Introduction to (shallow) Neural Networks

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Neural Networks: from biology to engineering

- Understanding and modelling of brain

↓

- Imitation to reproduce high-level functions

↓

- Mathematical tool for engineers

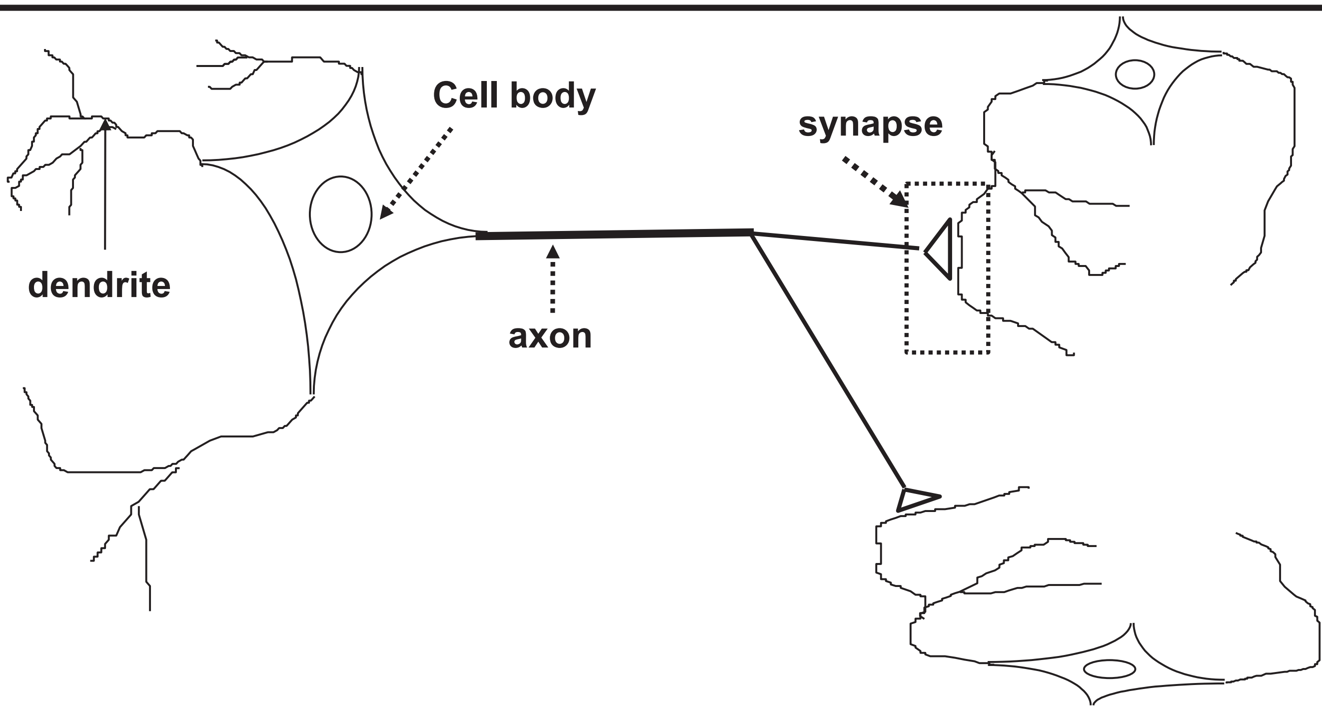
Application domains

Modelling any input-output function by "learning" from examples:

- Pattern recognition
- Voice recognition
- Classification, diagnosis

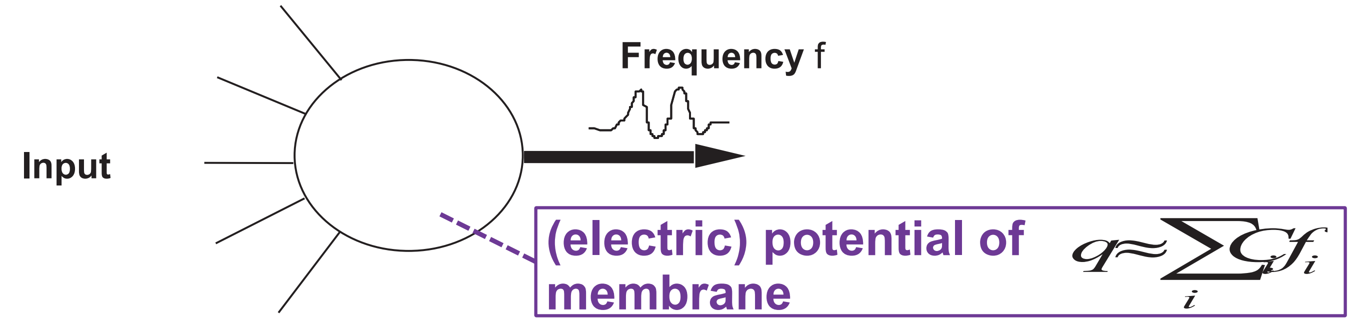
- Identification
- Forecasting
- Control, regulation

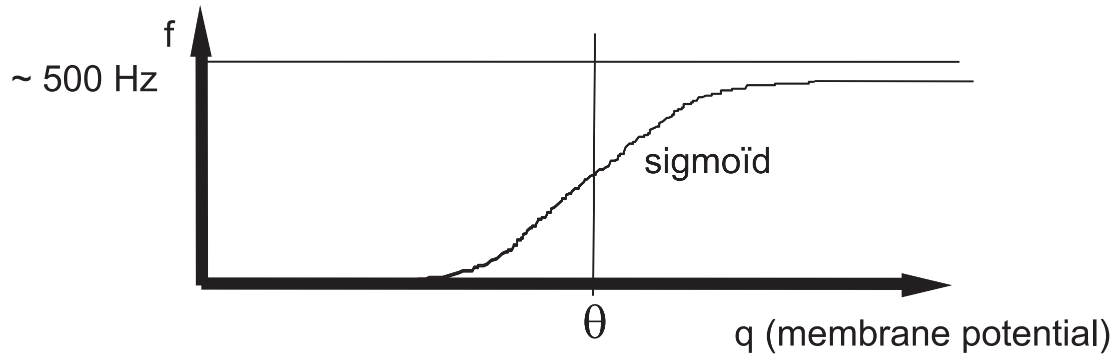
Biological neurons



- Electric signal: dendrites → cell body →> axon →synapses

Empirical model of *neurons*



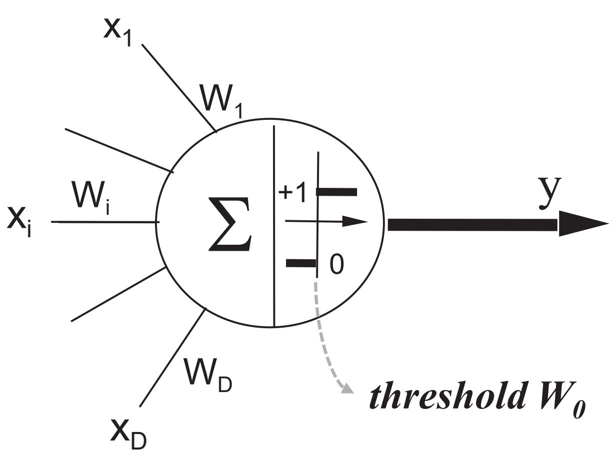


➔ **Neuron output = periodic signal with frequency f ≈ sigmoid(q) = sigmoid(Σ_i $C_i f_i$)**

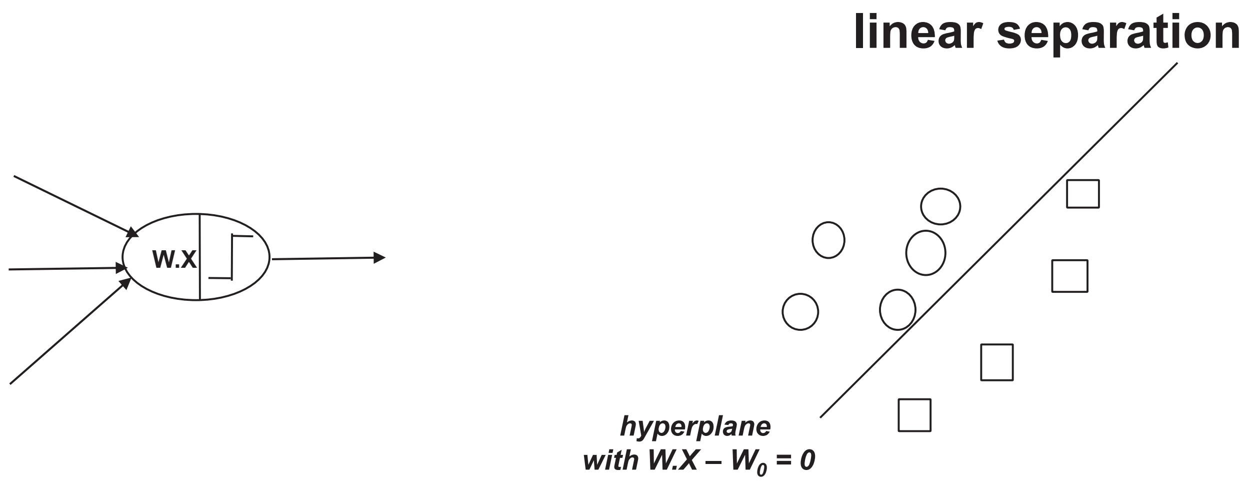
"Birth" of *formal* Neuron

- **Mc Culloch & Pitts (1943)**

  - **Simple model of neuron**
  - **goal: model the brain**



Linear separation by a single neuron



Theoretical model for *learning*

- **Hebb rule (1949)**

"*Cells that fire together wire together*", ie synaptic weight increases between neurons that activate *simultaneously*

$$W_{ij}(t+dt) = W_{ij}(t) + \lambda y_i(t) y_j(t)$$

First formal Neural *Networks*

(en français : Réseaux de Neurones)

- **PERCEPTRON (Rosenblatt, 1957)**
- **ADALINE (Widrow, 1962)**

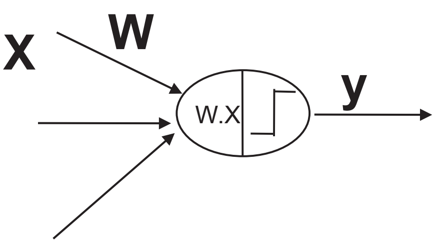
Formal neuron of Mac Culloch & Pitts

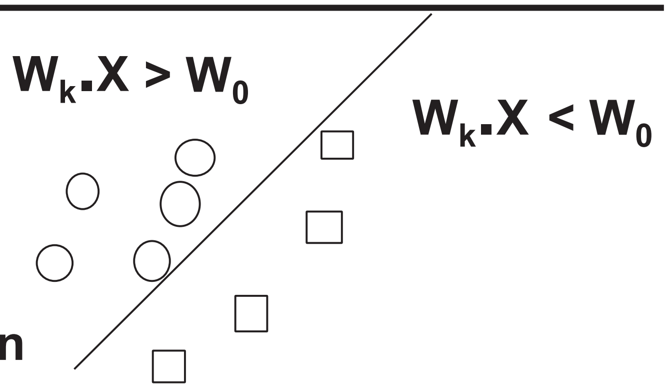
+

Hebb rule for learning

Possible to "learn" Boolean functions by training from examples

Training of Perceptron





➔ **Linear separation**

Training algorithm:

$W_{k+1} = W_k + vX$ if X incorrectly classified (v: target value)

$W_{k+1} = W_k$ if X correctly classified

- **Convergence if linearly-separable problem**
- **?? if NOT linearly-separable**

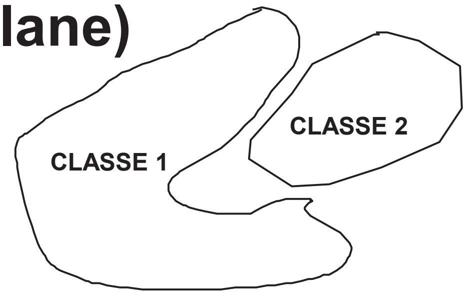
Limits of first models, necessity of "hidden" neurons

- **PERCEPTRONS, book by Minsky & Papert (1969)**

  Detailed study on Perceptrons and their intrinsic limits:

  - can NOT learn some types of Boolean functions (even simple one like XOR)
  - can do ONLY LINEAR separations

But many classes cannot be linearly-separated (by a single hyper-plane)



➔ Necessity of ***several*** layers in the Neural Network

➔ Requires new training algorithm

1st revival of Neural Nets

USE OF DERIVABLE NEURONS
\+
APPLY GRADIENT DESCENT METHOD

- **GRADIENT BACK-PROPAGATION** (Rumelhart 1986, Le Cun 85) (en français : *Rétro-propagation du gradient*)

→ Overcome Credit Assignment Problem by training Neural Networks with HIDDEN layers

- Empirical solutions for MANY real-world applications

- Some strong theoretical results: Multi-Layer Perceptrons are UNIVERSAL (and parsimonious) approximators

- around years 2000's: still used, but much less popular than SVMs and boosting

2nd recent « revival »: Deep-Learning

- Since ~2006, rising interest for, and excellent results with <u>*”deep”*</u> *neural networks*, consisting in MANY layers:
  - Unsupervised ”intelligent” initialization of weights
  - Standard gradient descent, and/or fine-tuning from initial values of weights
  - Hidden layers ➔ learnt hierarchy of features
- In particular, since ~2013 dramatic progresses in visual recognition (and voice recognition), with deep <u>*Convolutional* Neural Networks</u>

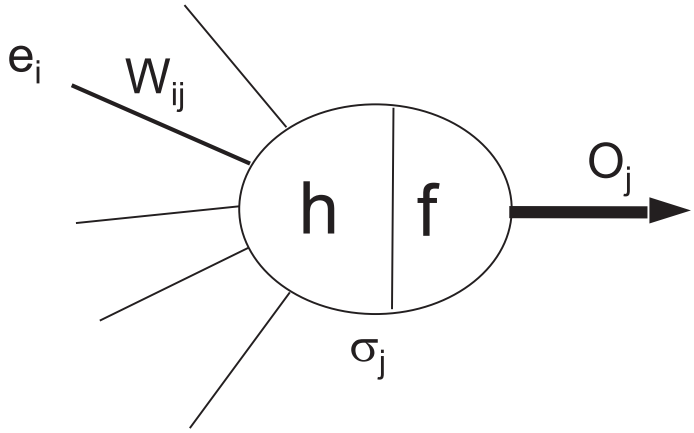
What is a FORMAL neuron?

DEFINITIONS OF FORMAL NEURONS

<u>In general:</u> a processing “unit” applying a simple operation to its inputs, and which can be “connected” to others to build a networks able to realize any input-output function

<u>“Usual” definition:</u> a “unit” computing a weighted sum of its inputs, and then applying some non-linearity (sigmoïd, ReLU, Gaussian, …)

General formal neuron



e_i: inputs of neuron
σ_j: potential of neuron
O_j: output of neuron

W_{ij}: (synaptic) weights
h: input function (computation of
potential = Σ, dist, kernel, …)
f: activation (or transfer) function

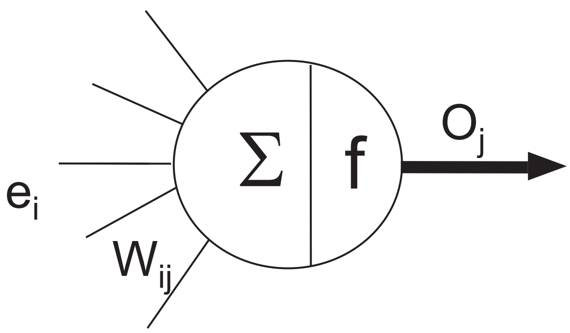
$$\sigma_j = h\left(e_i, \{W_{ij},\ i=0 \text{ à } k_j\}\right)$$

$$O_j = f(\sigma_j)$$

The combination of particular h and f functions defines the *type* of formal neuron

Summating artificial "neurons"

PRINCIPLE

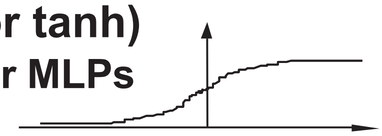


$$O_j = f\left(W_{0j} + \sum_{i=1}^{n_j} W_{ij} e_i\right)$$

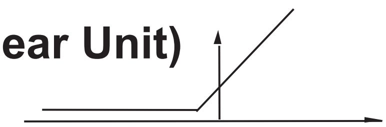
W_{0j} = "bias"

ACTIVATION FUNCTIONS

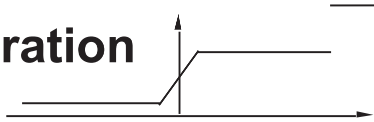
- **Threshold (Heaviside or sign)**
  → ***binary*** **neurons**
- **Sigmoïd (logistic or tanh)**
  → **most common for MLPs**



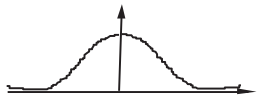
- **Identity** → ***linear*** **neurons**
- **ReLU (Rectified Linear Unit)**



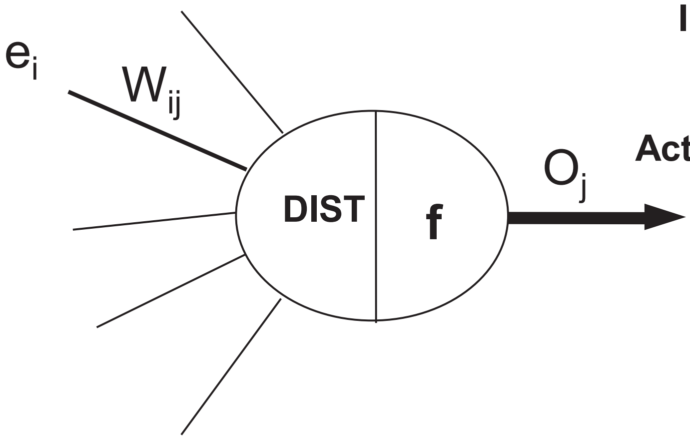
- **Saturation**



- **Gaussian**



"Distance" formal neurons

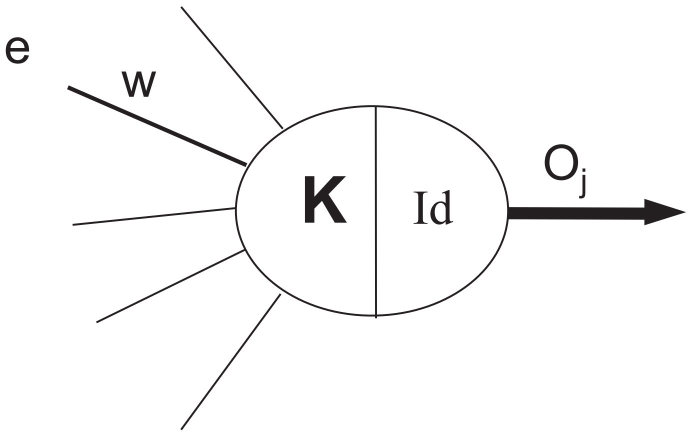


Input function: $h\left(\begin{pmatrix} e_1 \\ \dots \\ e_k \end{pmatrix}, \begin{pmatrix} W_{1j} \\ \dots \\ W_{kj} \end{pmatrix}\right) = \sum_i \left(e_i - W_{ij}\right)^2$

Activation function = Identity of Gaussian

The potential of these neurons is the Euclidian DISTANCE between input vector $(e_i)_i$ and weight vector $(W_{ij})_i$

Kernel-type formal neurons



Input function: $h(e,w) = K(e,w)$
with K symmetric and "positive"
in Mercer sense: $\forall \psi$ tq $\int \psi^2(x)dx < \infty$,
$\int K(u,v)\psi(u)\psi(v)dudv \geq 0$

Activation function = Identity

Examples of possible kernels:

- **Polynomial:** `K(u,v)=[u.v + 1]^p`
- **Radial Basis Function:** `K(u,v)=exp(-||u-v||² / 2σ²)`
  - ➔ *equivalent to distance-neuron+gaussian-activation*
- **Sigmoïd:** `K(u,v)=tanh(u.v+θ)`
  - ➔ *equivalent to summating-neurons+sigmoïd-activation*

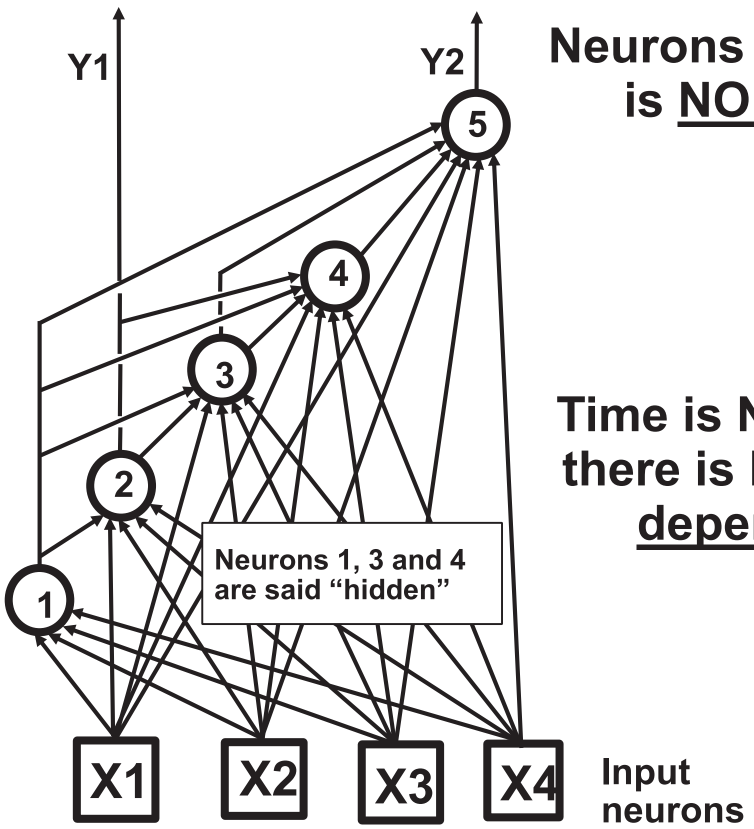
TWO FAMILIES OF NETWORKS

- **FEED-FORWARD NETWORKS**
  (en français, "*réseaux non bouclés*"):
  NO feedback connection,
  The output depends only on current input (NO memory)

- **FEEDBACK OR RECURRENT NETWORKS**
  (en français, "réseaux *bouclés*"):
  Some internal feedback/backwards connection
  ➔ output depends on current input
  AND ON ALL PREVIOUS INPUTS (some memory inside!)

Feed-forward networks

(en français : réseau "NON-bouclé")



Neurons can be ordered so that there is <u>NO "backwards" connection</u>

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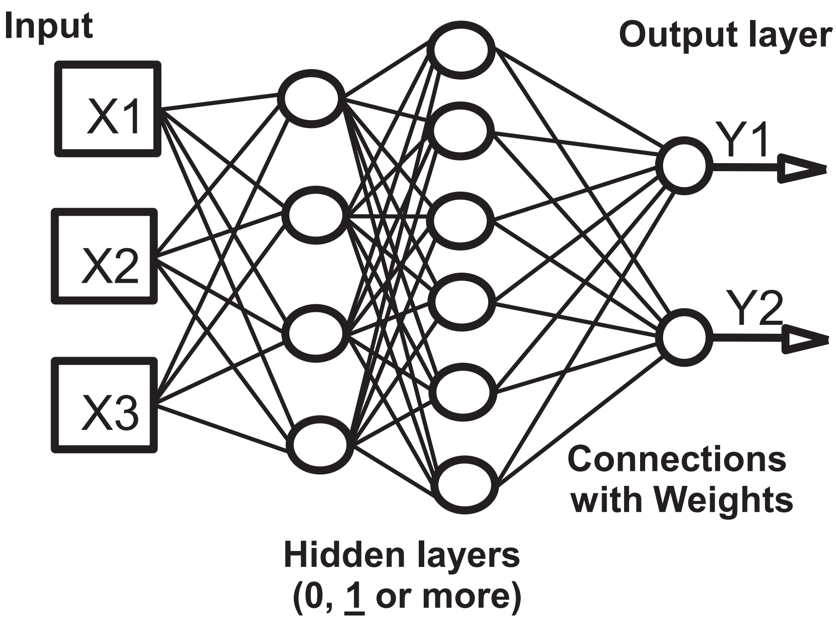
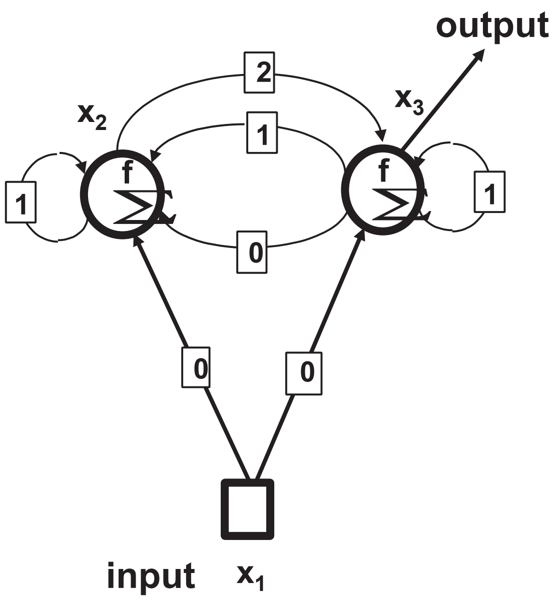
Time is NOT a functional variable, i.e. there is NO MEMORY, and <u>the output depends only on current input</u>

Feed-forward Multi-layer Neural Networks

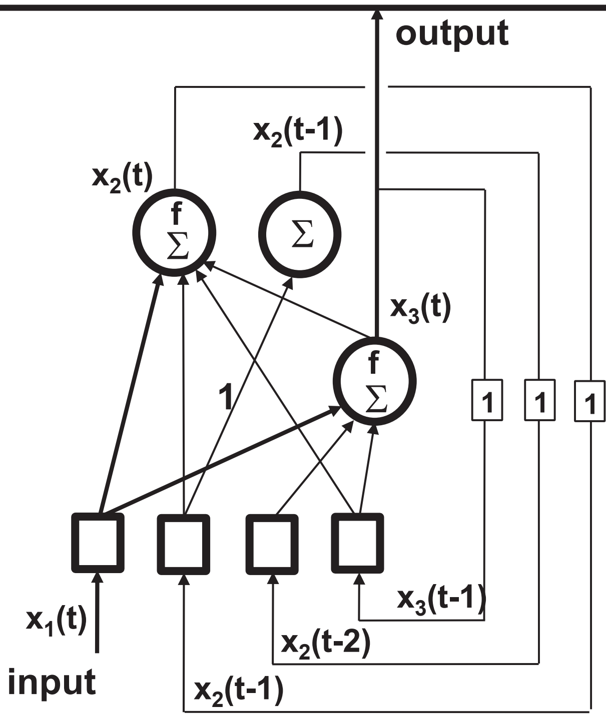


For "<u>Multi-Layer Perceptron" (MLP)</u>,
neurons type generally "summating with sigmoid activation"
[terme français pour MLP : "<u>Réseau Neuronal à couches</u>"]

Recurrent Neural Networks

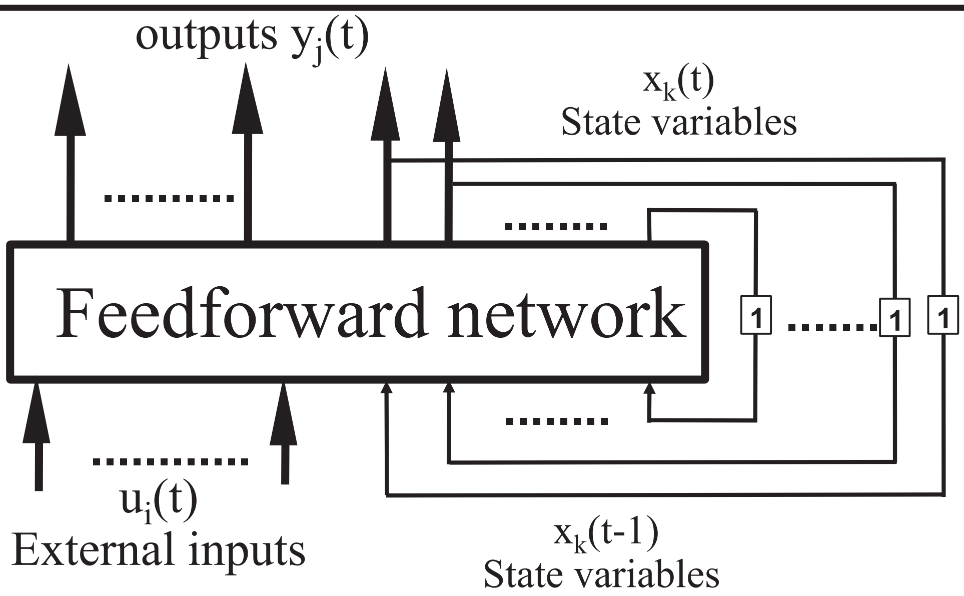


A time-delay is associated to each connection



Equivalent form

Canonical form of Recurrent Neural Networks



The output at time t depend not only on external inputs U(t), but also (via internal "state variables") on the whole sequence of previous inputs (and on initialization of state variables)

Use of a Neural Network

input x → network: **weights W**, **architecture A** → output **$y = F_{A,W}(x)$**

- **Two modes:**
  - **<u>training:</u> based on examples of (input,output) couples, the network modifies**
    - **Its parameters W (synaptic weights of connections)**
    - **And also potentially its architecture A (by creating/eliminating neurons or connections)**
  - **<u>recognition:</u>**
    computation of output associated to a given input (architecture and weights remaining frozen)

Training principle for Neural Networks

- Supervised training = adaptation of synaptic weights of the network so that its output is close to target value for each example

- Given n examples (X_p; D_p), and the network outputs Yp=NN(Xp), the average quadratic error is

$$E(W) = \sum_p \left(Y_p - D_p\right)^2$$

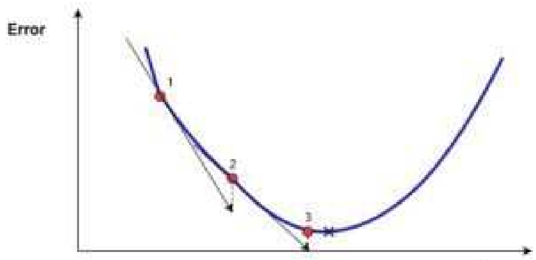
Training ~ finding W* =ArgMin(E), ie minimize the cost function E(W)

- Generally this is done by using gradient descent (total, partial or stochastic):

$W(t+1) = W(t) -$ [illegible] *[+ $\mu(t)(W(t)-W(t-1))$]*

Usual training algo for Multi Layer Perceptrons (MLP)

Training a Neural Network
= optimizing values of its weights&biases



- ***Random*** **initialization**
- Training by Stochastic Gradient Descent (SGD), using *back-propagation*:
  - Input 1 (or a few) random training sample(s)
  - Propagate
  - Calculate error (loss)
  - Back-propagate through all layers from end to input, to compute gradient and update weights

Back-propagation principle

Smart method for efficient computing of gradient (w.r.t. weights) of a Neural Network cost function, based on chain rule for derivation.

Cost function is $Q(t) = \Sigma_m \text{loss}(Y_m,D_m)$, where m runs over training set examples

Usually, $\text{loss}(Y_m,D_m) = ||Y_m-D_m||^2$ [quadratic error]

<u>Total</u> gradient:

$$W(t+1) = W(t) - \lambda(t)\,\text{grad}_W(Q(t)) + \mu(t)(W(t)-W(t-1))$$

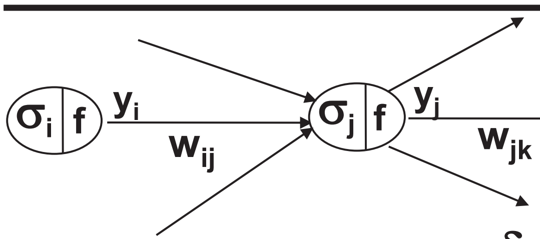
<u>Stochastic</u> gradient:

$$W(t+1) = W(t) - \lambda(t)\,\text{grad}_W(Q_m(t)) + \mu(t)(W(t)-W(t-1))$$

where $Q_m=\text{loss}(Y_m,D_m)$, is error computed on <u>only ONE</u> example randomly drawn from training set at every iteration and <u>$\lambda(t)$ = *learning rate*</u> (fixed, decreasing or adaptive), <u>$\mu(t)$ = momentum</u>

Now, how to compute dQ_m/dW_{ij}?

Backprop through fully-connected layers: use of chain rule derivative computation



$dE_m/dW_{ij} = (dE_m/d\sigma_j)(d\sigma_j/dW_{ij}) = (dE_m/d\sigma_j)\, y_i$

Let $\delta_j = (dE_m/d\sigma_j)$. Then $\boxed{W_{ij}(t+1) = W_{ij}(t) - \lambda(t)\, y_i\, \delta_j}$

(and $W_{0j}(t+1) = W_{0j}(t) - \lambda(t)\delta_j$)

<u>If neuron j is output</u>, $\delta_j = (dE_m/d\sigma_j) = (dE_m/dy_j)(dy_j/d\sigma_j)$ with $E_m=||Y_m-D_m||^2$

so $\boxed{\delta_j = 2(y_j-D_j)f'(\sigma_j) \text{ if neuron j is an output}}$

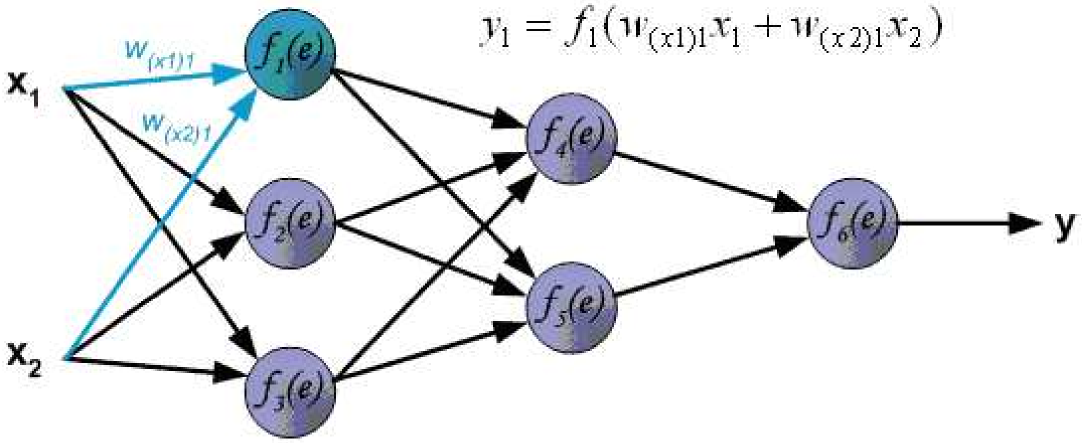
<u>Otherwise</u>, $\delta_j=(dE_m/d\sigma_j)=\Sigma_k (dE_m/d\sigma_k)(d\sigma_k/d\sigma_j)=\Sigma_k \delta_k(d\sigma_k/d\sigma_j) =\Sigma_k \delta_k W_{jk}(dy_j/d\sigma_j)$

so $\boxed{\delta_j = (\Sigma_k W_{jk}\delta_k)f'(\sigma_j) \text{ if neuron j is "hidden"}}$

➔ **all the δ_j can be computed successively from last layer to upstream layers by "error backpropagation" from output**

Animated illustration of Back-Propagation

FP



Animated GIF from the good tutorial
https://medium.com/datadriveninvestor/what-is-gradient-descent-intuitively-42f10dfb293f

Universal approximation theorem

Cybenko 1989

- For any continuous function F defined and bounded on a bounded set, and for any ε, there exists a layered Neural Network with ONLY ONE HIDDEN LAYER (of *sigmoïd* neurons) which approximates F with error < ε

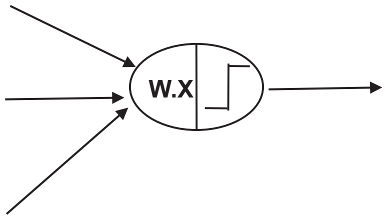
…But the theorem does not provide any clue about how to find this one_hidden-layer NN, nor about its size!
And the size of hidden layer might be huge…

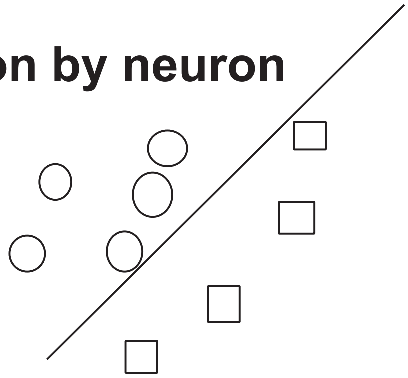
Sussman 92

- The set of MLPs with ONE hidden layer of sigmoid neurons is a family of PARCIMONIOUS approximators: for equal number of parameters, more functions can be correctly approximated than with polynoms

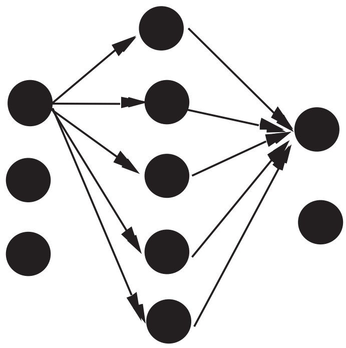
Multi-layer (MLP) v.s. single-layer (perceptron)

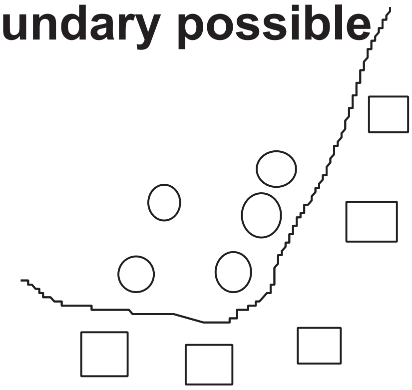
Single-layer → one linear separation by neuron





Multi-layer: any shape of boundary possible





Pros and cons of MLPs

ADVANTAGES

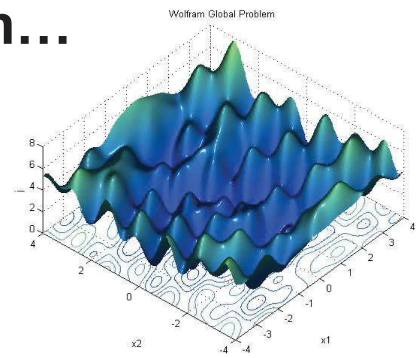
- Universal and parsimonious approximators (& classifiers)
- Fast to compute
- Robustness to data noise
- Rather easy to train and program

DRAWBACKS

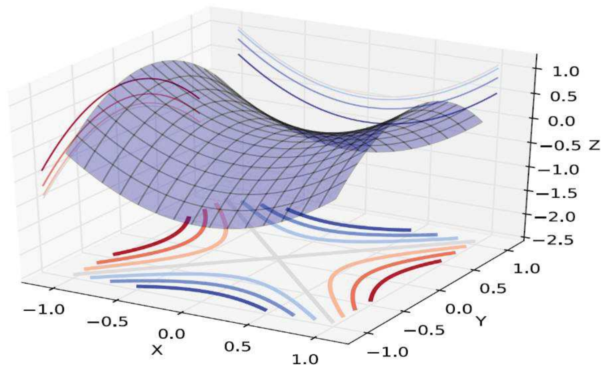
- *Choice of ARCHITECTURE (# of neurons in hidden layer) is CRITICAL, and empiric!*
- Many other critical hyper-parameters (learning rate, # of iterations, initialization of weights, etc…)
- *Many local minima in cost function*
- Blackbox: difficult to interpret the model

Why gradient descent works *despites non-convexity*?

- **Local minima dominate in low-Dim…**

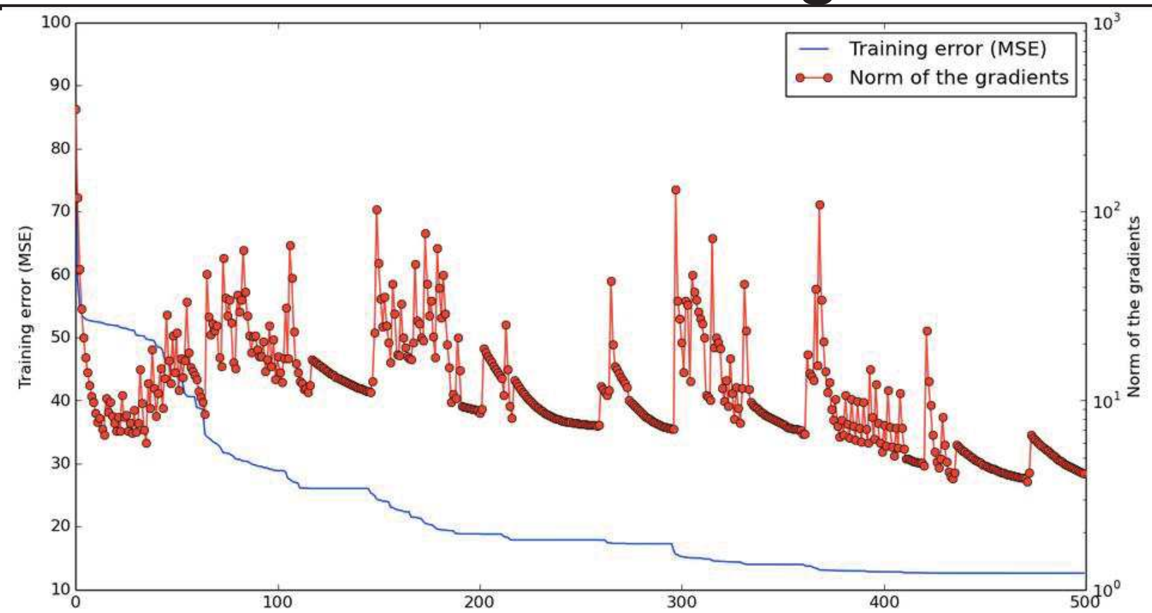


- **…but recent work has shown *saddle points* dominate in high-Dim**



- **Furthermore, most local minima are close to the global minimum**

Saddle points in training curves



- **Oscillating between two behaviors:**
  - **Slowly approaching a saddle point**
  - **Escaping it**

METHODOLOGY FOR SUPERVISED TRAINING OF MULTI-LAYER NEURAL NETWORKS

Training set vs. TEST set

- Space of possible input values usually infinite, and training set is only a FINITE subset
- Zero error on all training examples ≠ <u>good results on whole space of possible inputs</u> (cf generalization error ≠ empirical error…)

↓

- Need to collect enough and representative examples
- Essential to keep aside a subset of examples that shall be used only as TEST SET for estimating final generalization (when training finished)
- Need also to use some "validation set" independant from training set, in order to tune all hyper-parameters (layer sizes, number of iterations, etc…)

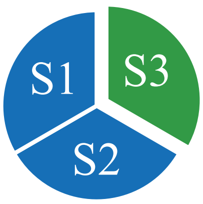
Optimize hyper-parameters by "VALIDATION"

To avoid over-fitting and maximize generalization, absolutely ***essential to use some VALIDATION estimation,*** for optimizing training hyper-parameters (and stopping criterion):

– either use a *separate validation dataset* (random split of data into Training-set + Validation-set)

– or use ***CROSS-VALIDATION***:

- Repeat k times: train on (k-1)/k proportion of data + estimate error on remaining 1/k portion
- Average the k error estimations



3-fold cross-validation:

- Train on S1∪S2 then estimate errS3 error on S3
- Train on S1∪S3 then estimate errS2 error on S2
- Train on S2∪S3 then estimate errS1 error on S1
- Average validation error: (errS1+errS2+errS3)/3

Some Neural Networks training "tricks"

- Importance of **input normalization**

  (zero mean, unit variance)

- Importance of **weights initialization**

  random but SMALL and prop. to 1/sqrt(nbInputs)

- Decreasing (or adaptive) **learning rate**

- Importance of **training set size**

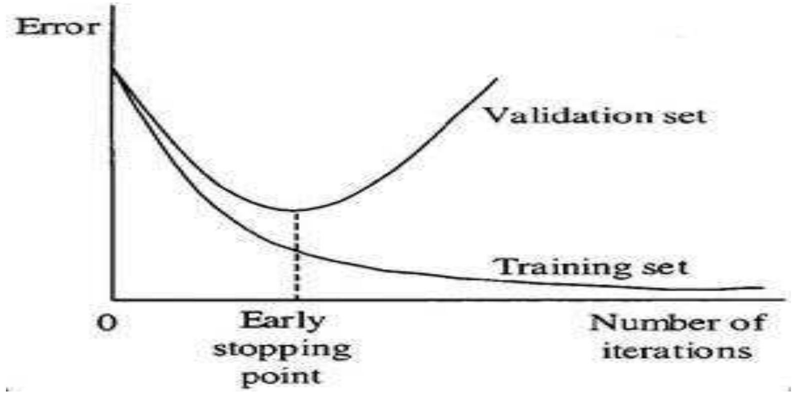
  If a Neural Net has a LARGE number of free parameters,
  ➔ train it with a sufficiently large training-set!

- Avoid overfitting by **Early Stopping** of training iterations

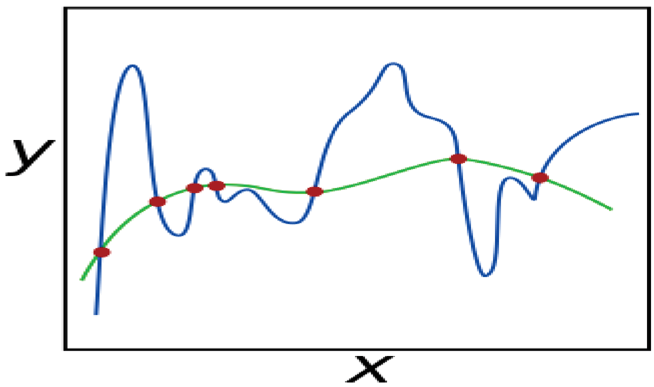
- Avoid overfitting by use of L1 or L2 **regularization**

Avoid overfitting by EARLY STOPPING

- For Neural Networks, a first method to avoid overfitting is to STOP LEARNING iterations as soon as the *validation*_error stops decreasing
- Generally, not a good idea to decide the number of iterations beforehand. Better to **ALWAYS USE EARLY STOPPING**



Avoid overfitting using regularization penalty (weight decay)



Trying to fit too many free parameters with not enough information can lead to overfitting

Regularization = penalizing too complex models
Often done by adding a special term to cost function

For neural network, the regularization term is just norm L2 or L1 of vector of all weights:

$$K = \Sigma_m(\mathrm{loss}(Y_m,D_m)) + \beta \, \Sigma_{ij} |W_{ij}|^p \quad \text{with } p=2 \text{ (L2) or } p=1 \text{ (L1)}$$

→ name "Weight decay"

MLP hyper-parameters

- Number and sizes of hidden layers!!
- Activation functions
- Learning rate (& momentum) [optimizer]
- Number of gradient iterations!! (& early_stopping)
- Regularization factor
- Weight initialization

Tuning hyper-parameters of MLPs in practice

- Use 'adam' optimizer
- Test/compare *WIDELY VARIED* <u>HIDDEN LAYER SIZES</u>
  `(typically 30;100;300;1000;30-30;100-100)`
- Test/compare *SEVERAL INITIAL* <u>LEARNING RATES</u>
  `(typically 0.1;0.03;0.01;0.003;0.001)`
- Make sure ENOUGH ITERATIONS for convergence `(typically >200 epochs)`, but EARLY STOPPING on validation_error to avoid overfitting
  `(→ check by plotting learning curves!!)`

Some (old) references on (*shallow, i.e. non deep*) Neural Networks

- *Réseaux de neurones : méthodologie et applications*, G. Dreyfus et al., Eyrolles, 2002.
- *Réseaux de neurones formels pour la modélisation, la commande, et la classification*, L. Personnaz et I. Rivals, CNRS éditions, collection Sciences et Techniques de l'Ingénieur, 2003.
- *Réseaux de neurones : de la physique à la psychologie*, J.-P. Nadal, Armand Colin, 1993.