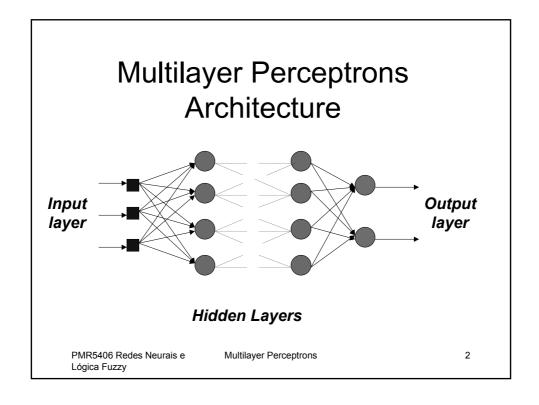
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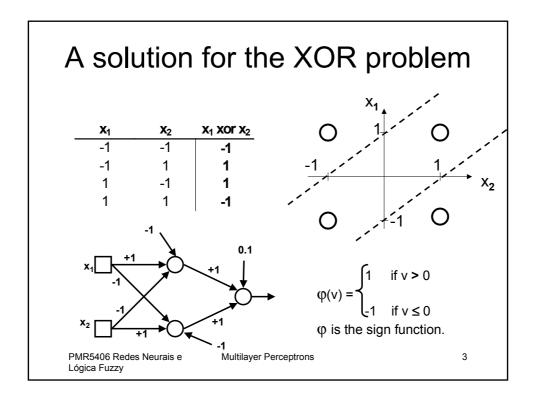
Aula 3 Multilayer Percetrons

Baseado em:

Neural Networks, Simon Haykin, Prentice-Hall, 2nd edition

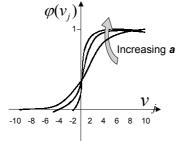
Slides do curso por Elena Marchiori, Vrije Unviersity





NEURON MODEL

Sigmoidal Function



$$\varphi(\mathbf{v}_{j}) = \frac{1}{1 + e^{-av_{j}}}$$

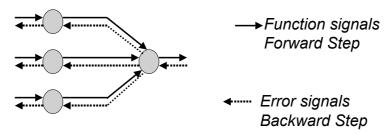
$$\mathbf{v}_{\mathbf{j}} = \sum_{i=0,\dots,m} w_{\mathbf{j}\mathbf{i}} \mathbf{y}_{\mathbf{i}}$$

- v_j induced field of neuron j
- · Most common form of activation function
- a $\rightarrow \infty \Rightarrow \phi \rightarrow$ threshold function
- Differentiable

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LEARNING ALGORITHM

Back-propagation algorithm



 It adjusts the weights of the NN in order to minimize the average squared error.

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Multilayer Perceptrons

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Average Squared Error

- Error signal of output neuron *j* at presentation of *n-th* training example:
- Total energy at time *n*:

$$e_{j}(n) = d_{j}(n) - y_{j}(n)$$

Average squared error:
$$E(n) = \frac{1}{2} \sum_{j \in C} e_j^2(n)$$

Measure of learning performance:

N: size of training set

$$E_{\text{AV}} = \frac{1}{N} \sum_{n=1}^{N} E(n)$$

Goal: Adjust weights of NN to minimize E_{AV}

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Notation

e_i Error at output of neuron j

y_j Output of neuron j

$$\mathbf{v}_{j} = \sum_{i=0,\dots,m} w_{ji} y_{i}$$
 Induced local field of neuron j

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Weight Update Rule

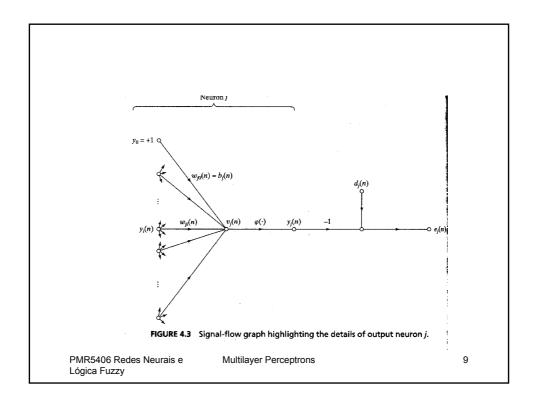
Update rule is based on the gradient descent method take a step in the direction yielding the maximum decrease of E

$$\Delta w_{ji} = -\eta rac{\partial E}{\partial w_{ji}}$$
 Step in direction opposite to the gradient

With W_{ji} weight associated to the link from neuron i to neuron j

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Definition of the Local Gradient of neuron j

$$\delta_{\rm j} = - \frac{\partial E}{\partial {\rm v}_{\rm j}}$$
 Local Gradient

We obtain
$$\delta_{j} = e_{j} \varphi'(v_{j})$$

because

$$-\frac{\partial E}{\partial \mathbf{v}_{j}} = -\frac{\partial E}{\partial \mathbf{e}_{j}} \frac{\partial \mathbf{e}_{j}}{\partial \mathbf{v}_{j}} \frac{\partial \mathbf{v}_{j}}{\partial \mathbf{v}_{j}} = -\mathbf{e}_{j} (-1) \varphi'(\mathbf{v}_{j})$$

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Update Rule

• We obtain

$$\Delta \mathbf{w}_{ji} = \eta \delta_j y_i$$

because

$$\frac{\partial E}{\partial \mathbf{w}_{ji}} = \frac{\partial E}{\partial \mathbf{v}_{j}} \frac{\partial \mathbf{v}_{j}}{\partial \mathbf{w}_{ji}}$$
$$-\frac{\partial E}{\partial \mathbf{v}_{j}} = \delta_{j} \frac{\partial \mathbf{v}_{j}}{\partial \mathbf{w}_{ji}} = y_{i}$$

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Compute local gradient of neuron j

- The key factor is the calculation of **e**_i
- There are two cases:
 - Case 1): j is a output neuron
 - Case 2): j is a hidden neuron

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Error e_i of output neuron

• Case 1: j output neuron

$$e_j = d_j - y_j$$

Then

$$\delta_{j} = (d_{j} - y_{j})\varphi'(v_{j})$$

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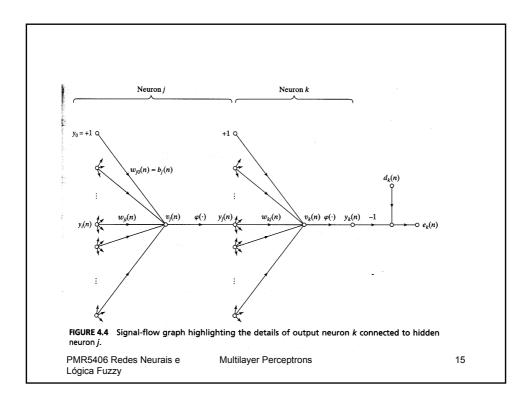
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Local gradient of hidden neuron

- Case 2: j hidden neuron
- the local gradient for neuron j is recursively determined in terms of the local gradients of all neurons to which neuron j is directly connected

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Use the Chain Rule

$$\delta_{j} = -\frac{\partial E}{\partial y_{j}} \frac{\partial y_{j}}{\partial v_{j}} \qquad \qquad \frac{\partial y_{j}}{\partial v_{j}} = \varphi'(v_{j})$$

$$E(n) = \frac{1}{2} \sum_{k \in C} e_{k}^{2}(n)$$

$$-\frac{\partial E}{\partial y_{j}} = -\sum_{k \in C} e_{k} \frac{\partial e_{k}}{\partial y_{j}} = \sum_{k \in C} e_{k} \left[\frac{-\partial e_{k}}{\partial v_{k}} \right] \frac{\partial v_{k}}{\partial y_{j}}$$

$$from \qquad -\frac{\partial e_{k}}{\partial v_{k}} = \varphi'(v_{k}) \qquad \frac{\partial v_{k}}{\partial y_{j}} = w_{kj}$$

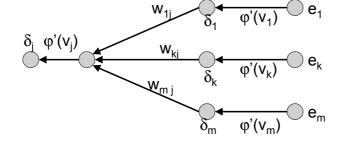
We obtain $-\frac{\partial E}{\partial y_j} = \sum_{k \in C} \delta_k w_{kj}$

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Local Gradient of hidden neuron j

Hence $\delta_{j} = \varphi'(v_{j}) \sum_{k \in C} \delta_{k} w_{kj}$



Signal-flow graph of backpropagation error signals to neuron *j*

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Delta Rule

• Delta rule $\Delta w_{ji} = \eta \delta_j y_i$

$$\mathcal{S}_{j} = \begin{cases} & \phi'(v_{j})(d_{j} - y_{j}) & \text{IF j output node} \\ & \phi'(v_{j}) \sum_{k \in C} \mathcal{S}_{k} w_{kj} & \text{IF j hidden node} \end{cases}$$

C: Set of neurons in the layer following the one containing *j*

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Local Gradient of neurons

$$\varphi'(v_j) = ay_j[1 - y_j]$$

a > 0

$$\delta_{j} = \begin{cases} ay_{j}[1 - y_{j}] \sum_{j} \delta_{k} w_{kj} & \text{if j hidden node} \\ ay_{j}[1 - y_{j}][d_{j}^{k} - y_{j}] & \text{If j output node} \end{cases}$$

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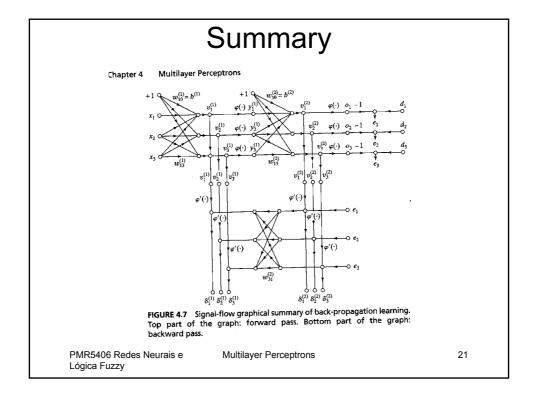
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Backpropagation algorithm

- · Two phases of computation:
 - Forward pass: run the NN and compute the error for each neuron of the output layer.
 - Backward pass: start at the output layer, and pass the errors backwards through the network, layer by layer, by recursively computing the local gradient of each neuron.

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Training

- Sequential mode (on-line, pattern or stochastic mode):
 - (x(1), d(1)) is presented, a sequence of forward and backward computations is performed, and the weights are updated using the delta rule.
 - Same for (x(2), d(2)), ..., (x(N), d(N)).

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Training

- The learning process continues on an epochby-epoch basis until the stopping condition is satisfied.
- From one epoch to the next choose a randomized ordering for selecting examples in the training set.

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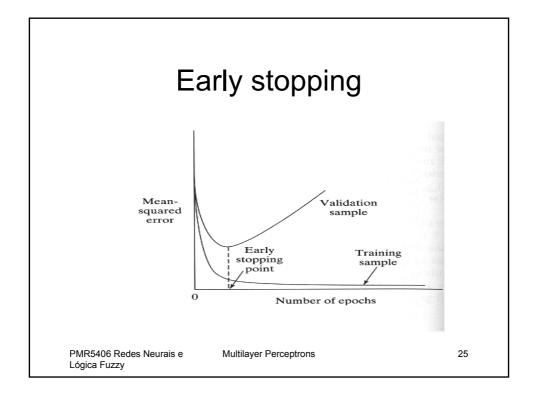
Stopping criterions

- Sensible stopping criterions:
 - Average squared error change:

 Back-prop is considered to have converged when the absolute rate of change in the average squared error per epoch is sufficiently small (in the range [0.1, 0.01]).
 - Generalization based criterion:
 After each epoch the NN is tested for generalization. If the generalization performance is adequate then stop.

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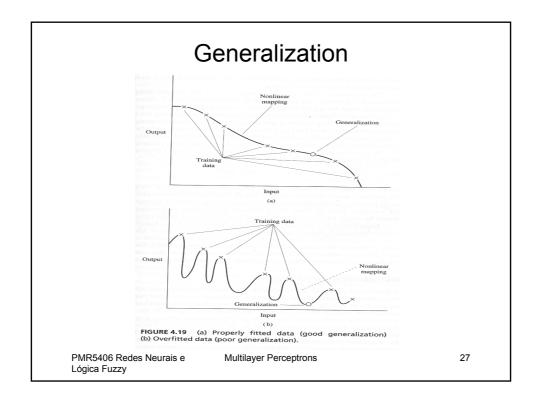


Generalization

- Generalization: NN generalizes well if the I/O mapping computed by the network is nearly correct for new data (test set).
- Factors that influence generalization:
 - the size of the training set.
 - the architecture of the NN.
 - the complexity of the problem at hand.
- Overfitting (overtraining): when the NN learns too many I/O examples it may end up memorizing the training data.

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Expressive capabilities of NN

Boolean functions:

- Every boolean function can be represented by network with single hidden layer
- · but might require exponential hidden units

Continuous functions:

- Every bounded continuous function can be approximated with arbitrarily small error, by network with one hidden layer
- Any function can be approximated with arbitrary accuracy by a network with two hidden layers

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Generalized Delta Rule

- If η small ⇒ Slow rate of learning
 If η large ⇒ Large changes of weights
 ⇒ NN can become unstable (oscillatory)
- Method to overcome above drawback: include a momentum term in the delta

$$\Delta w_{ji}(n) = \alpha \Delta w_{ji}(n-1) + \eta \delta_j(n) y_i(n) \label{eq:delta_function} \text{Generalized}$$

$$\text{delta}$$
 function} momentum constant

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Generalized delta rule

- the momentum accelerates the descent in steady downhill directions.
- the momentum has a stabilizing effect in directions that oscillate in time.

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η adaptation

Heuristics for accelerating the convergence of the back-prop algorithm through η adaptation:

- Heuristic 1: Every weight should have its own η.
- Heuristic 2: Every η should be allowed to vary from one iteration to the next.

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NN DESIGN

- Data representation
- Network Topology
- Network Parameters
- Training
- Validation

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Setting the parameters

- · How are the weights initialised?
- · How is the learning rate chosen?
- · How many hidden layers and how many neurons?
- · Which activation function?
- How to preprocess the data?
- How many examples in the training data set?

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Some heuristics (1)

 Sequential x Batch algorithms: the sequential mode (pattern by pattern) is computationally faster than the batch mode (epoch by epoch)

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Some heuristics (2)

- Maximization of information content: every training example presented to the backpropagation algorithm must maximize the information content.
 - The use of an example that results in the largest training error.
 - The use of an example that is radically different from all those previously used.

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Some heuristics (3)

 Activation function: network learns faster with antisymmetric functions when compared to nonsymmetric functions.

$$\varphi(\mathbf{v}) = \frac{1}{1 + e^{-av}}$$

Sigmoidal function is nonsymmetric

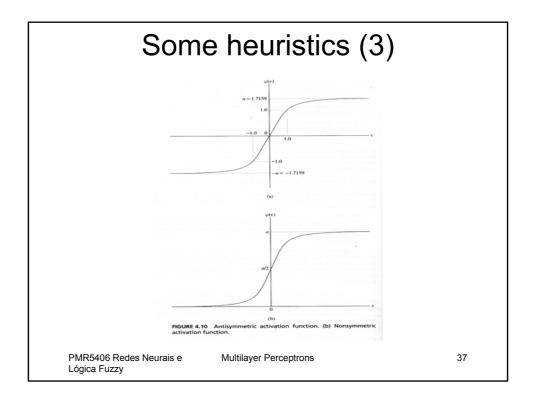
$$\varphi(\mathbf{v}) = a \tanh(b\mathbf{v})$$

Hyperbolic tangent function is nonsymmetric

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Some heuristics (4)

- Target values: target values must be chosen within the range of the sigmoidal activation function.
- Otherwise, hidden neurons can be driven into saturation which slows down learning

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Some heuristics (4)

- For the antisymmetric activation function it is necessary to design E
- For a+: $d_i = a \varepsilon$
- For –a: $d_i = -a + \varepsilon$
- If a=1.7159 we can set €=0.7159 then d=±1

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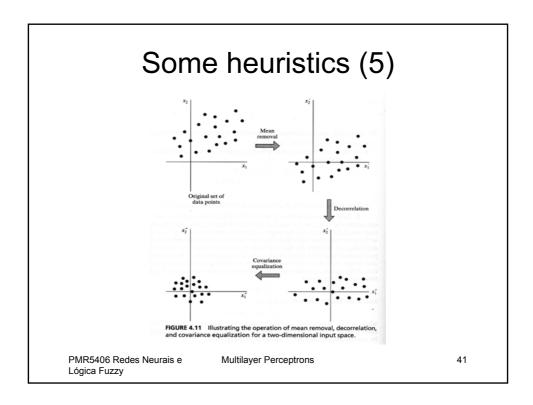
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Some heuristics (5)

- Inputs normalisation:
 - Each input variable should be processed so that the mean value is small or close to zero or at least very small when compared to the standard deviation.
 - Input variables should be uncorrelated.
 - Decorrelated input variables should be scaled so their covariances are approximately equal.

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Some heuristics (6)

- · Initialisation of weights:
 - If synaptic weights are assigned large initial values neurons are driven into saturation. Local gradients become small so learning rate becomes small.
 - If synaptic weights are assigned small initial values algorithms operate around the origin. For the hyperbolic activation function the origin is a saddle point.

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Some heuristics (6)

 Weights must be initialised for the standard deviation of the local induced field v lies in the transition between the linear and saturated parts.

$$\sigma_{v} = 1$$

$$\sigma_w = m^{-1/2}$$
 m=number of weights

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Some heuristics (7)

- · Learning rate:
 - The right value of η depends on the application. Values between 0.1 and 0.9 have been used in many applications.
 - Other heuristics adapt η during the training as described in previous slides.

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Some heuristics (8)

- · How many layers and neurons
 - The number of layers and of neurons depend on the specific task. In practice this issue is solved by trial and error.
 - Two types of adaptive algorithms can be used:
 - start from a large network and successively remove some neurons and links until network performance degrades.
 - begin with a small network and introduce new neurons until performance is satisfactory.

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Some heuristics (9)

- · How many training data?
 - Rule of thumb: the number of training examples should be at least five to ten times the number of weights of the network.

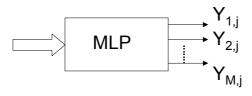
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Output representation and decision rule

• M-class classification problem

$$Y_{k,j}(x_j) = F_k(x_j), k=1,...,M$$



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Data representation

$$d_{k,j} = \begin{cases} 1, x_j \in C_k \\ 0, x_j \notin C_k \end{cases} \qquad \begin{bmatrix} 0 \\ \vdots \\ 1 \\ 0 \end{bmatrix} \leftarrow \text{ Kth element }$$

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MLP and the a posteriori class probability

 A multilayer perceptron classifier (using the logistic function) aproximate the a posteriori class probabilities, provided that the size of the training set is large enough.

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The Bayes rule

- An appropriate output decision rule is the (approximate) Bayes rule generated by the a *posteriori* probability estimates:
- $x \in C_k$ if $F_k(x) > F_i(x)$ for all $j \neq k$

$$F(x) = \begin{bmatrix} F_1(x) \\ F_2(x) \\ \dots \\ F_M(x) \end{bmatrix}$$

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