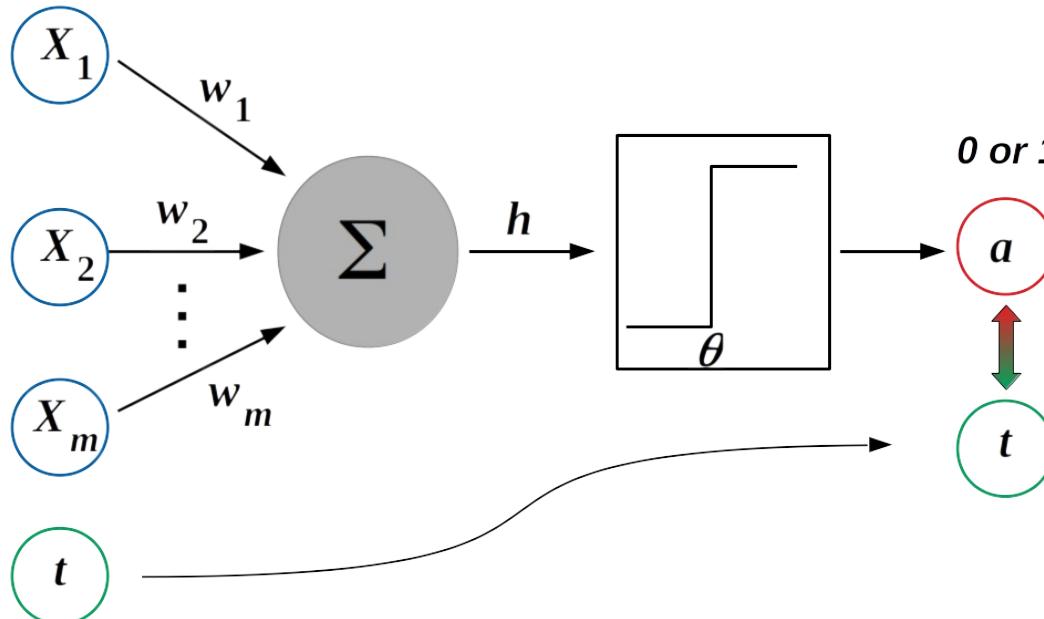


$$h = \sum_{i=1}^m X_i w_i \quad a = g(h) = \begin{cases} 1 & \text{if } h > \theta \\ 0 & \text{if } h \leq \theta \end{cases}$$

Its main components are:

- An **input vector X_i** that represents the dimensions of a given object
- A **set of weights w_i** that links the various input dimensions to the neuron
- A **sum function h** that defines how these weights are combined with the input dimensions
- An **activation function $g(h)$** that defines if the network should remain in a “0” state or should be activated to a “1” state, depending on the results of the sum.

Training a Neuron



The learning process for this model is supervised
→ Each **input vector** is associated to a **target value**

So what is the purpose of the neuron if the expected value is already known ?

→ **Generalization**

Find **patterns in the data distribution** in the parameter space so it can perform prediction on vectors with unseen (but close) values.

In practice, such a simple neuron **optimizes a linear separation** in the parameter space (**hyperplane**).

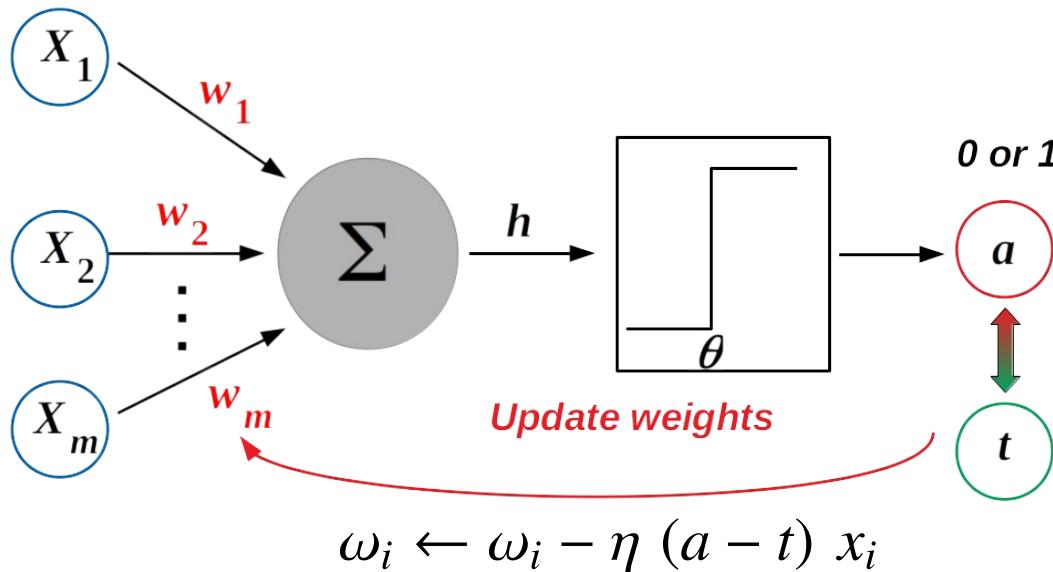
How does this model learn ?

Which parameters can or cannot be modified ?

The **input, output, and targets are fixed**, so the learning relies on modifying the **weights and the activation threshold**.

$$h = \sum_{i=1}^m X_i w_i \quad a = g(h) = \begin{cases} 1 & \text{if } h > \theta \\ 0 & \text{if } h \leq \theta \end{cases}$$

Training a Neuron



$$h = \sum_{i=1}^m X_i w_i \quad a = g(h) = \begin{cases} 1 & \text{if } h > \theta \\ 0 & \text{if } h \leq \theta \end{cases}$$

How to proceed when the output does not correspond to the target ?

There are m weights w_i associated with the network corresponding to the input dimensions.

How to modify the weights?

- If the output state is 1 while it should be 0, the weights need to be **lowered**
- If the output state is 0 while it should be 1, the weights need to be **increased**

To quantify this modification, one needs to choose an **error function E** .

$$E = 0.5 \times (a - t)^2$$

In the end, the weight update is defined as proportional to the **input value**, to the **derivative of the error function** for each dimension, and scaled by a **learning rate*** factor.

$$\omega_i \leftarrow \omega_i - \eta (a - t) x_i$$

*Typically between 0.1 and 0.4, details will be given later. 7 / 38

The bias node

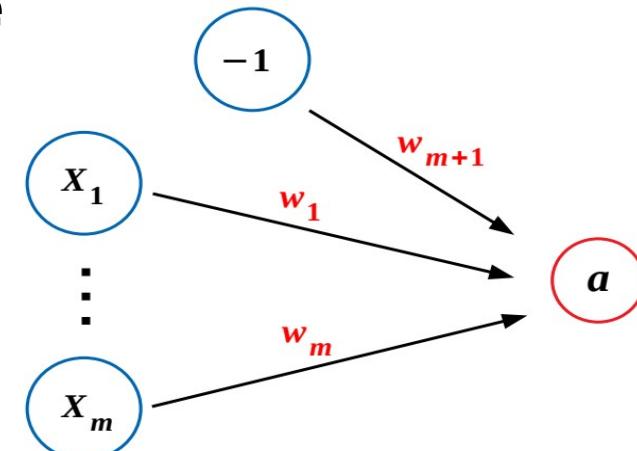
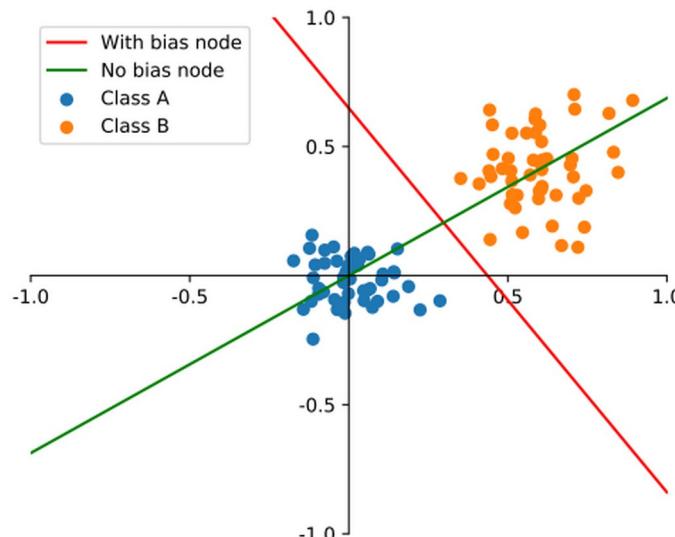
Problem with the previous formalism

The linear separation presents a **fixed $f(0) = 0$ point**.

The weight correction is also 0, regardless of the input value.

Solution

Add a **bias input node** that acts as an additional input with a **constant value** (usually -1). It has its own **variable weight** so it can learn the shift of the intercept position. The size of both the input vector and the weights vector is now $m+1$.



To plot the found linear separation of a neuron, we need to find where in the parameter space the neuron changes state, which corresponds to:

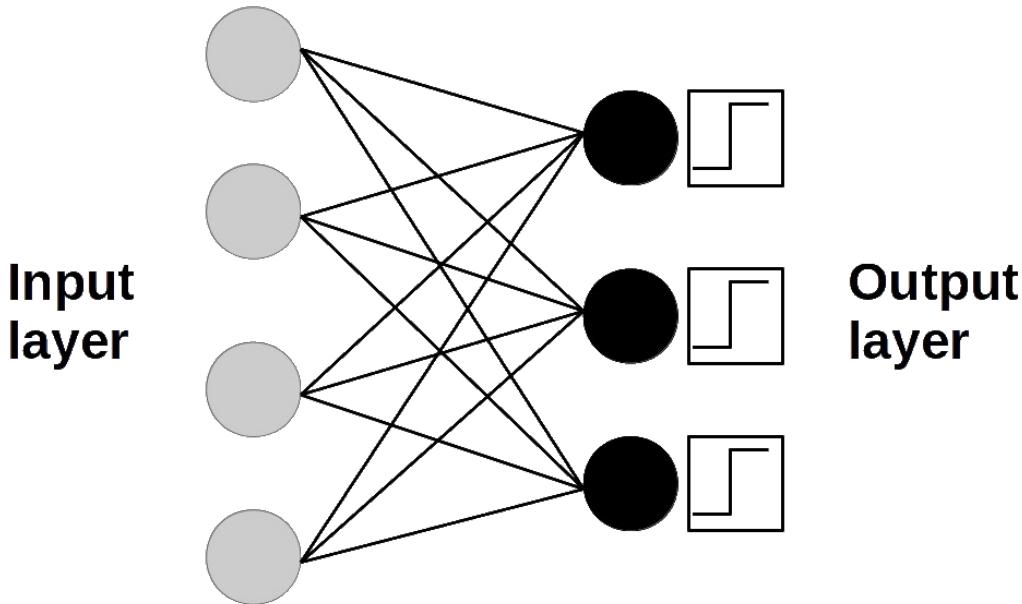
$$\sum_{i=1}^m X_i w_i = h = 0$$

For a 2D parameter space it results in:

$$X_1 = (W_b - X_0 W_0) / W_1$$

Note that the direction of activation is orthogonal to the linear separation.

The Perceptron algorithm



A single neuron **only performs a linear separation**, which is insufficient for many applications.

The simplest way to combine neurons on a single problem is to **stack them independently**. Each neuron is connected to the input vector with **its own set of weights**.

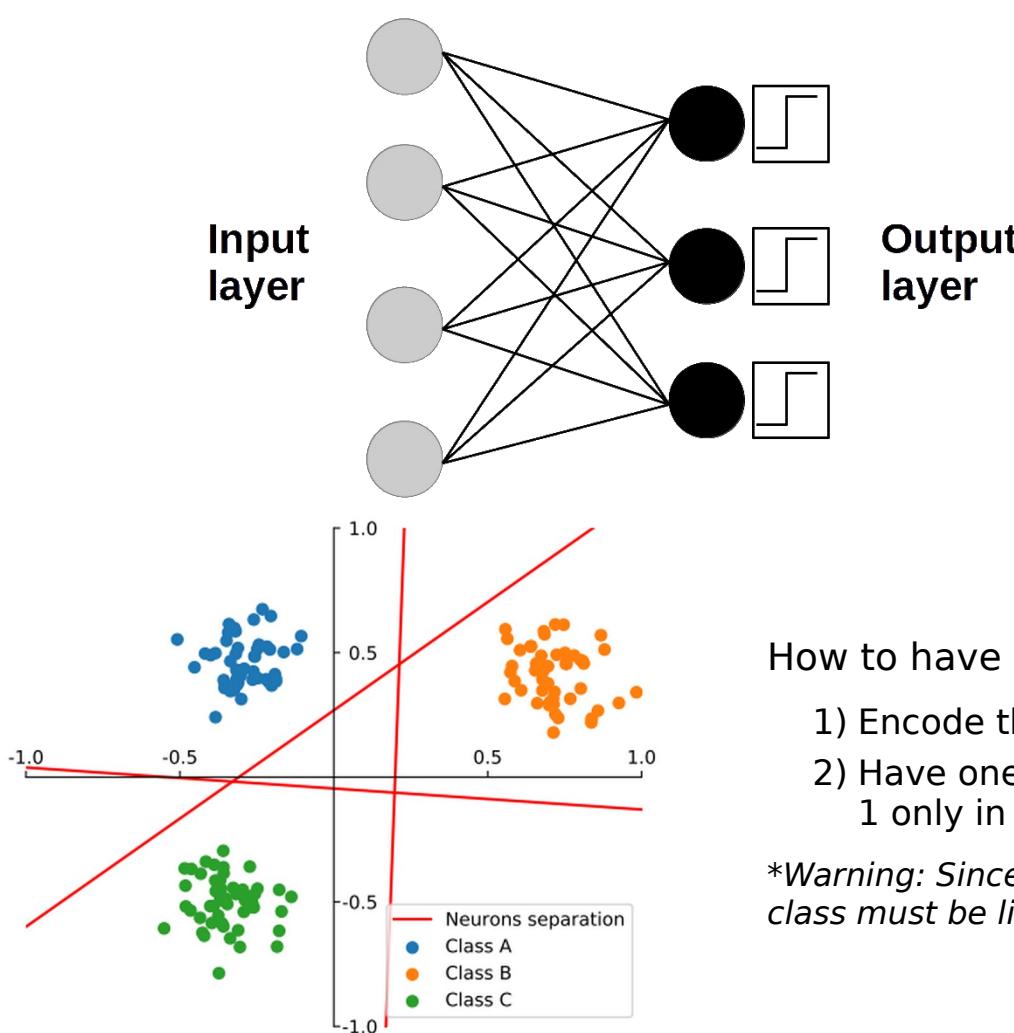
The training procedure is identical, but this time there is an index j to represent the neurons, and **the weights are now in the form of a 2D matrix**.

$$h_j = \sum_{i=1}^{m+1} x_i \omega_{ij} \quad a_j = g(h_j) = \begin{cases} 1 & \text{if } h_j > \theta \\ 0 & \text{if } h_j \leq \theta \end{cases}$$

$$\omega_{ij} \leftarrow \omega_{ij} - \eta (a_j - t_j) \times x_i$$

The combination of this training procedure and this neuron connection scheme is called the single layer “Perceptron” (Rosenblatt 1958).

The Perceptron algorithm



C1	C2	C3
1	0	0
0	1	0
0	0	1

How to have multiple neurons work on the same problem ?

- 1) Encode the output vector (e.g in binary format)
- 2) Have one neuron per output class and target a format with a 1 only in the appropriate class, e.g [1,0,0]-[0,1,0]-[0,0,1]

*Warning: Since each neuron only performs a *linear separation*, each class must be *linearly separable* from all the others.

The Perceptron algorithm

- **Initialization**

- Set the starting weights to small random values (positive and negative).
Can be drawn from a uniform or Gaussian distribution centered on zero.

- **Training**

- For a given number of steps T, or until the output is “correct”
 - For each input vector
 - Compute the activation of each neuron j using the activation function g :

$$a_j = g\left(\sum_{i=0}^{m+1} w_{ij}x_i\right) = \begin{cases} 1 & \text{if } \sum_{i=0}^{m+1} w_{ij}x_i > 0 \\ 0 & \text{if } \sum_{i=0}^{m+1} w_{ij}x_i \leq 0 \end{cases}$$

- Update each weight individually using :

$$\omega_{ij} \leftarrow \omega_{ij} - \eta (a_j - t_j) \times x_i$$

- **Inference**

- Compute the final activation of each neuron j for each input vector to test

First application : logical gates

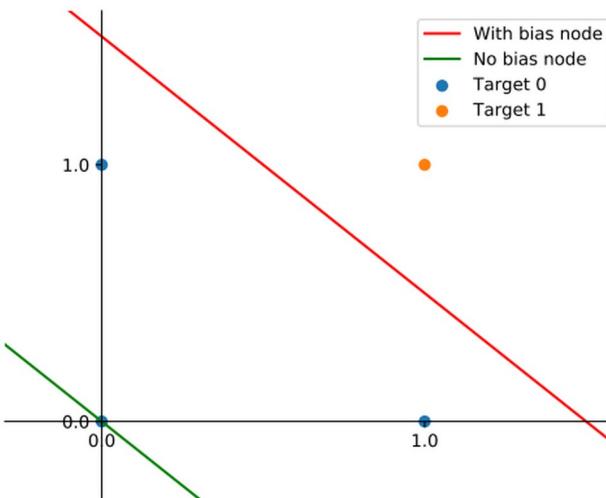
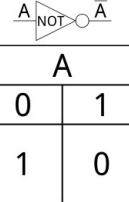
		A
		0 1
B		0 0 1
A	B	1 1

		A
		0 1
B		0 0 0
A	B	1 0 1

		A
		0 1
B		0 0 1
A	B	1 1 0

		A
		0 1
B		0 1 0
A	B	1 0 0

		A
		0 1
B		0 1 1
A	B	1 1 0



A straightforward application of this algorithm is to make it learn a logical door, here the **OR or AND gate**. For this simple application, the Perceptron has a two-dimensional input vector and 4 possibilities as input-target pairs.

The output is made of a single binary neuron to predict either the 0 or 1 state of the gate.

As a first exercise:

- Write a simple program that declares an array with all the possible inputs and the associated targets.
- Identify all the necessary variables and initialize the weights with small values.
- Try to train this neuron over a few iterations following the Perceptron algorithm.

Do not forget the bias node!

- Display the output at each iteration to watch the network converge toward a stable solution.

Why is the **XOR gate** problematic with this algorithm?
How to solve the problem?

The Pima Indian dataset

Dataset from the UCI Machine Learning repository.

Provides 8 physiological measurements for 768 female native Americans and provides a class depending on whether the individual has developed diabetes.

This exercise aims to implement a Perceptron to **predict if a person has diabetes** based solely on the 8 input measurements.

Despite its limitations, a simple Perceptron can reach up to **70% accuracy** on this dataset.

- Modify your program to read the Pima dataset.
- Adapt the input dimension (including bias).
- Adapt the corresponding computations.
- Find a method to compute the “**accuracy**” and its evolution during training.
- Question the limits of your accuracy definition, and find a way to ensure that you are testing the generalization capabilities of the method.

Attribute Number	Attribute
1	Patient age
2	Body mass index (kg/m ²)
3	Concentration of plasma glucose
4	2-h serum insulin (mu U/mL)
5	Thickness of triceps skin-fold (mm)
6	Pedigree function of diabetes
7	Number of times patient pregnant
8	Diastolic blood pressure (mmHg)
9	Class 0 or 1

Input dimension : 8 (+1)

*Output dimension : 1
(or 2 if using one neuron per class)*

Number of example : 768

Class distribution : 500 class 0; and 268 class 1

The Iris dataset

Dataset from the UCI Machine Learning repository.

Provides 4 sizes for a set of 150 Iris flowers and provides membership to one of 3 classes.

This exercise aims to implement a Perceptron to **predict the corresponding class** based on the 4 input measurements for each flower.

Despite its limitations, a simple Perceptron can reach up to **80% accuracy** on this dataset.

- Modify your program to read the Pima dataset.
- Adapt the input dimension (including bias).
- Adapt the corresponding computations.
- Find a method to compute the “**accuracy**” and its evolution during the training phase.
- Question the limits of your accuracy definition, and find a way to ensure that you are testing the generalization capabilities of the method.

iris setosa



iris versicolor



iris virginica



Samples
(instances, observations)

	Sepal length	Sepal width	Petal length	Petal width	Class label
1	5.1	3.5	1.4	0.2	Setosa
2	4.9	3.0	1.4	0.2	Setosa
...					
50	6.4	3.5	4.5	1.2	Versicolor
...					
150	5.9	3.0	5.0	1.8	Virginica

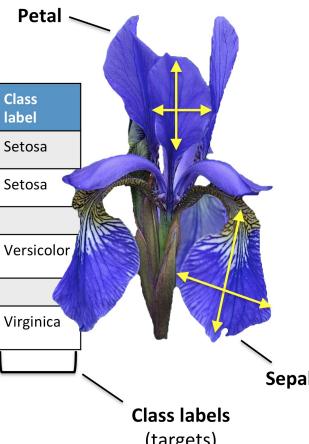
Features
(attributes, measurements, dimensions)

Input dimension : 4 (+1)

Output dimension : 3

Number of example : 150

Class distribution : 50 examples per class



The Spectra dataset

This dataset contains **stellar spectra** obtained with the 0.9m Coudé Feed telescope at Kitt Peak National Observatory, classified into various spectral types.

The provided dataset here is a simplification that only keeps 1115 homogeneous spectra with half the resolution (3753 “pixels” remains).

The target only provides the 7 regular spectral types for classification to increase the number of examples per class. Still, the dataset remains highly imbalanced!

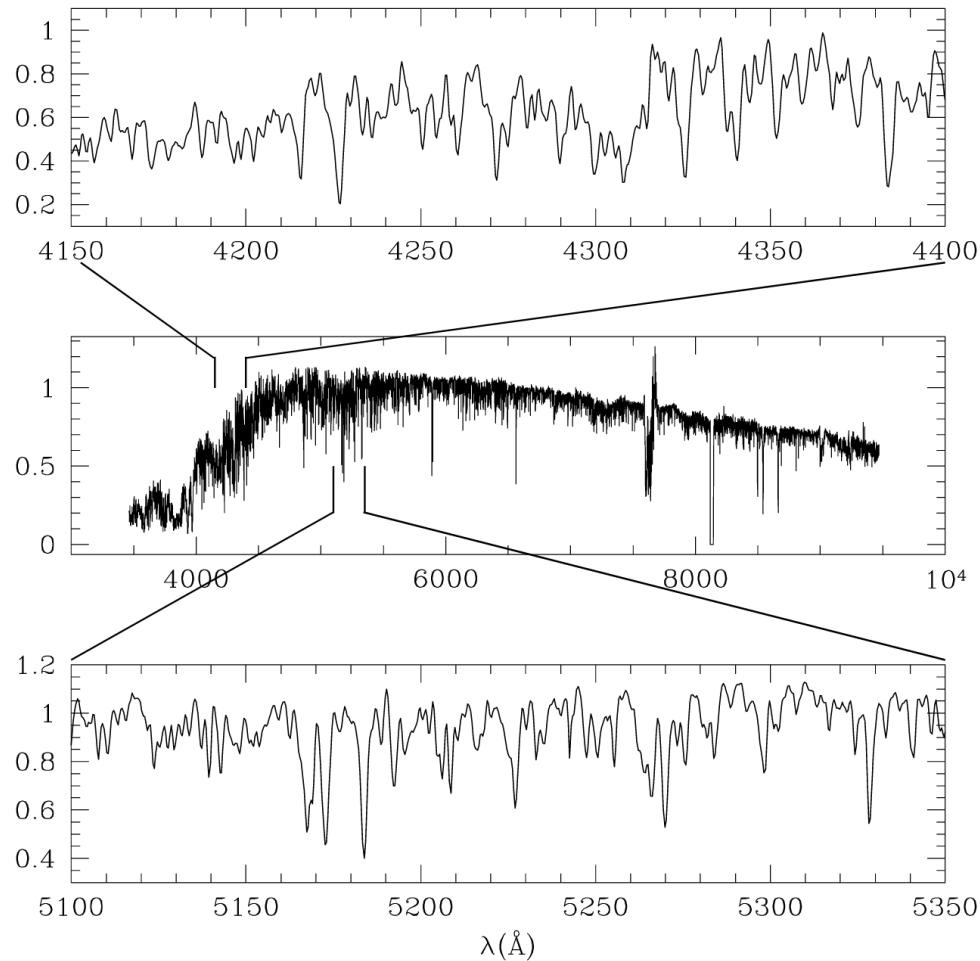
Infos about the dataset and the reference paper (*F. Valdes et al. 2004*) are in the info file.

Input dimension : 3753 (+1)

Output dimension : 7

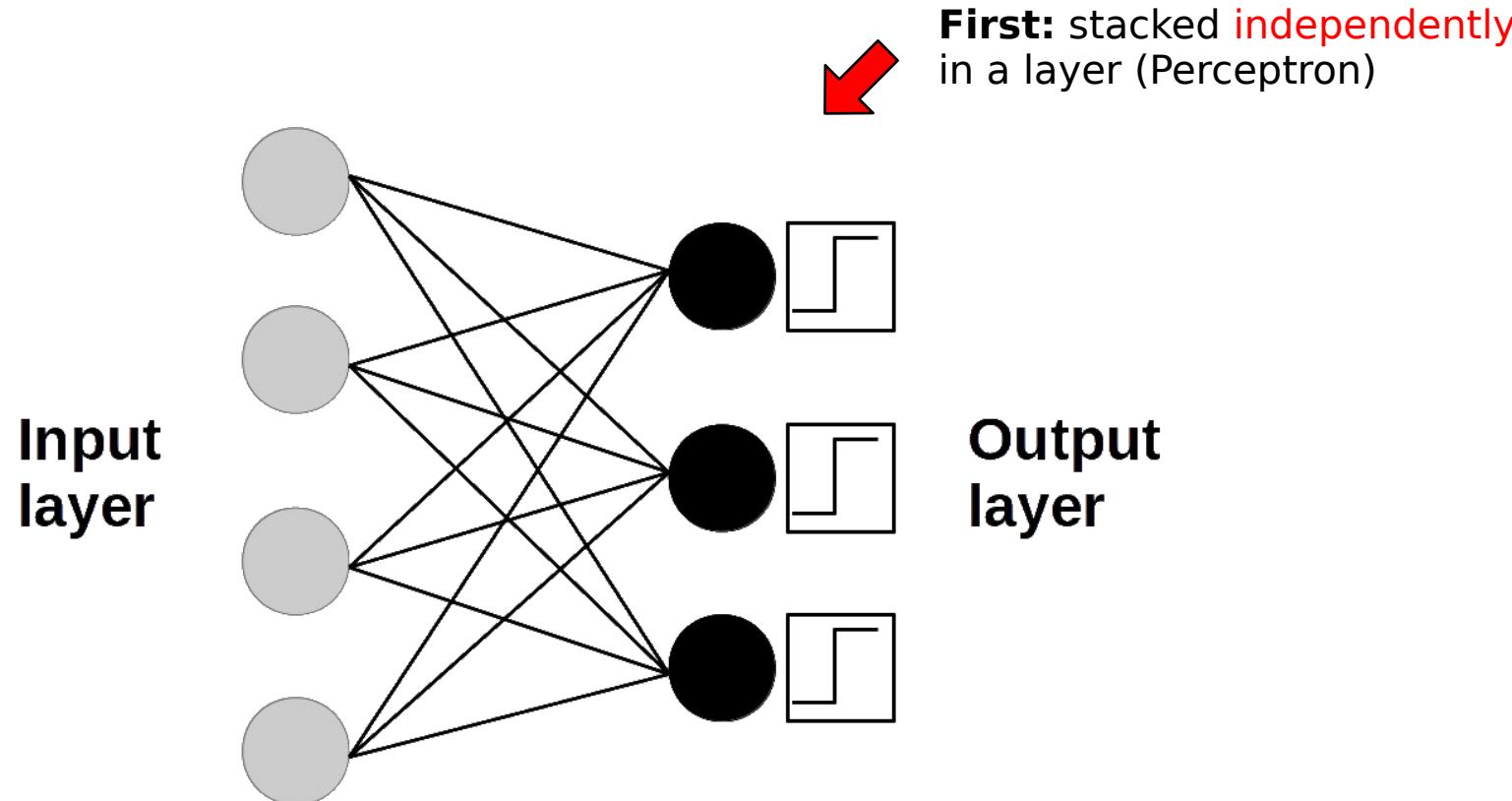
Number of example : 1115

Class distribution : strong imbalance



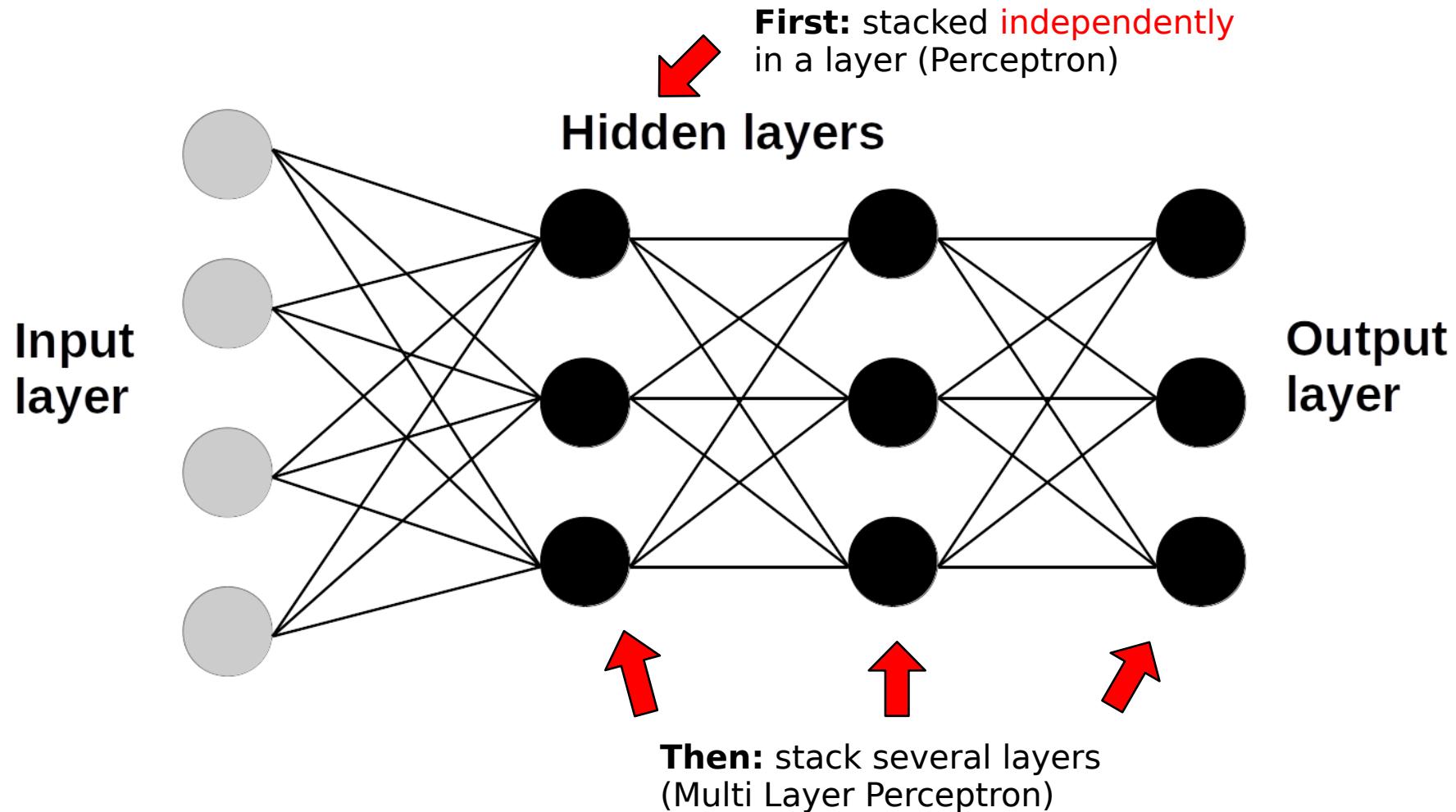
Constructing a “Deep” Neural Network

For more complex problems **more neurons must be used.**



Constructing a “Deep” Neural Network

For more complex problems **more neurons must be used.**



Constructing a “Deep” Neural Network

In addition to the MLP architecture, it is necessary to **change the activation** to allow **non-linear combinations**

→ **Change for a Sigmoid (logistic) function**

$$g(h) = \frac{1}{1 + \exp(-\beta h)}$$

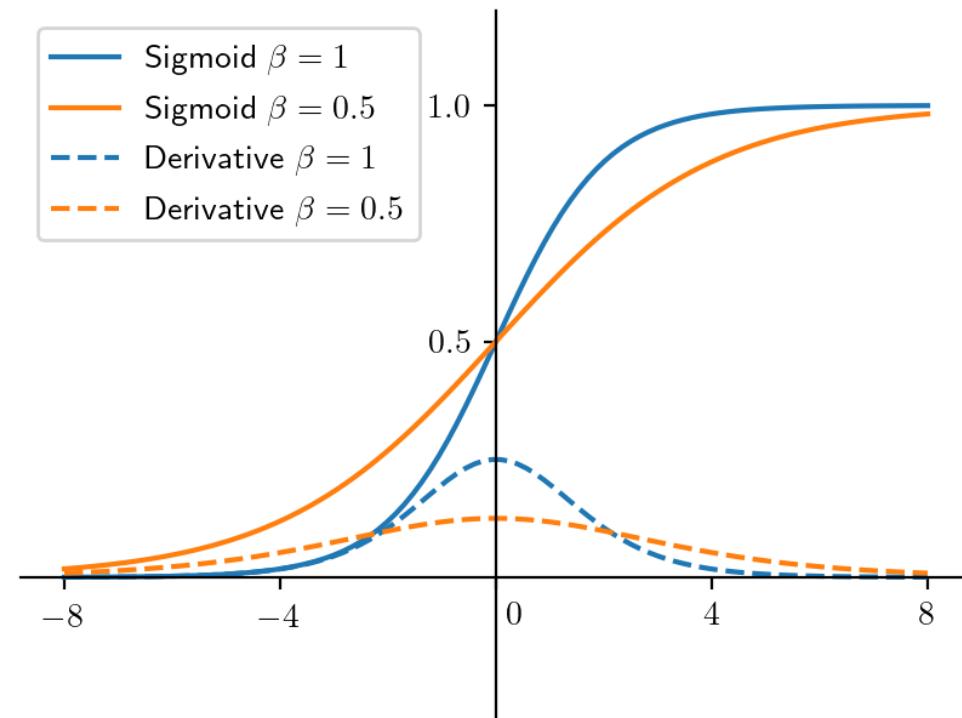
Beta represents the **slope** of the function.

The sigmoid is continuous while preserving the desired global binary behavior in its extremity.

It has a nice derivative form :

$$\frac{\partial a_j}{\partial h_j} = \beta a_j(1 - a_j)$$

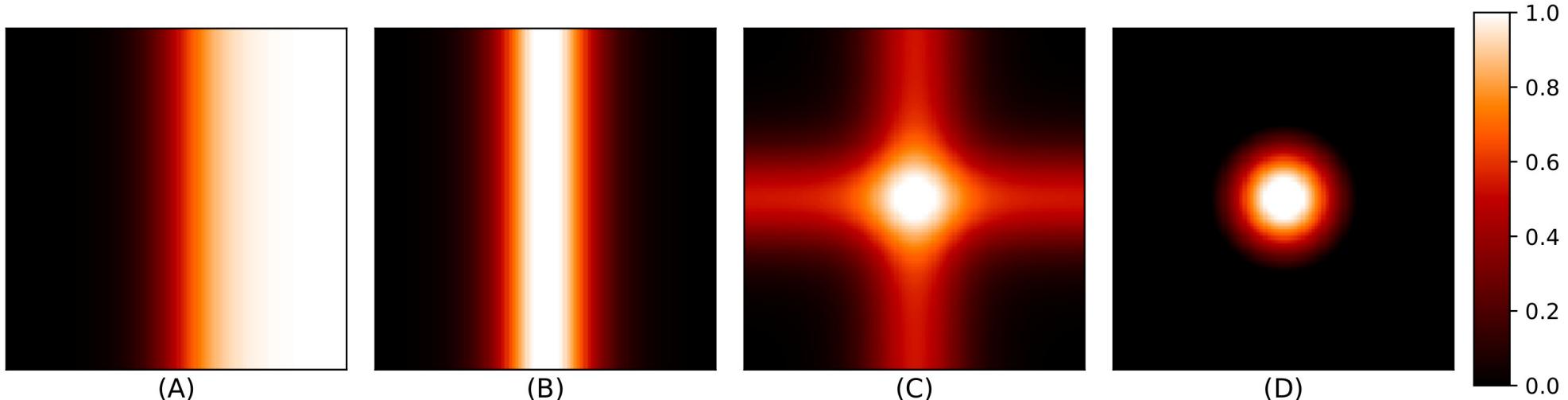
For regression problems, the output layer can either use sigmoids or simple linear activation functions since the previous layers will handle non-linearity.



Constructing a “Deep” Neural Network

Stacking layers that use a sigmoid activation allows the construction of **more and more complex functions**. The image below demonstrates that it is possible to reconstruct hill shapes (B), bumps (C), and point-like functions.

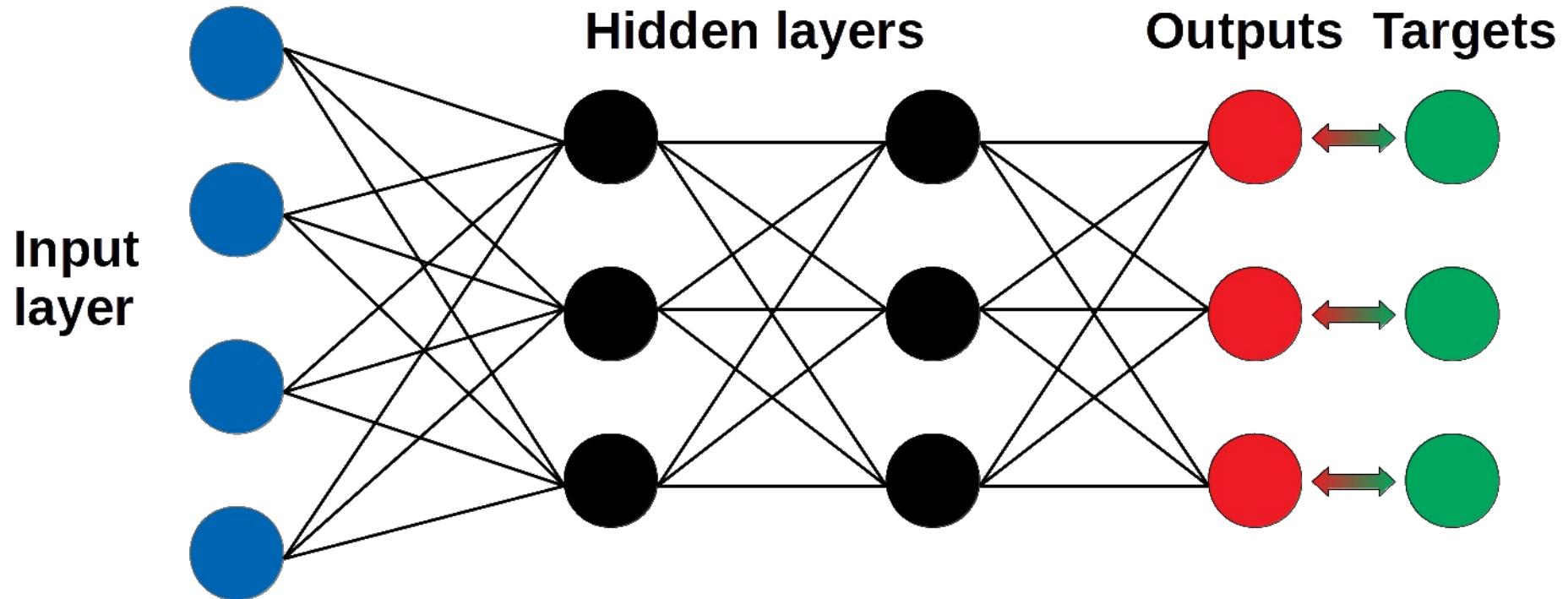
→ With these improvements, the MLP is a **Universal Function Approximator**



In practice, based on the universal approximation theorem, a MLP with a **single hidden layer** remains a UFA at the condition of having a large enough number of neurons.

Error gradient backpropagation

Problem : how to correct the output of neurons in the hidden layers ?



$$\omega_{ij} \leftarrow \omega_{ij} - \eta \frac{\partial E}{\partial \omega_{ij}} \quad \xrightarrow{\text{red arrow}} \quad \frac{\partial E}{\partial \omega_{ij}} = \delta_l(j) \frac{\partial h_j}{\partial \omega_{ij}} \quad \text{with} \quad \delta_l(j) \equiv \frac{\partial E}{\partial h_j} = \frac{\partial E}{\partial a_j} \frac{\partial a_j}{\partial h_j} = \frac{\partial a_j}{\partial h_j} \sum_k \omega_{kj} \delta_{l+1}(k)$$

Actual Network equations for an MLP with a single hidden layer

Changes in the Perceptron algorithm required to obtain the Multi-Layer Perceptron algorithm :

- Change the activation function of all neurons, with $\beta \geq 1$

$$g(h) = \frac{1}{1 + \exp(-\beta h)}$$

- Add a hidden layer with its own bias node (connect input \rightarrow hidden, and hidden \rightarrow output)
- Implement the “back-propagation” with $E(a^o, t) = \frac{1}{2} \sum_{k=1}^{N_o} (a_k^o - t_k)^2$ using the following equations:

$$\delta_o(k) = \beta a_k^o (1 - a_k^o) (a_k^o - t_k)$$

$$\delta_h(j) = \beta a_j^h (1 - a_j^h) \sum_{k=1}^{N_o} \delta_o(k) \omega_{jk}$$

$$\omega_{jk} \leftarrow \omega_{jk} - \eta \delta_o(k) a_j^h$$

$$v_{ij} \leftarrow v_{ij} - \eta \delta_h(j) x_i$$

Example with classification

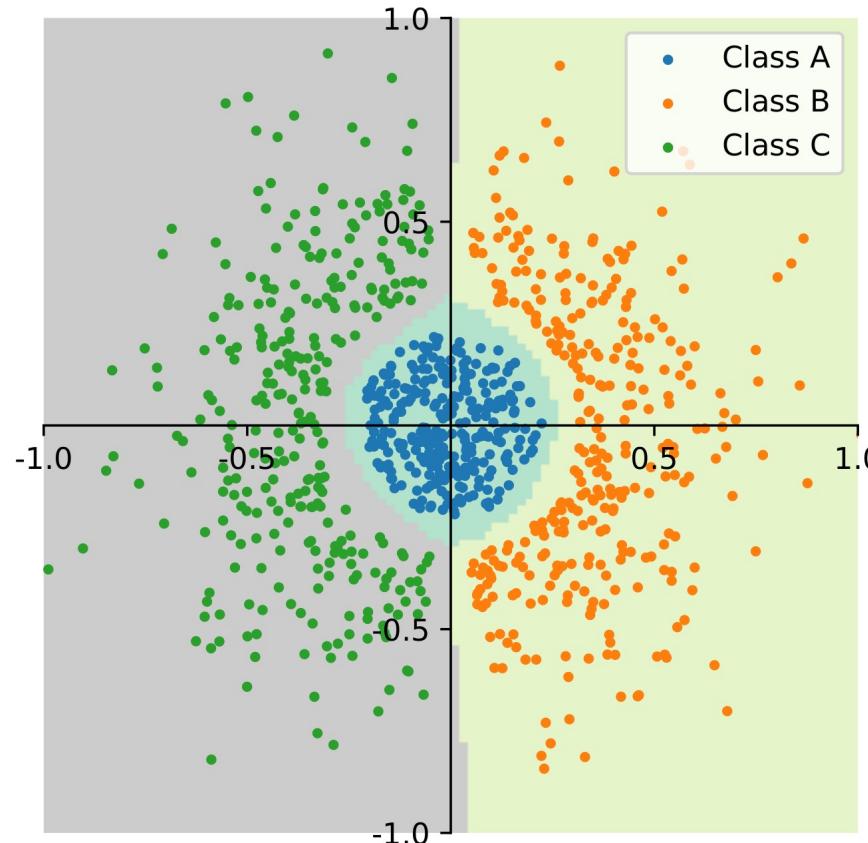


Illustration of a three-class separation in a two-dimensional feature space using a trained MLP with 3 output neurons and 8 hidden neurons, all with sigmoid activations. The light background colors indicate the regions of the feature space that the network has attributed to each class.

How to measure classification performance ?

→ Confusion Matrix

- Uses “**observational proportions**”
- Provides confusion between classes
- Is much more precise than the average accuracy

Predicted

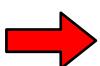
$$\text{Recall} = \frac{TP}{TP + FN}$$

Actual	Class	Positive	Negative	Recall
Positive	Positive	93	7	93.0%
Negative	Negative	46	954	95.4%
	Precision	66.9%	99.27%	95.18%

$$\text{Precision} = \frac{TP}{TP + FP}$$

$TP \equiv$ True Positive

$FP \equiv$ False Positive



$TN \equiv$ True Negative

$FN \equiv$ False Negative

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

ML methods usually learn better on balanced dataset **BUT**

the results must always be represented using “**observational proportions**”, with imbalance.

Learning rate

Choosing the **appropriate learning rate** for the task is very important and must consider several aspects of the error space.

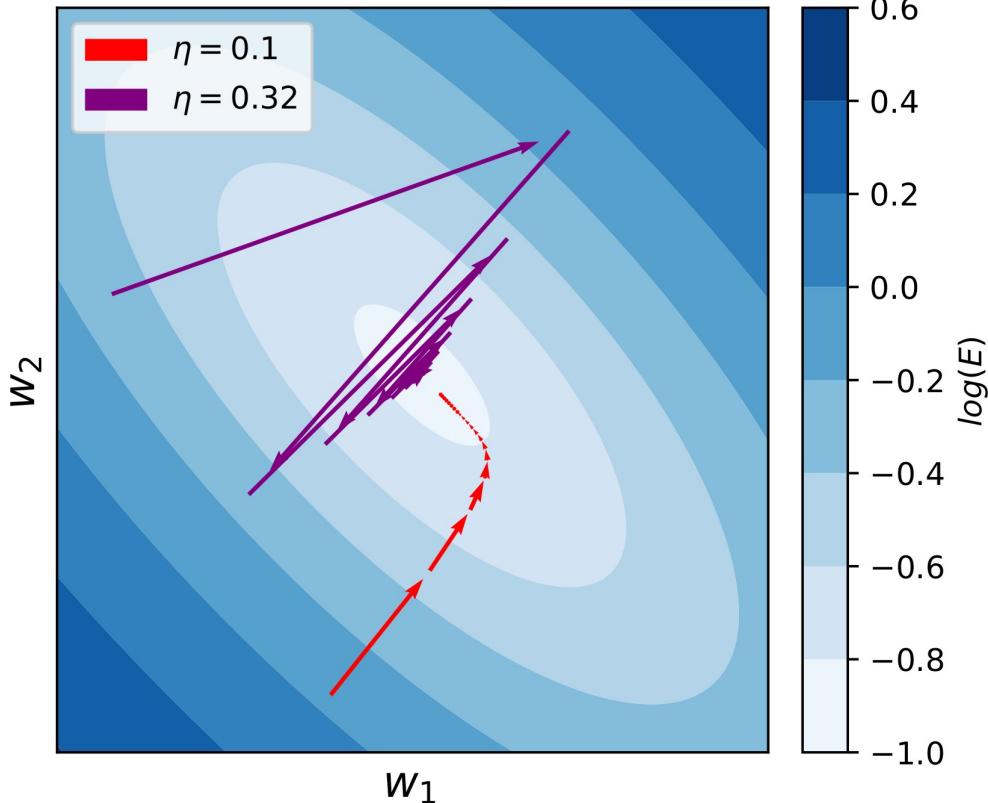
	Small η	Large η
Pros	<ul style="list-style-type: none">• Increase training stability• Can find narrower minima	<ul style="list-style-type: none">• Faster training• Easily switch from a local minima to another
Cons	<ul style="list-style-type: none">• Slow training• Might get stuck on local minima	<ul style="list-style-type: none">• Might fail to find a narrow minima• Training can be very unstable

The learning rate does not have to be a single value, it can **change** during the training phase.

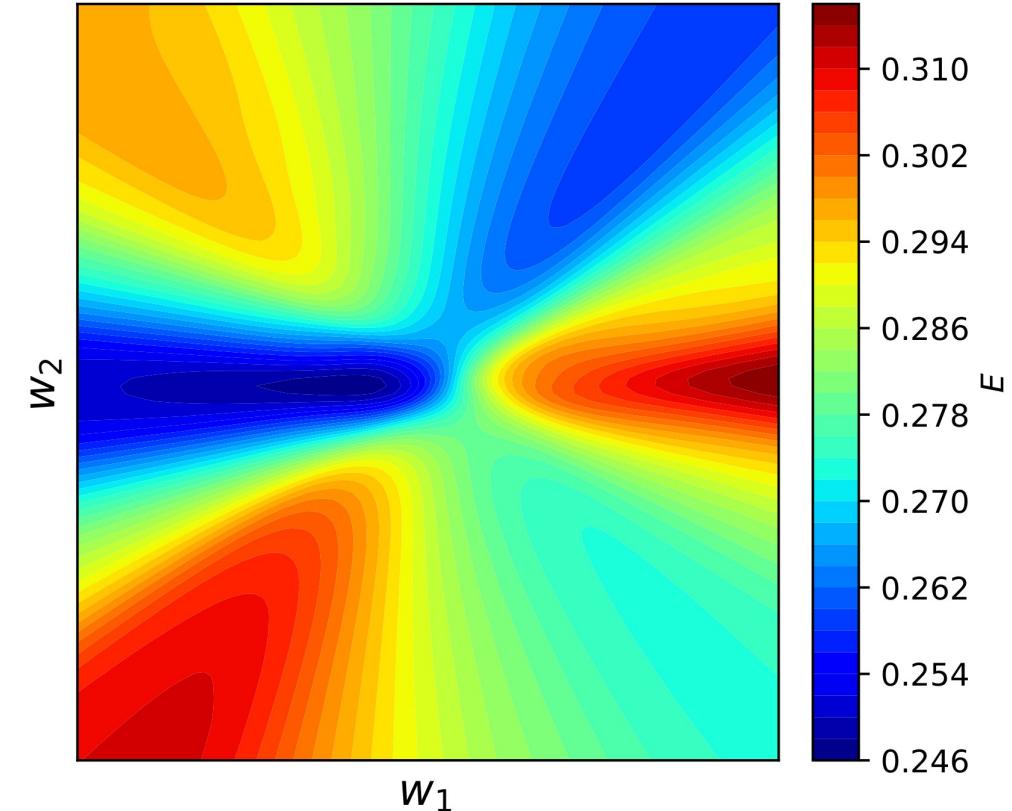
The simple approaches are: pre-established fixed values, linear decay, **exponential decay**, ...

Most frameworks allow the use of advanced gradient descent scheme that also automatically adapts the learning rate: Adam, RMSprop, Adagrad, etc ...

Learning rate



Logarithm of the error term in the weight space of a simple binary neuron with a two dimensional input parameter. The arrows represent the correction after each epoch for two different learning rates.



Error term in a 2D weight space of neuron in the hidden layer of a 3 class output MLP. The other weights of the network are frozen while exploring this 2D weight space.

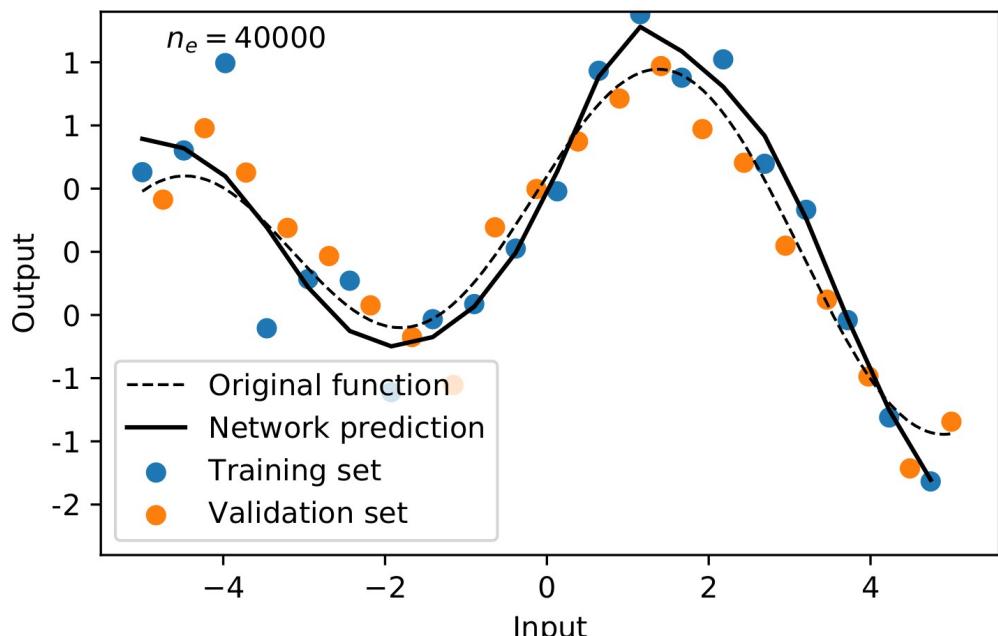
Overtraining



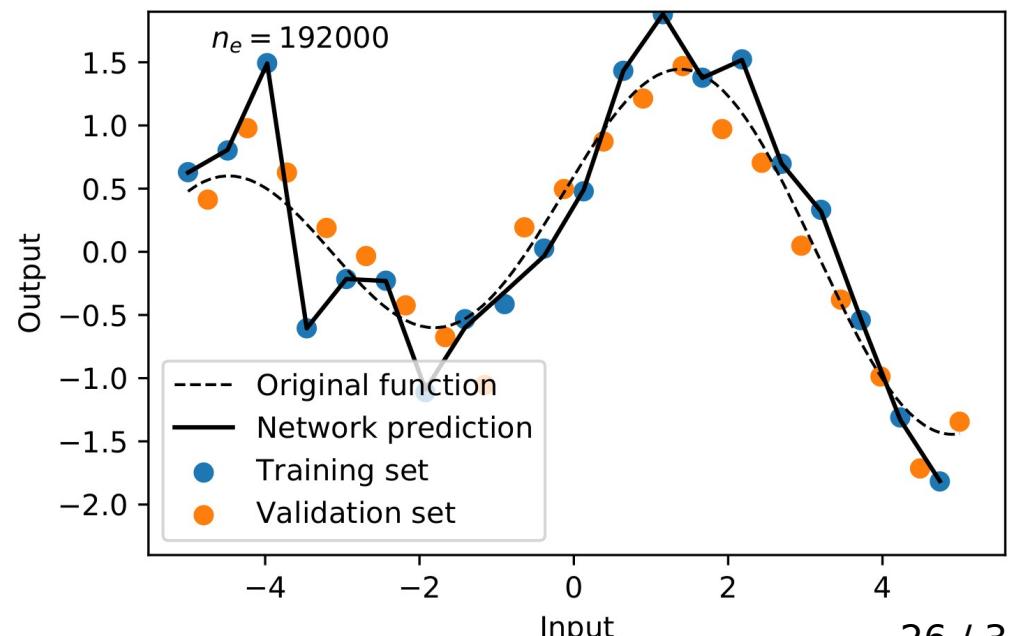
Overtraining: At some point during the training phase, the network that looks at the same data again and again, might start to over-fit!

It means that the network is learning specificities of the dataset that are no longer related to the average function that it should approximate.

Proper fit



Over-fitting

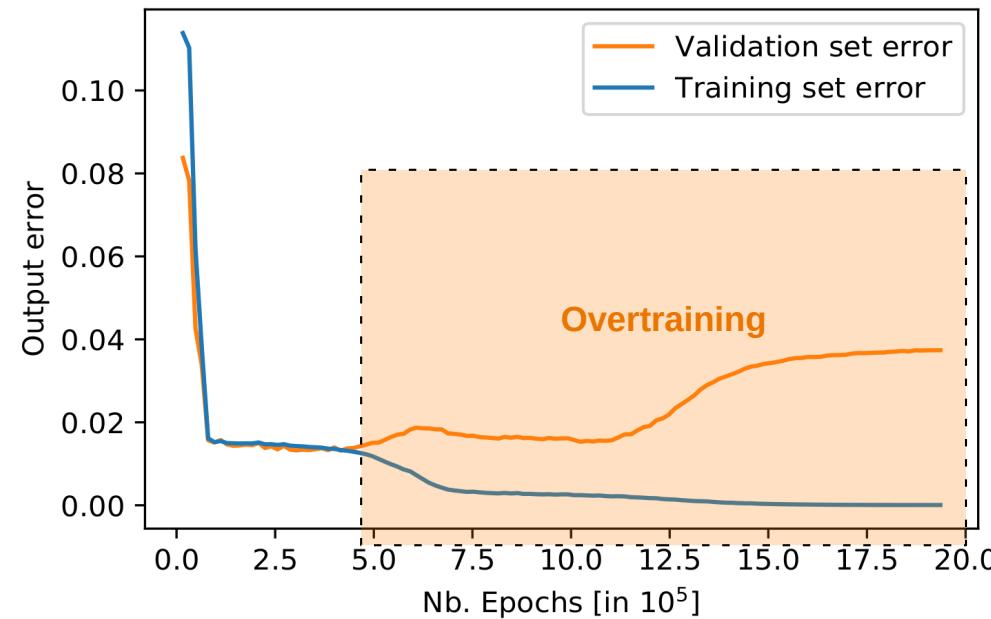
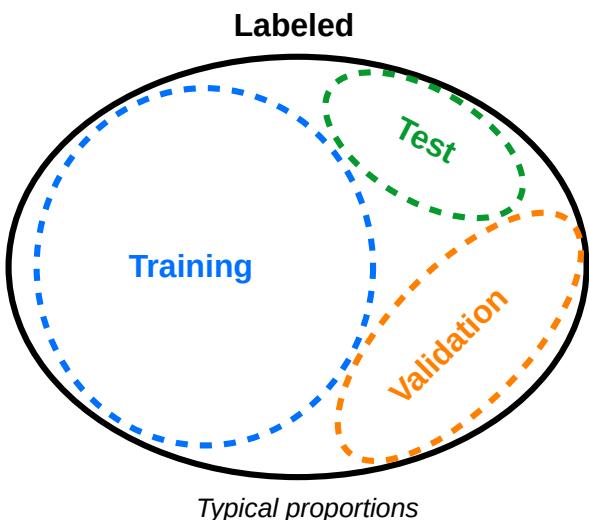


Monitoring overtraining

While several techniques can be used to moderate overtraining (like regularization), it is always **necessary to monitor it** to stop the training at the appropriate time.

Split **labeled dataset** into 3 subsets

- Training set** ➤ To train the network
- Validation set** ➤ To monitor the training process
- Test set** ➤ To assess the quality of the prediction



Network depth and size

How to choose the **network architecture**?

In the case of the MLP, how many layers and neurons should be used per layer?

In this context, the objective is to find a **trade-off between**:

The **strength of the network** (its expressive power) and the **difficulty of training the model**

A few ideas that help explore the architectures:

- More data allows to constrain more parameters

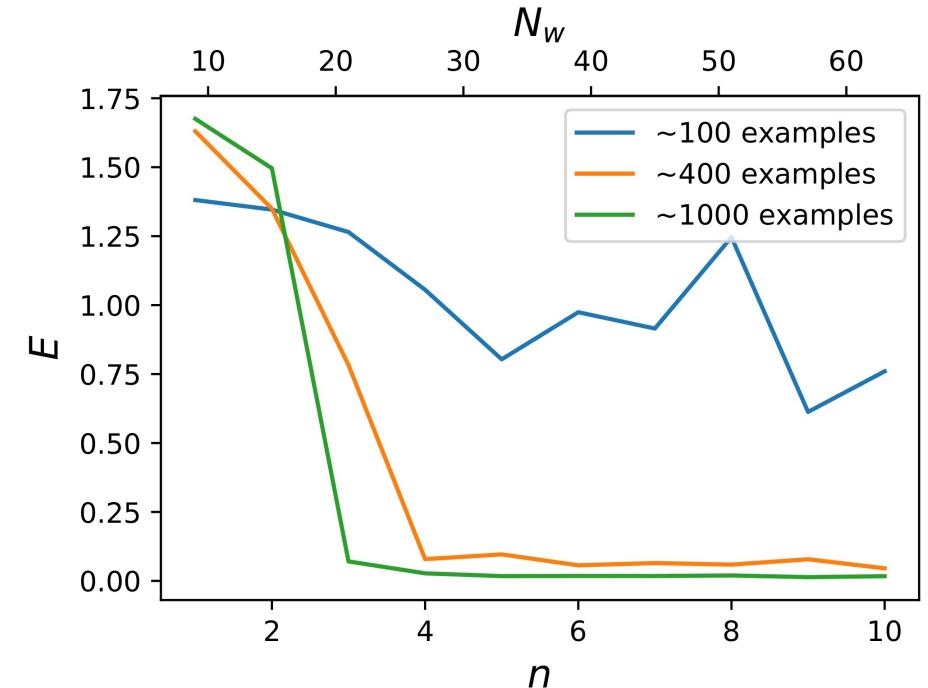
Rule of thumb: need roughly 10 times the number of weights as training examples

- More neurons increase the strength but add parameters to fit.

Reminder: a neuron is a linear separation in the parameter space → how many would you need by eye?
(starting point before exploration)

- More layers allow the construction of complex functions with fewer parameters, but increases training difficulty.

Reminder: a single hidden layer can approximate any function, but it is not always the optimal solution
(nb. of parameters, time to converge, etc.)



Finding the appropriate architecture is always an **exploratory and iterative process**.

Training different networks on the same data is almost always necessary to obtain good results.

MLP application

Use equations from slide 21 to implement **Multi-Layer Perceptron algorithm** with a single hidden layer.

Use datasets from the perception exercise to test your algorithm, and try to **optimize** its prediction performance by tweaking the described hyperparameters.

Your implementation must have the following properties:

- Easy change of the learning rate, number of epochs, **number of neurons in the hidden layer**
- An output encoding using one neuron per class
- A display of the results in the form of a **confusion matrix**
- Splitting of the labeled data to avoid overtraining

In addition, try to have:

- Generic functions for the forward and backprop operations that are independent of the dataset
- A way to re-balance the proportions of classes for the training phase (but test on true proportions)