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 »

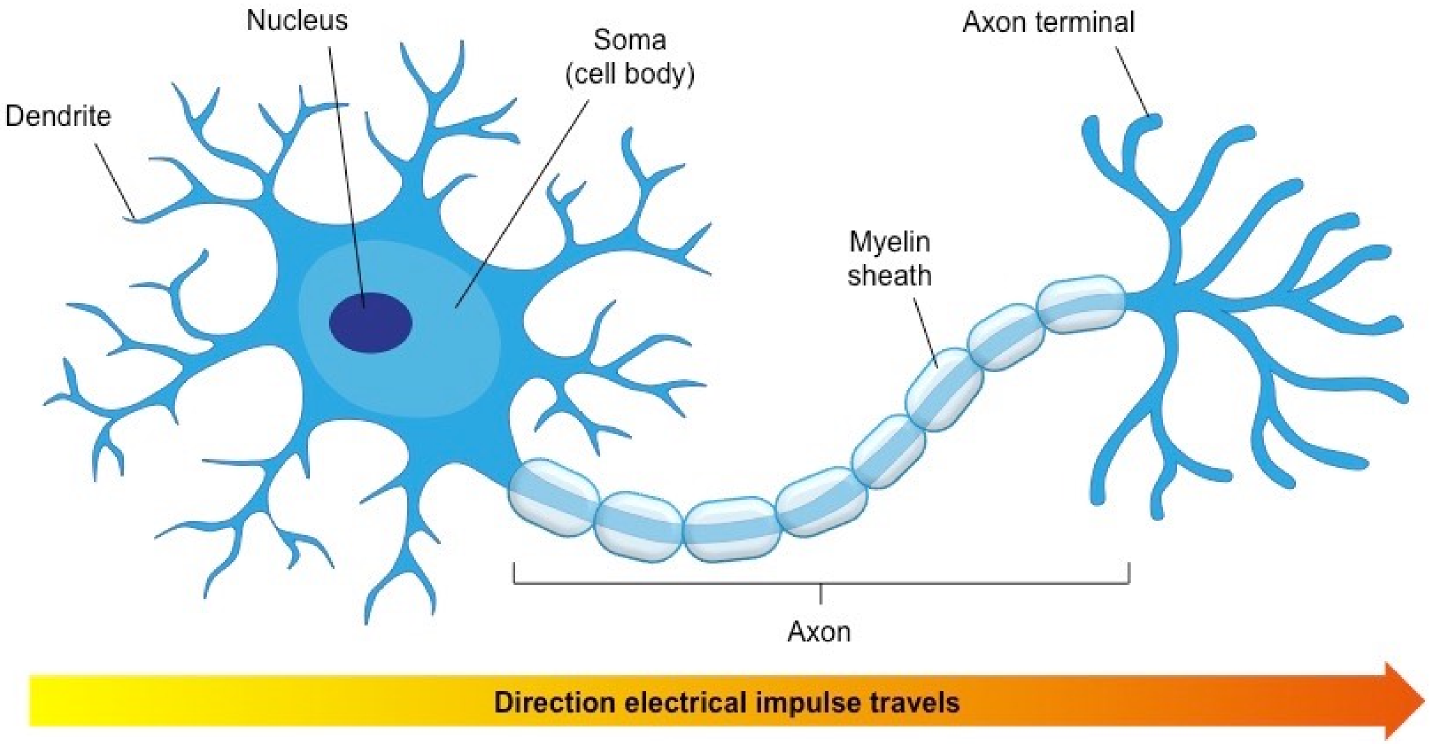
**Stephen Marsland*

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.

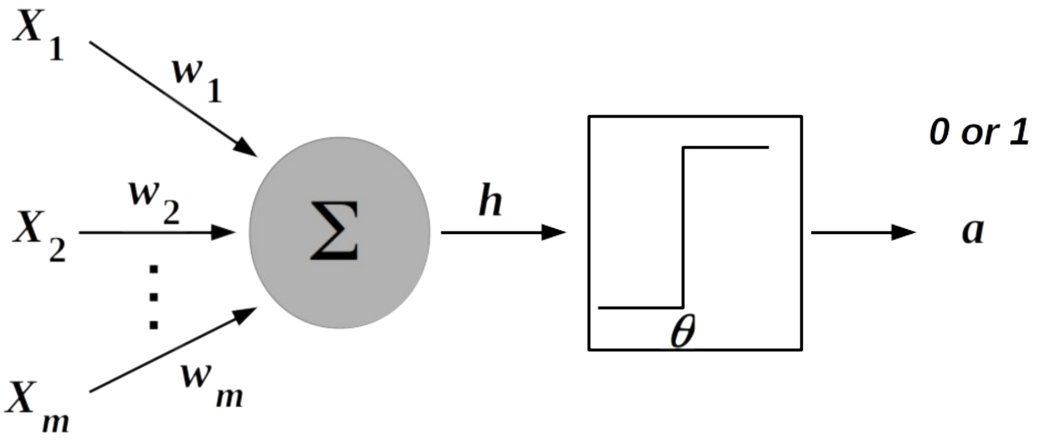
➡ **This is called conditioning**

**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.

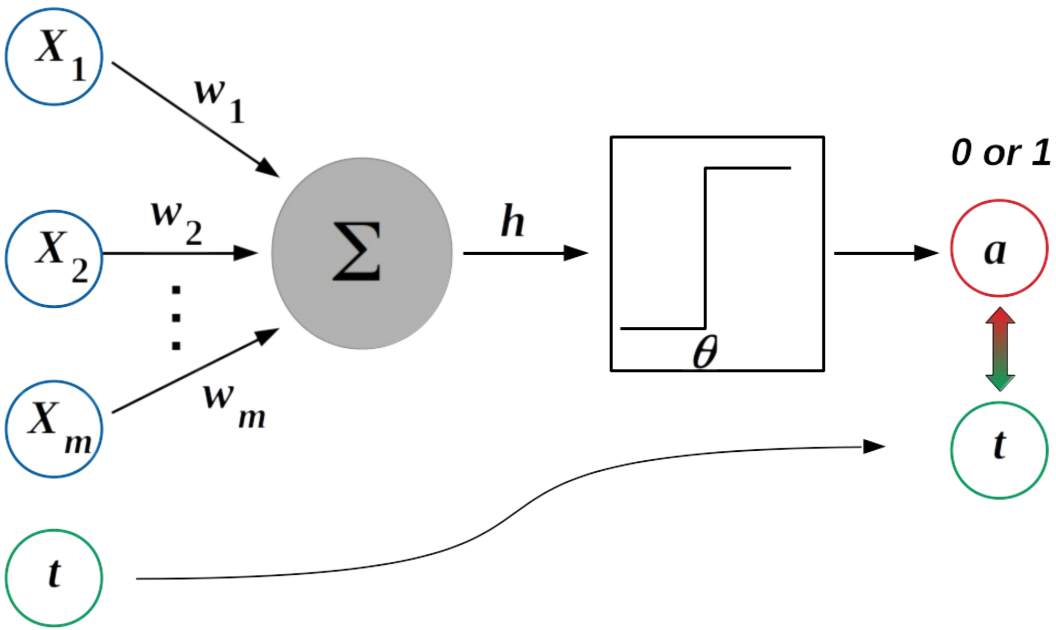


Its main components are:

- 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.

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

Training a Neuron



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

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.

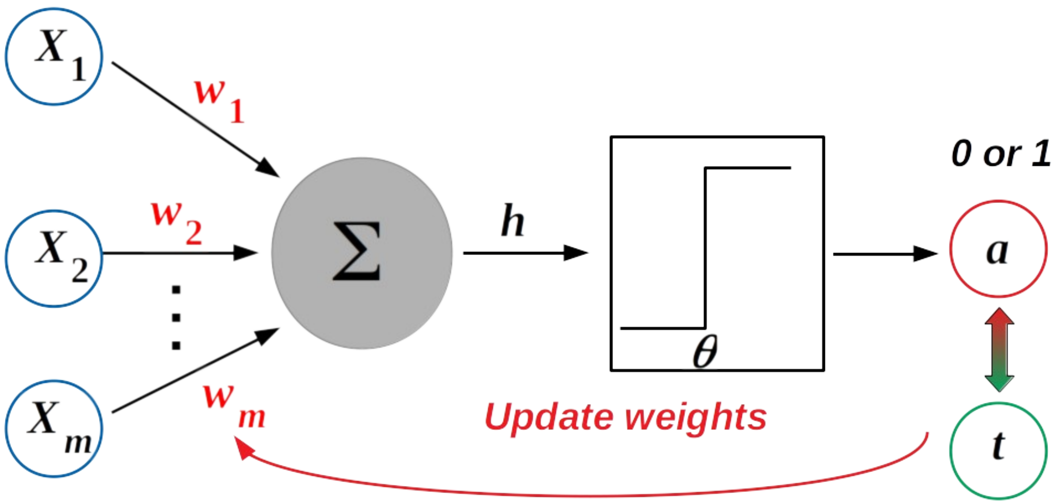
In practice, such a simple neuron optimizes a linear separation in the parameter space (**hyperplane**).

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**.

Training a Neuron



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

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

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.*

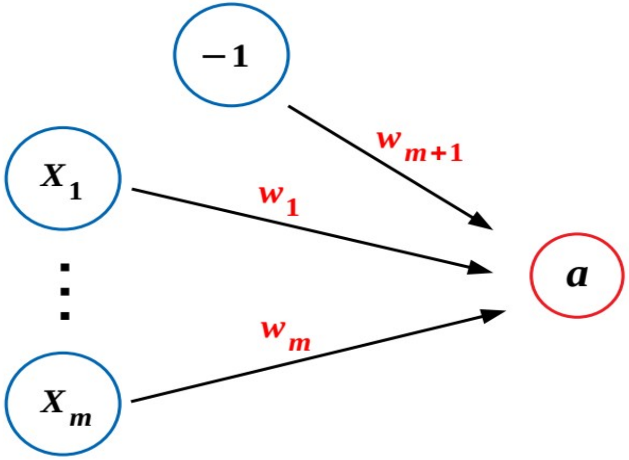
$$E = 0.5 \times (a - t)^2$$

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.*

The bias node

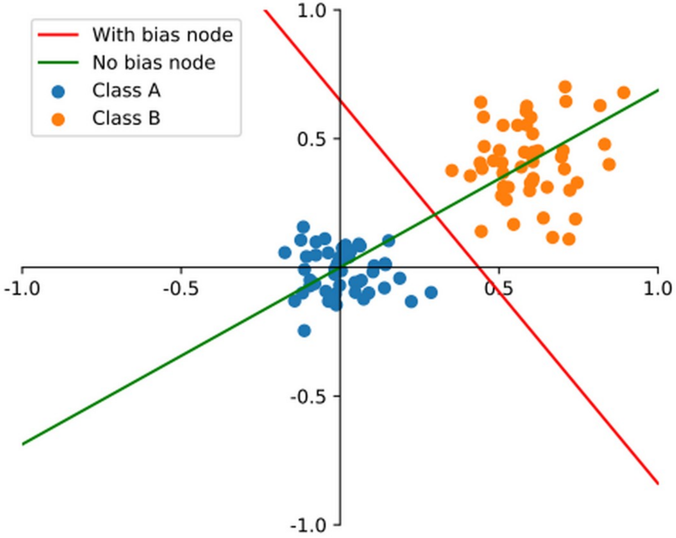


Problem with the previous formalism

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:

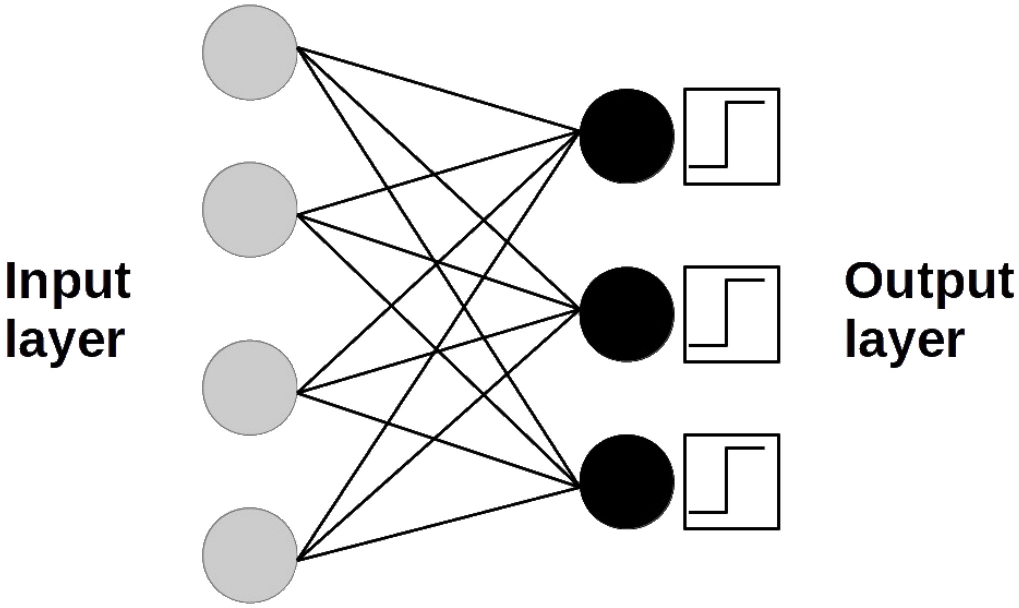
$$\sum_{i=1}^{m} X_i w_i = h = 0$$

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.

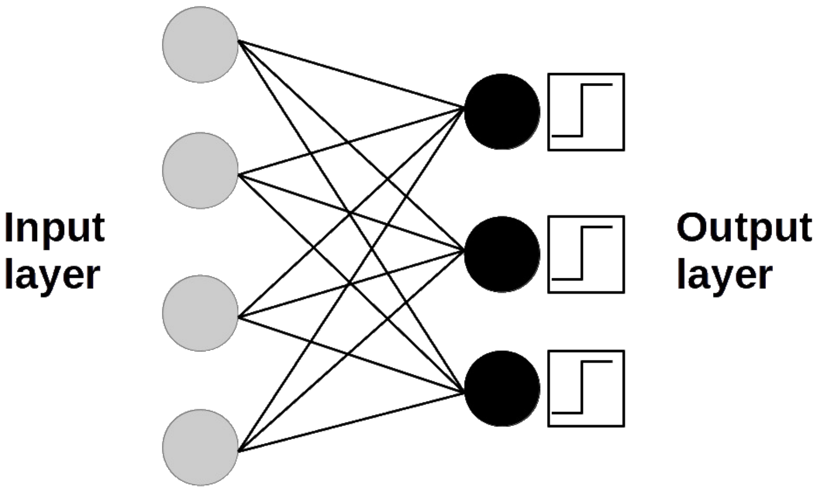
The training procedure is identical, but this time there is an index *j* to represent the neurons, and the weights are now in the form of a 2D matrix.

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

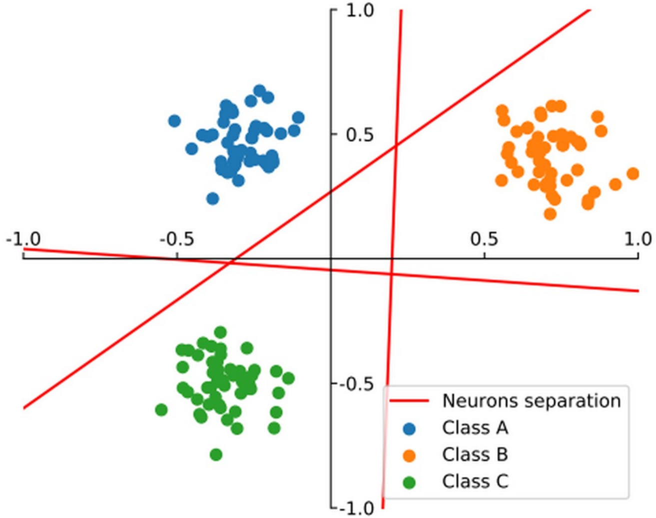
$$\omega_{ij} \leftarrow \omega_{ij} - \eta \left(a_j - t_j \right) \times x_i$$

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 :*

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

    - Update each weight individually using :

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

- **Inference**

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

First application : logical gates

OR		A	
		0	1
B	0	0	1
	1	1	1

AND		A	
		0	1
B	0	0	0
	1	0	1

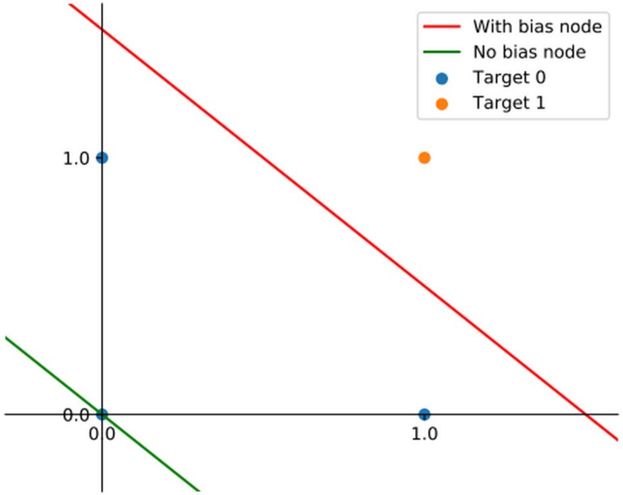
XOR		A	
		0	1
B	0	0	1
	1	1	0

NOR		A	
		0	1
B	0	1	0
	1	0	0

NAND		A	
		0	1
B	0	1	1
	1	1	0

NOT

A	
0	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/m2)
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

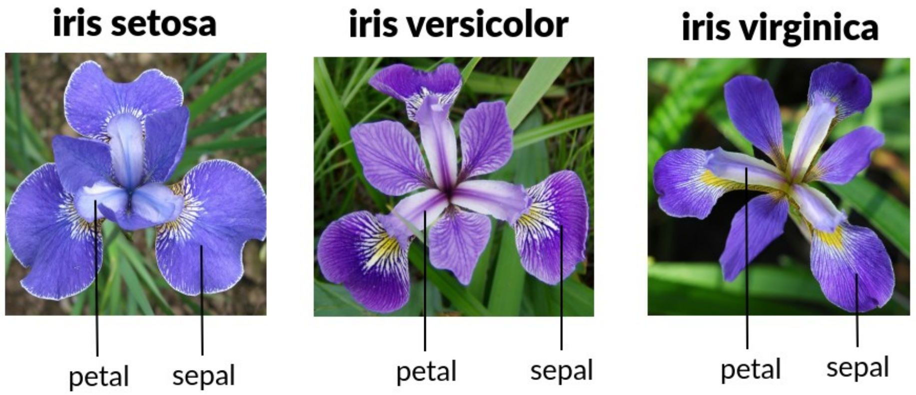
Dataset from the UCI Machine Learning repository.

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.

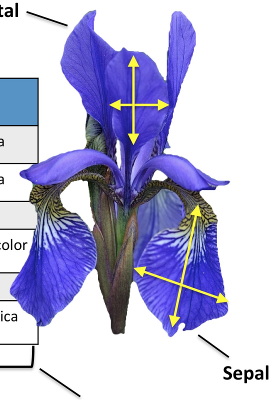
Despite its limitations, a simple Perceptron can reach up to **80% accuracy** on this dataset.

- 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.



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)

Class labels
(targets)

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