Artificial Neural Networks
MLP, Backpropagation

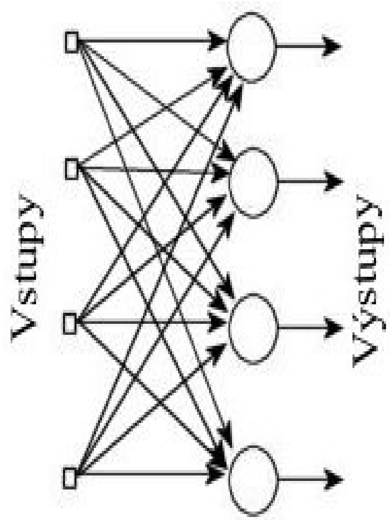
Jan Drchal
drchajan@fel.cvut.cz

Computational Intelligence Group
Department of Computer Science and Engineering
Faculty of Electrical Engineering
Czech Technical University in Prague

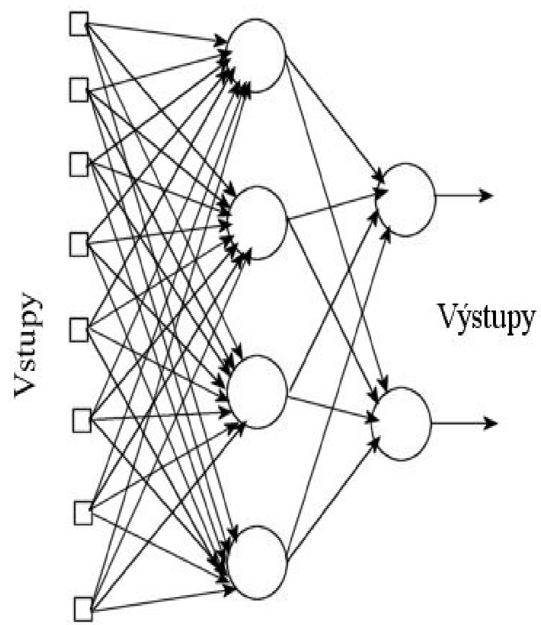
Outline

- MultiLayer Perceptron (MLP).
- How many layers and neurons?
- How to train ANNs?
- Backpropagation.
- Derived and other methods.

Layered ANNs

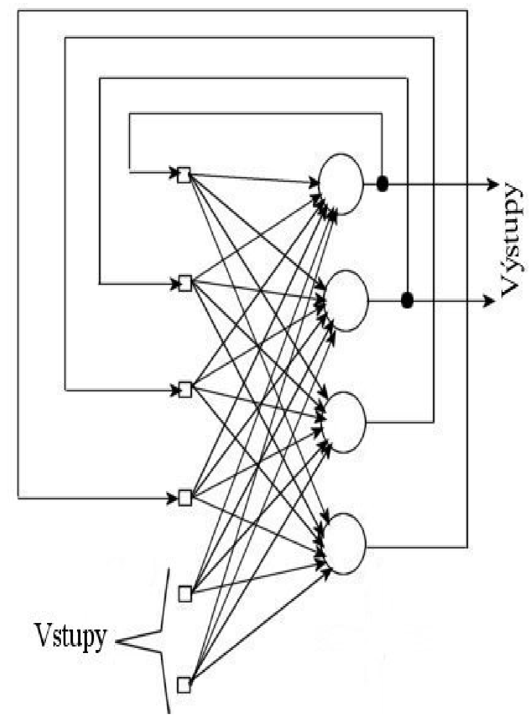


single layer



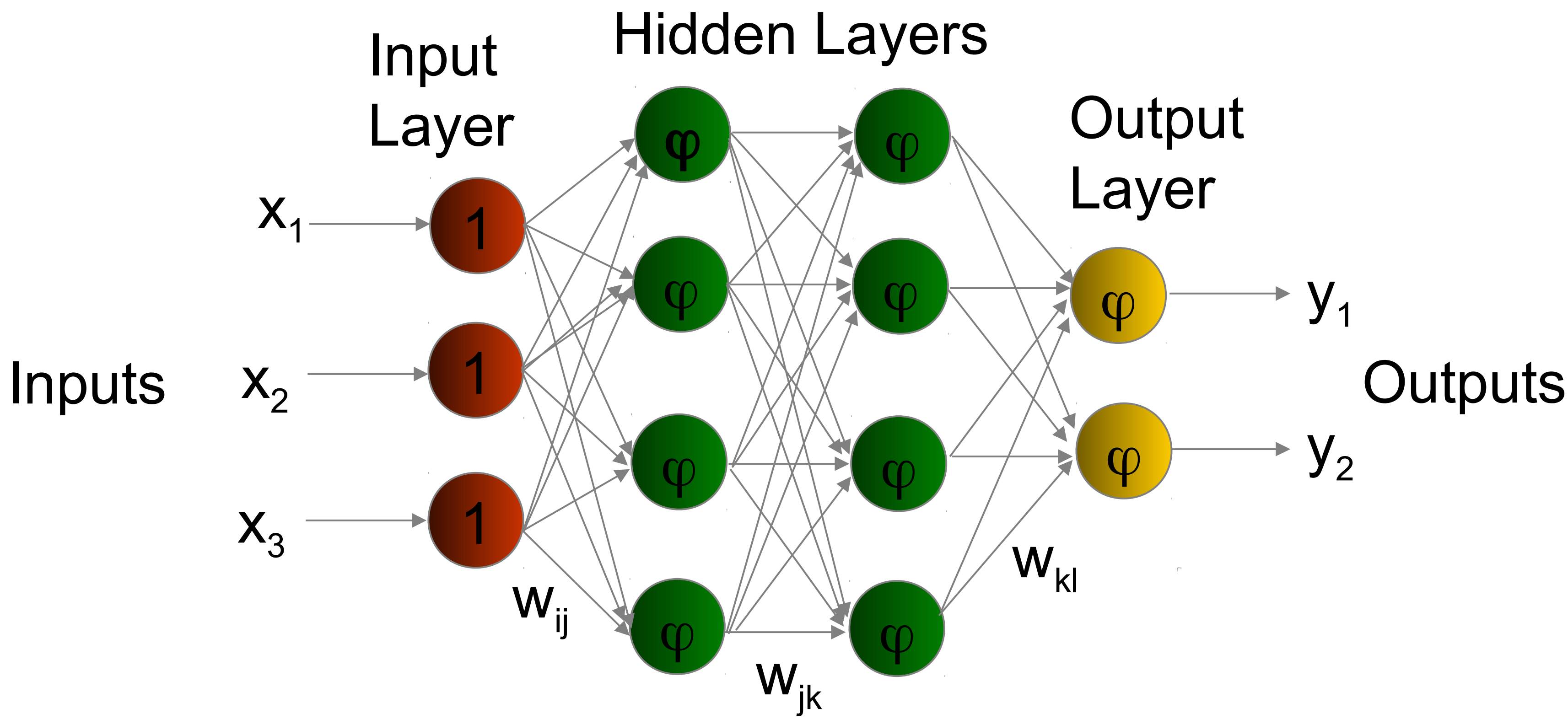
two layers

feed-forward networks

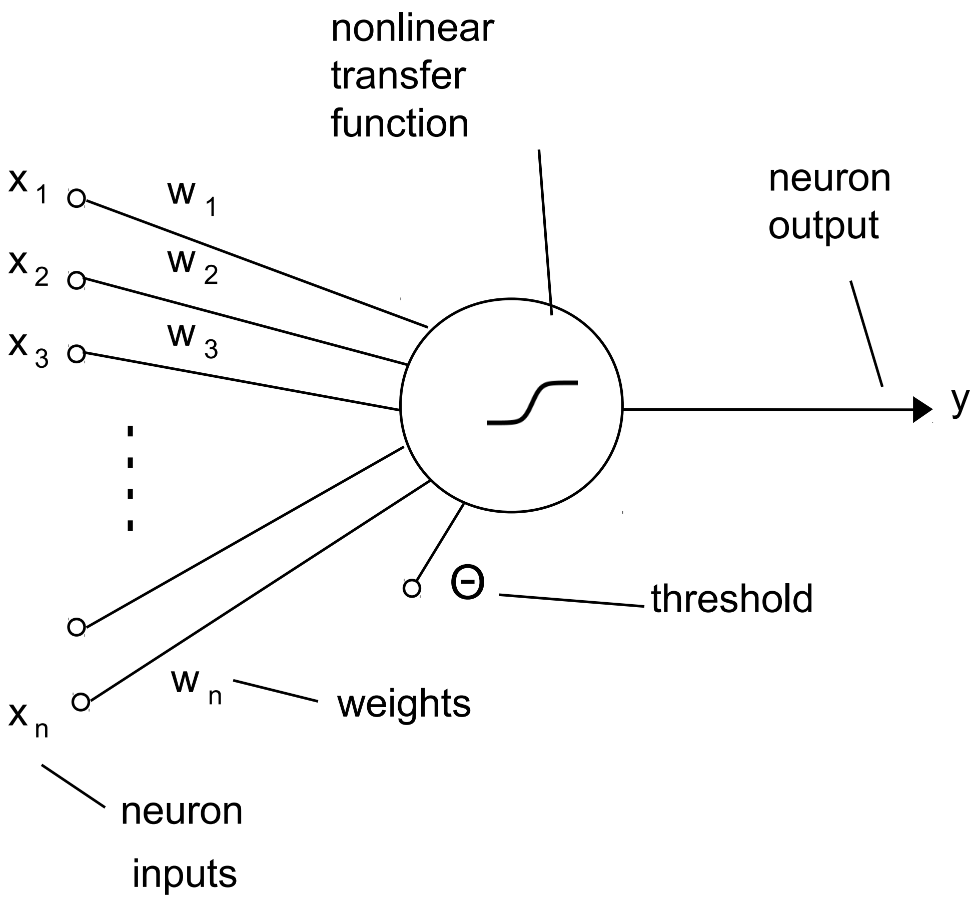


recurrent network

MultiLayer Perceptron (MLP)

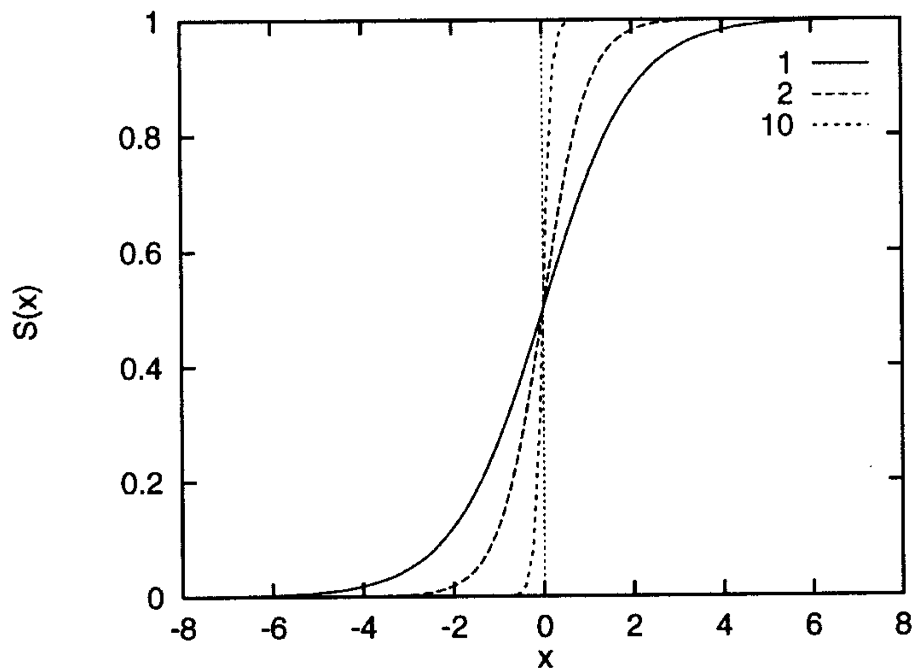


Neurons in MLPs



McCulloch-Pitts perceptron.

Logistic Sigmoid Function



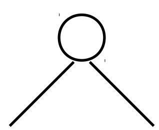
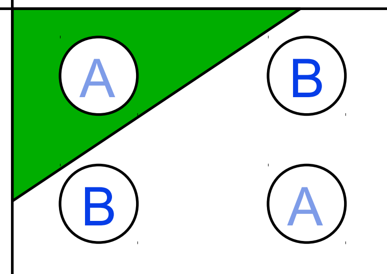
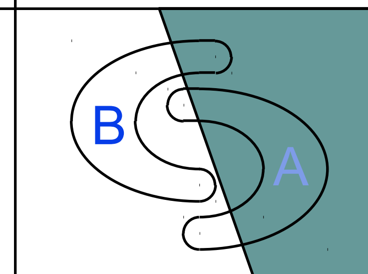
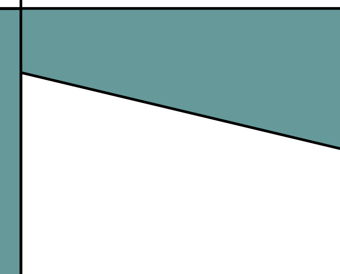
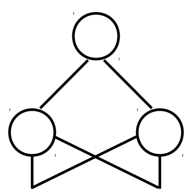
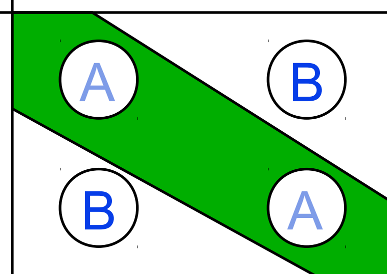
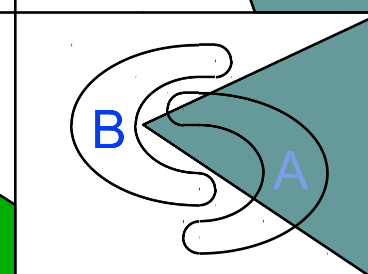
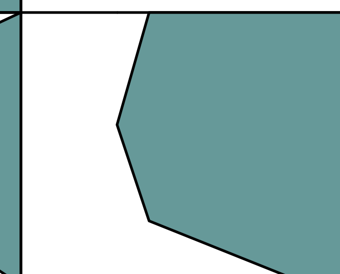
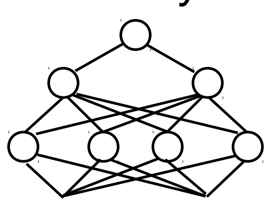
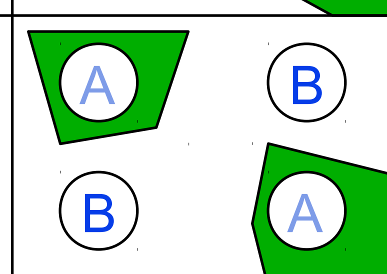
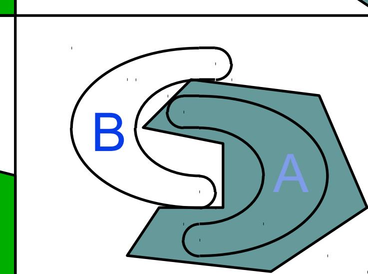
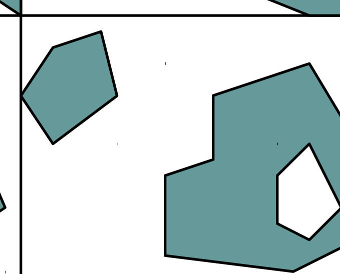
Sigmoid for different gain/slope parameter γ .

$$S(s) = \frac{1}{1+e^{-\gamma s}}$$

- But also many other (non)-linear functions...

How Many Hidden Layers? MLPs with Discrete Activation Functions

see ftp://ftp.sas.com/pub/neural/FAQ3.html#A_hl for overview

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)			

How Many Hidden Layers? Continuous MLPs

- **Universal Approximation** property.
- Kurt Hornik: “For MLP using **continuous, bounded, and non-constant** activation functions a **single hidden layer is enough** to approximate any function.”
- **Q**: what about linear activation?

How Many Hidden Layers? Continuous MLPs

- **Universal Approximation** property.
- Kurt Hornik: “For MLP using **continuous, bounded, and non-constant** activation functions a **single hidden layer is enough** to approximate any function.”
- **Q**: what about linear activation?
- **A**: it is continuous, non-constant but not bounded!
- We will get back to this topic later...

Continuous MLPs

- Although one hidden layer is enough for a continuous MLP:
  - we don't know how many neurons to use,
  - **fewer neurons are often sufficient for ANN architectures with two (or more) hidden layers.**

    See ftp://ftp.sas.com/pub/neural/FAQ3.html#A_hl for example.

How Many Neurons?

No one knows :(we have only rough estimates (upper bounds):

ANN with a **single hidden layer:**

$$N_{\mathrm{hid}} = \sqrt{N_{\mathrm{in}} . N_{\mathrm{out}}} \,,$$

ANN with two **hidden layers**:

$$N_{\mathrm{hid}-1} = N_{\mathrm{out}} \cdot \left(\sqrt[3]{\frac{N_{\mathrm{in}}}{N_{\mathrm{out}}}} \right)^2, \quad N_{\mathrm{hid}-2} = N_{\mathrm{out}} \cdot \left(\sqrt[3]{\frac{N_{\mathrm{in}}}{N_{\mathrm{out}}}} \right).$$

You have to experiment.

Generalization vs. Overfitting

- When training ANNs we typically want them to perform accurately on new previously unseen data.
- This ability is known as the **generalization**.
- When ANN rather memorizes the training data while giving bad results on new data, we talk about **overfitting (overtraining)**.

Training/Testing Sets

Training set | Testing set

Random samples.

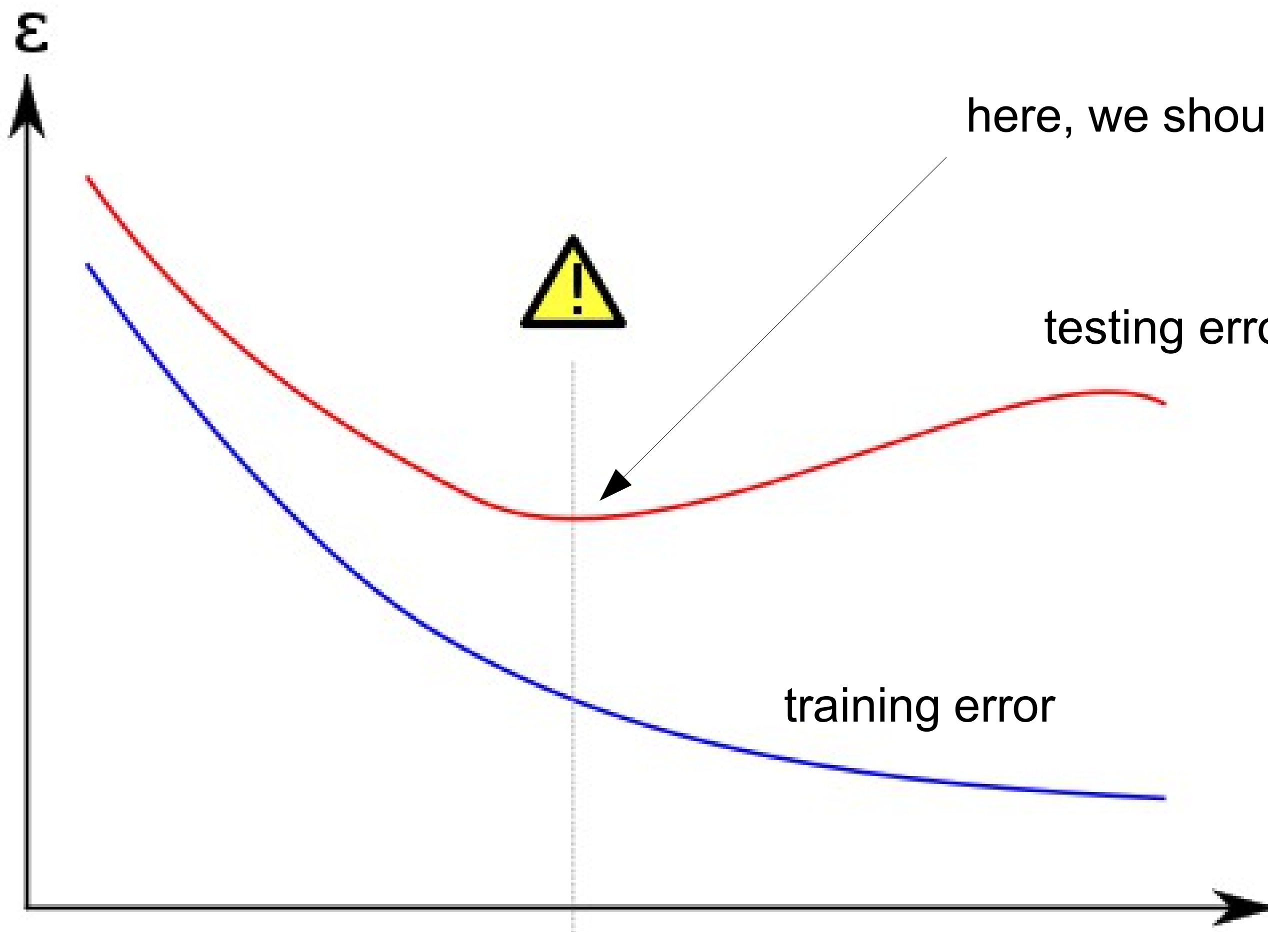
~70% ~30%

Used to train ANN model.

Testing set error
→ generalization

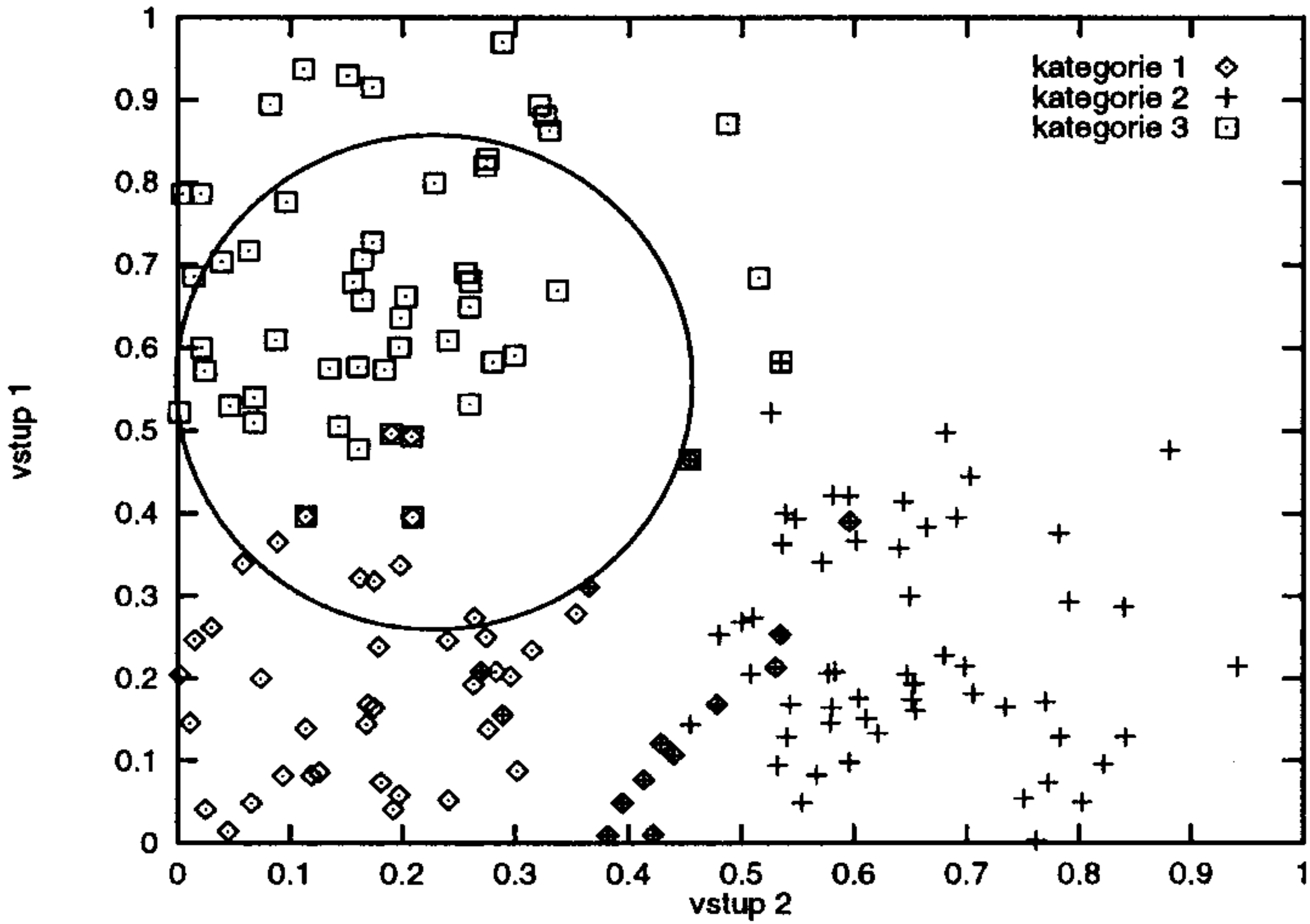
Jan Drchal, drchajan@fel.cvut.cz, http://cig.felk.cvut.cz

Overfitting Example



http://upload.wikimedia.org/wikipedia/commons/1/1f/Overfitting_svg.svg

Example: Bad Choice of A Training Set

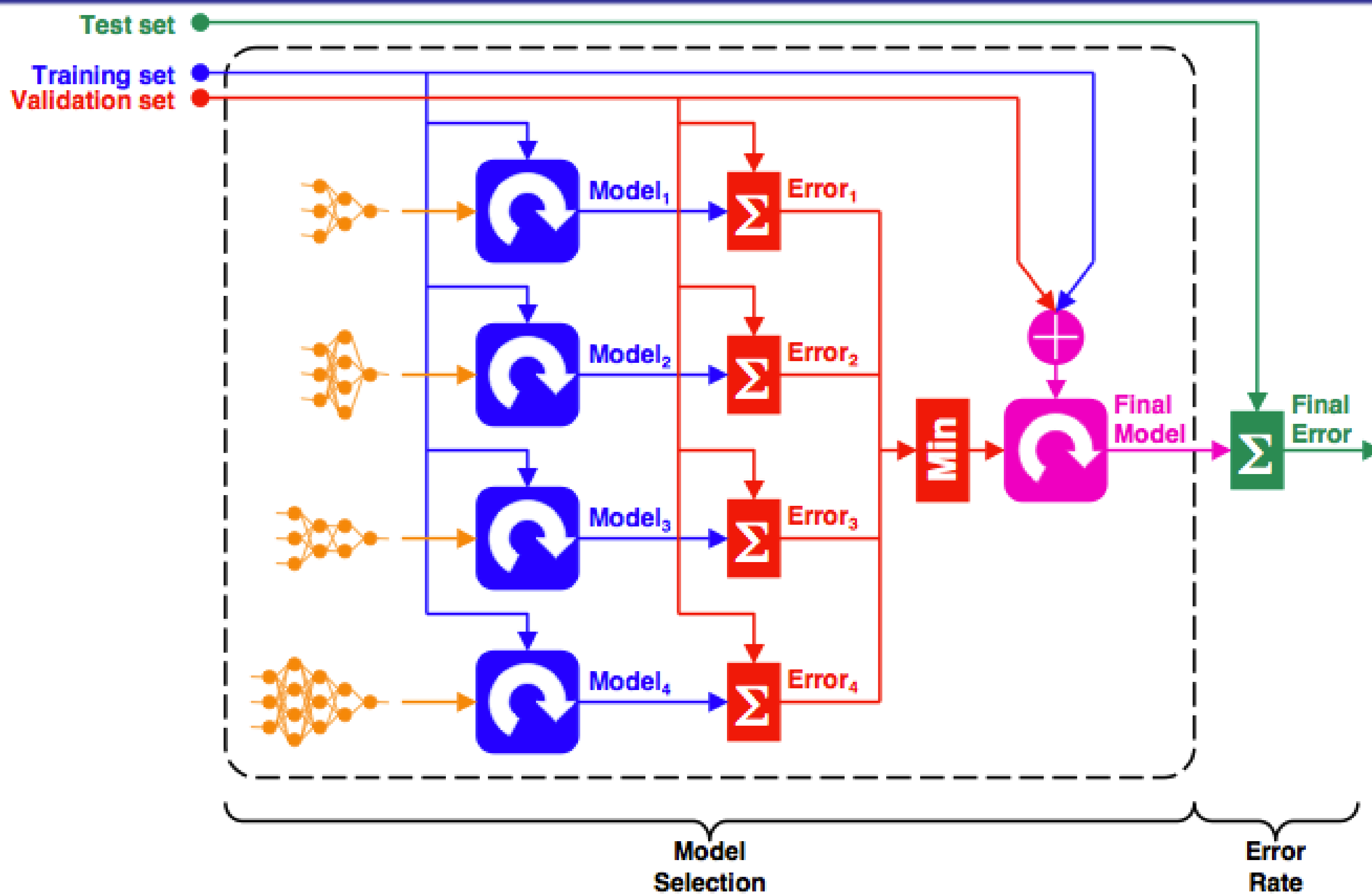


Training/Validation/Testing Sets

- Ripley "Pattern Recognition and Neural Networks", 1996:
  - **Training set**: A set of examples used for learning, that is to fit the parameters [i.e., weights] of the ANN.
  - **Validation set**: A set of examples used to tune the parameters [i.e., architecture, not weights] of an ANN, for example to choose the number of hidden units.
  - **Test set**: A set of examples used only to assess the performance (generalization) of a fully-specified ANN.
- Separated: ~60%, ~20%, ~20%.
- Note: meaning of the validation and test sets is often reversed in literature (machine-learning vs. statististics).

For example see Priddy, Keller: Artificial neural networks: an introduction (Google books, p. 44)

Training/Validation/Testing Sets II



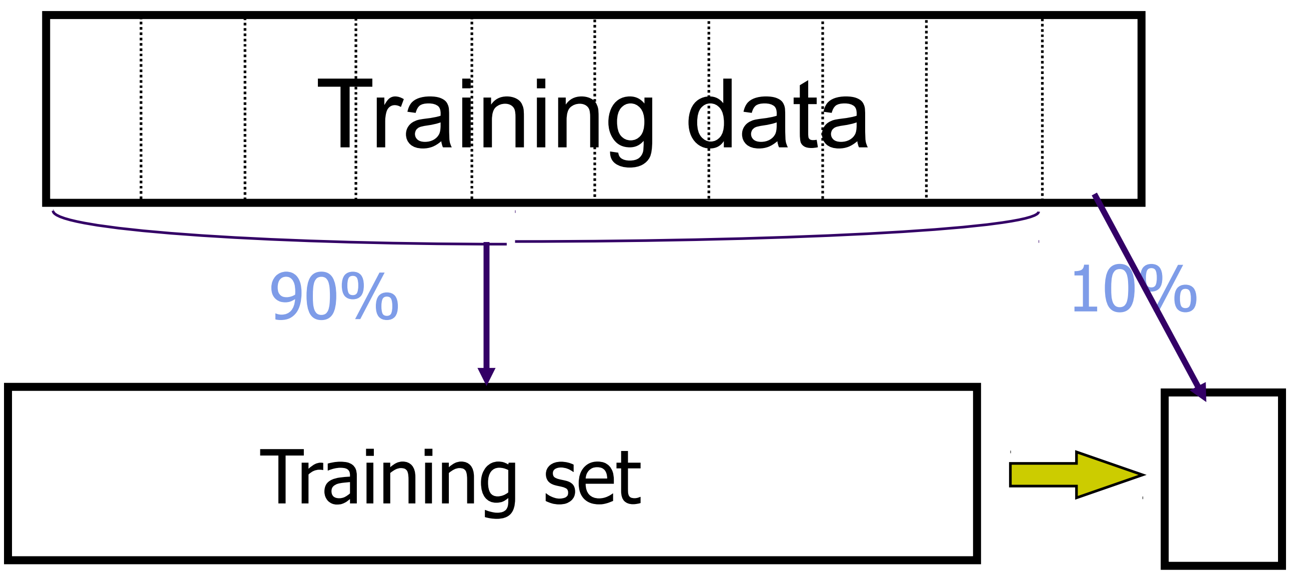
•Taken from Ricardo Gutierrez-Osuna's slides: http://courses.cs.tamu.edu/rgutier/ceg499_s02/l13.pdf

k-fold Cross-validation

Example 10-fold cross-validation:

Split training data to 10 folds of equal size.

Repeat 10 times, always chose different fold for validation set (1 of 10).



Validation set

Create 10 ANN models.

The cross-validation error is the average over all (10) validation sets.

Suitable for small datasets, reduces the problems caused by random selection of training/testing sets

"Cleaning" Dataset

- Imputing missing values.
- Outlier identification:
  - the instance of the data distant from the rest of the data
- Smoothing-out the noisy data.

Data Reduction

- Often needed for large data sets.
- The reduced dataset should be representative sample of the original dataset.
- The simplest algorithm: randomly remove data instances.

Data Transformation

- Normalization:
  - scaling/shifting values to fit given interval or distribution
- Aggregation:
  - i.e. “binning” - discretization (continuous values to classes).

Learning Process Notes

- We don't have to choose instances sequentially → random selection.
- We can apply certain instances more frequently than others.
- We need often hundreds to thousands epochs to train the network.
- Good strategy might speed things up.

Backpropagation (BP)

- Paul Werbos,
- 1974, Harvard, PhD thesis.
- Still popular method,
- many modifications.
- **BP is a learning method for MLP:**
  - **continuous, differentiable activation functions!**

BP Overview

random weight initialization
repeat
  repeat *// epoch*
    choose an instance from the training set
    apply it to the network
    evaluate network outputs
    compare outputs to desired values
    modify the weights
  until all instances selected from the training set
until global error < criterion

ANN Energy

Backpropagation is based on a minimalization of ANN *energy* (= error). Energy is a measure describing how the network is trained on given data. For BP we define the energy function:

$$E_{TOTAL} = \sum_p E_p$$

The total sum computed over all patterns of the training set.

where

$$E_p = \frac{1}{2} \sum_{i=1}^{N_o} (d_i^o - y_i^o)^2$$

we will omit “p” in following slides

Note, ½ – only for convenience – we will see later...

ANN Energy II

The energy/error is a function of:

$$E = f\left(\vec{X}, \vec{W}\right)$$

$\vec{W}$ weights (thresholds) → **variable**,

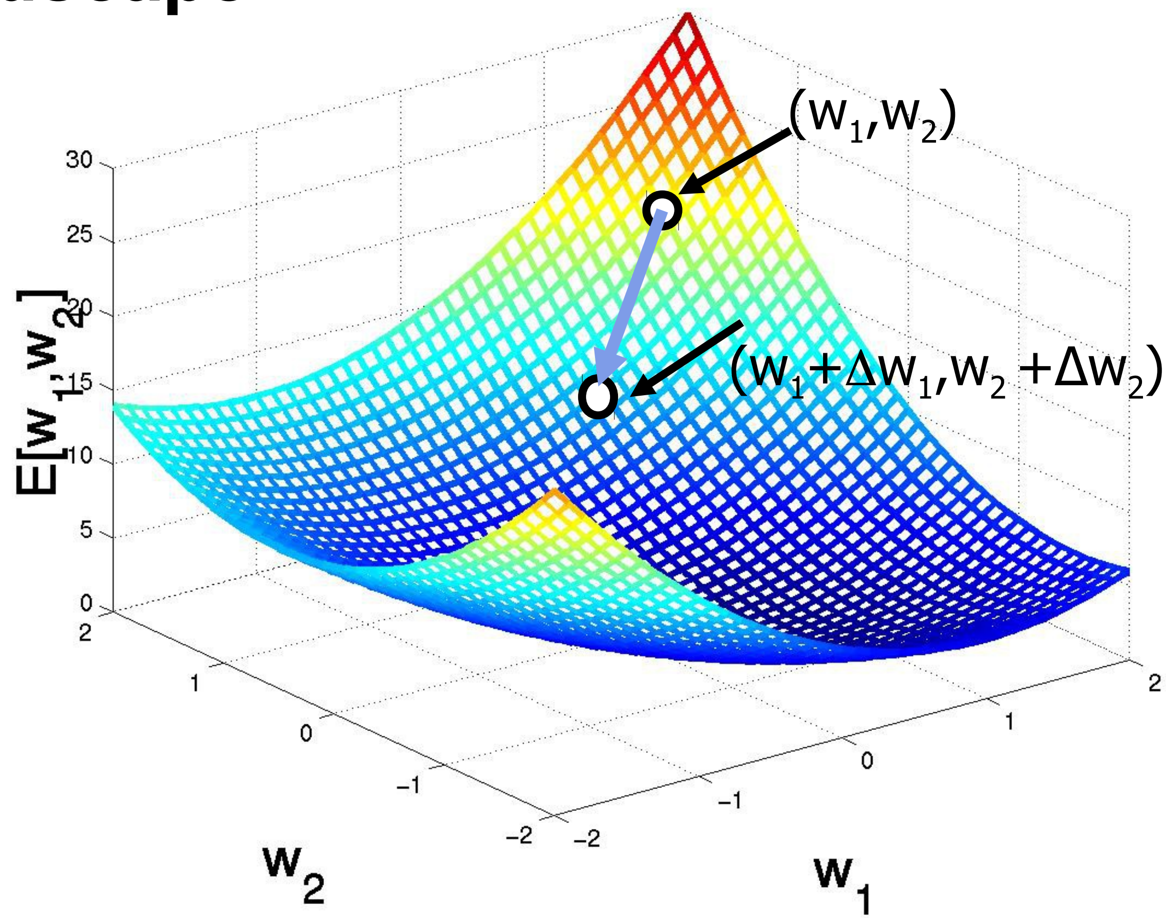
$\vec{X}$ inputs → **fixed (for given pattern)**.

Backpropagation Keynote

- For given values at network inputs we obtain an energy value.
- Our task is to minimize this value.
- The minimization is done via modification of weights and thresholds.
- We have to identify how the energy changes when a certain weight is changed by Δw.
- This corresponds to partial derivatives $\frac{\partial E}{\partial w}$.
- We employ a **gradient method**.

Gradient Descent in Energy Landscape

Energy/Error Landscape



Weight Update

- We want to update weights in opposite direction to the gradient:

$$\Delta w_{jk} = -\eta \frac{\partial E}{\partial w_{jk}}$$

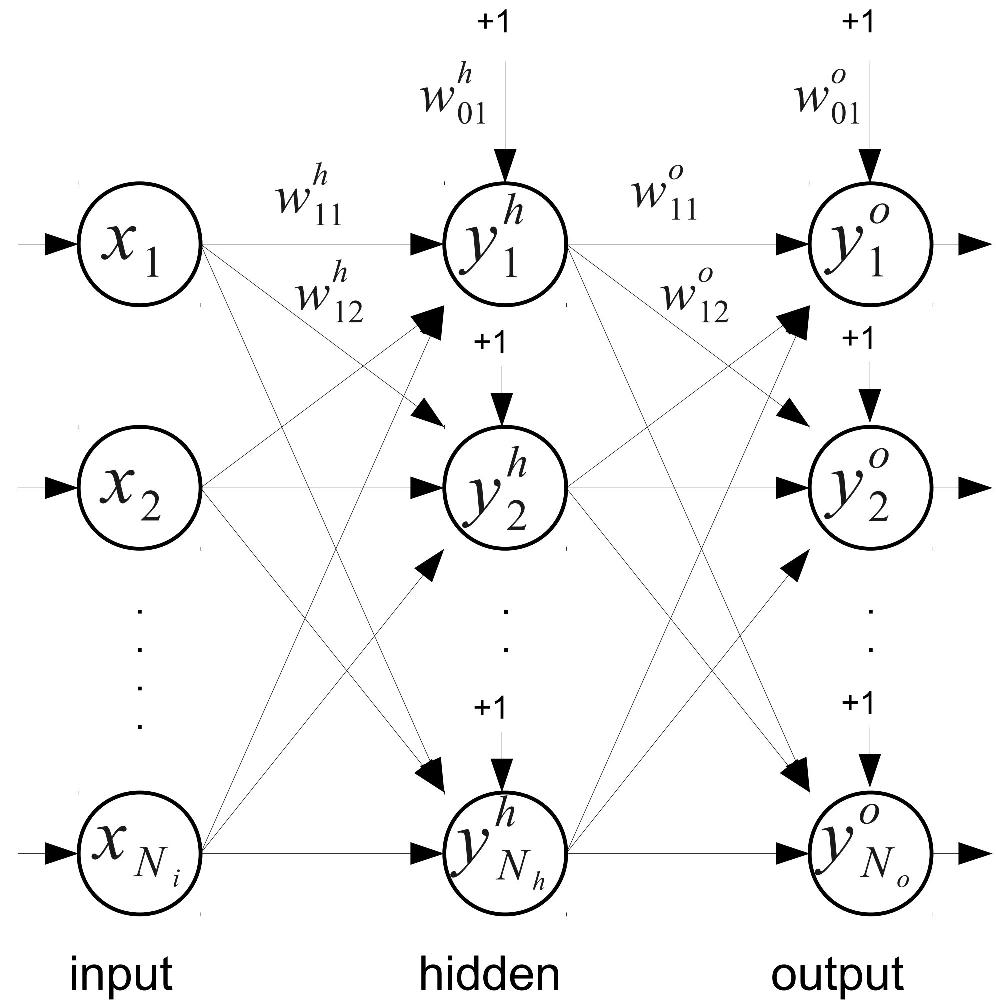
weight "delta"

learning rate

Note: gradient of energy function is a vector which contains partial derivatives for all weights (thresholds)

Notation

w_{jk}	weight of connection from neuron *j* to neuron *k*
$w^{m}_{0\mathrm{k}}$	threshold of neuron *k* in layer *m*
w^{m}_{jk}	weight of connection from layer *m-1* to *m*
s^{m}_{k}	inner potential of neuron *k* in layer *m*
y^{m}_{k}	output of neuron *k* in layer *m*
x_k	*k*-th input
$N_i,\ N_h,\ N_o$	number of neurons in input, hidden and output layers



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Energy as a Function Composition

$$\frac{\partial E}{\partial w_{jk}} = \frac{\partial E}{\partial s_k} \frac{\partial s_k}{\partial w_{jk}}$$

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$$s_k = \sum_j w_{jk} y_j$$

use

$$\frac{\partial s_k}{\partial w_{jk}} = y_j$$

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denote

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$$\delta_k = -\frac{\partial E}{\partial s_k}$$

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Energy as a Function Composition

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use

denote

$$\frac{\partial s_k}{\partial w_{jk}} = y_j$$

$$\delta_k = -\frac{\partial E}{\partial s_k}$$

$$\Delta w_{jk} = \eta \delta_k y_j$$

Remember the delta rule?

Output Layer

$$\delta_k = -\frac{\partial E}{\partial s_k} \quad \xrightarrow{\text{output layer}} \quad \delta_k^o = -\frac{\partial E}{\partial s_k^o}$$

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Output Layer

$$\delta_k = -\frac{\partial E}{\partial s_k}$$

output layer →

$$\delta_k^o = -\frac{\partial E}{\partial s_k^o}$$

$$\frac{\partial E}{\partial s_k^o} = \frac{\partial E}{\partial y_k^o} \frac{\partial y_k^o}{\partial s_k^o}$$

derivate of activation function

$$\frac{\partial y_k^o}{\partial s_k^o} = S'(s_k^o)$$

Output Layer

$$\delta_k = -\frac{\partial E}{\partial s_k}$$

output layer

$$\delta_k^o = -\frac{\partial E}{\partial s_k^o}$$

$$E = \frac{1}{2}\sum_{i=1}^{N_o}(d_i^o - y_i^o)^2$$

$$\frac{\partial E}{\partial s_k^o} = \frac{\partial E}{\partial y_k^o}\frac{\partial y_k^o}{\partial s_k^o}$$

use

$$\frac{\partial E}{\partial y_k^o} = -(d_k^o - y_k^o)$$

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dependency of energy on a network output

$$\frac{\partial E}{\partial y_k^o} = -(d_k^o - y_k^o)$$

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use

dependency of energy on a network output

$$\frac{\partial E}{\partial y_k^o} = -(d_k^o - y_k^o)$$

That is why we used the ½ in energy definition.

derivate of activation function

$$\frac{\partial y_k^o}{\partial s_k^o} = S'(s_k^o)$$

Output Layer

$$\delta_k = -\frac{\partial E}{\partial s_k}$$

output layer →

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dependency of energy on a network output

$$\frac{\partial E}{\partial y_k^o} = -(d_k^o - y_k^o)$$

That is why we used 1/2.

Again, remember the delta rule?

derivate of activation function

$$\frac{\partial y_k^o}{\partial s_k^o} = S'(s_k^o)$$

Output Layer

$$\delta_k = -\frac{\partial E}{\partial s_k}$$ output layer → $$\delta_k^o = -\frac{\partial E}{\partial s_k^o}$$

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derivate of activation function

$$\frac{\partial y_k^o}{\partial s_k^o} = S'(s_k^o)$$

$$\Delta w_{jk}^o = \eta \delta_k^o y_j^h = \eta (d_k - y_k^o) S'(s_k^o) y_j^h$$

Hidden Layer

$$\delta_k = -\frac{\partial E}{\partial s_k} \xrightarrow{\text{hidden layer}} \delta_k^h = -\frac{\partial E}{\partial s_k^h}$$

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$$\frac{\partial y_k^h}{\partial s_k^h} = S'(s_k^h)$$

Same as output layer.

Hidden Layer

$$\delta_k = -\frac{\partial E}{\partial s_k}$$

hidden layer →

$$\delta_k^h = -\frac{\partial E}{\partial s_k^h}$$

$$\frac{\partial E}{\partial s_k^h} = \frac{\partial E}{\partial y_k^h} \frac{\partial y_k^h}{\partial s_k^h}$$

Note, this is output of a **hidden** neuron.

$$\frac{\partial y_k^h}{\partial s_k^h} = S'(s_k^h)$$

Same as output layer.

Hidden Layer

$$\delta_k = -\frac{\partial E}{\partial s_k}$$

hidden layer →

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Note, this is output of a **hidden** neuron.

$$\frac{\partial y_k^h}{\partial s_k^h} = S'(s_k^h)$$

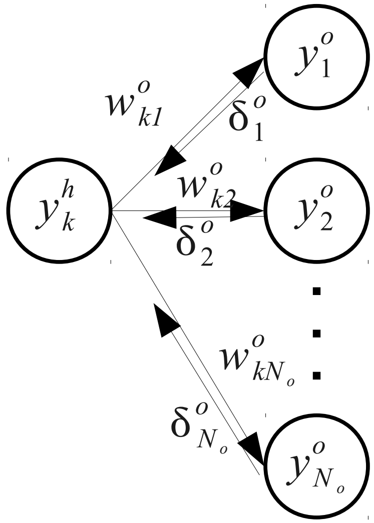
Same as output layer.

? let's look at this partial derivation

Hidden Layer II

$$\frac{\partial E}{\partial y_k^h} = \sum_{l=1}^{N_o} \frac{\partial E}{\partial s_l^o} \frac{\partial s_l^o}{\partial y_k^h} = \sum_{l=1}^{N_o} \frac{\partial E}{\partial s_l^o} \frac{\partial}{\partial y_k^h} \left(\sum_{i=1}^{N_h} w_{il}^o y_i^h \right) =$$

Apply the chain rule
(http://en.wikipedia.org/wiki/Chain_rule).



$$= \sum_{l=1}^{N_o} \frac{\partial E}{\partial s_l^o} w_{kl}^o = - \sum_{l=1}^{N_o} \delta_l^o w_{kl}^o$$

Hidden Layer II

$$\frac{\partial E}{\partial y_k^h}=\sum_{l=1}^{N_o}\frac{\partial E}{\partial s_l^o}\frac{\partial s_l^o}{\partial y_k^h}=\sum_{l=1}^{N_o}\frac{\partial E}{\partial s_l^o}\frac{\partial}{\partial y_k^h}\left(\sum_{i=1}^{N_h}w_{il}^o y_i^h\right)=$$

Apply the chain rule
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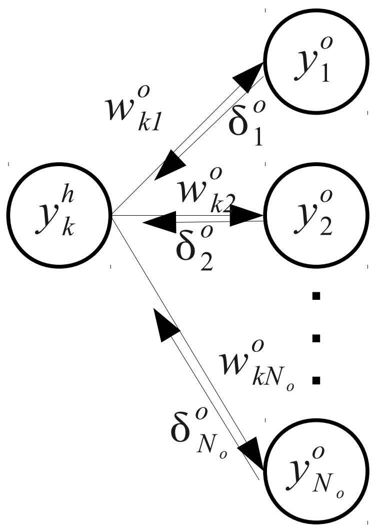

But we know
this already.

$$\delta_k^o=-\frac{\partial E}{\partial s_k^o}$$

Hidden Layer II

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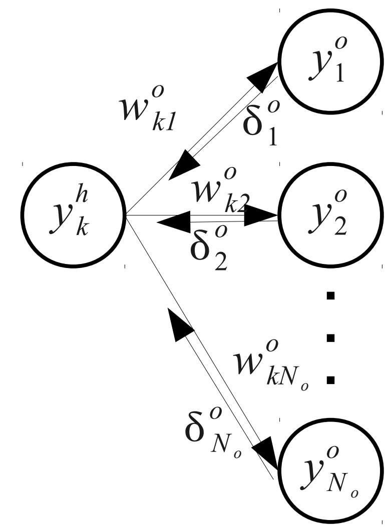


$$= \sum_{l=1}^{N_o} \frac{\partial E}{\partial s_l^o} w_{kl}^o = -\sum_{l=1}^{N_o} \delta_l^o w_{kl}^o$$

But we know this already.

Take the error of the output neuron

and multiply it by the input weight.

$$\delta_k^o = -\frac{\partial E}{\partial s_k^o}$$

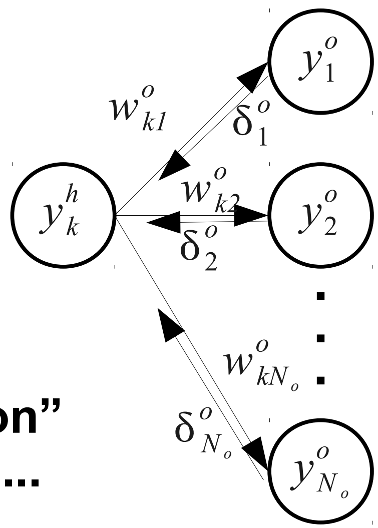
Hidden Layer II

$$\frac{\partial E}{\partial y_k^h} = \sum_{l=1}^{N_o} \frac{\partial E}{\partial s_l^o} \frac{\partial s_l^o}{\partial y_k^h} = \sum_{l=1}^{N_o} \frac{\partial E}{\partial s_l^o} \frac{\partial}{\partial y_k^h} \left(\sum_{i=1}^{N_h} w_{il}^o y_i^h \right) =$$

Apply the chain rule
(http://en.wikipedia.org/wiki/Chain_rule).

$$= \sum_{l=1}^{N_o} \frac{\partial E}{\partial s_l^o} w_{kl}^o = - \sum_{l=1}^{N_o} \delta_l^o w_{kl}^o$$

Here the "back-propagation" actually happens...



But we know this already.

$$\delta_k^o = - \frac{\partial E}{\partial s_k^o}$$

Take the error of the output neuron

and multiply it by the input weight.

Hidden Layer III

Now, let's put it all together!

$$\frac{\partial E}{\partial s_k^h} = \frac{\partial E}{\partial y_k^h} \frac{\partial y_k^h}{\partial s_k^h} = -\left(\sum_{l=1}^{N_o} \delta_l^o w_{kl}^o \right) S'(s_k^h)$$

Hidden Layer III

Now, let's put it all together!

$$\frac{\partial E}{\partial s_k^h} = \frac{\partial E}{\partial y_k^h} \frac{\partial y_k^h}{\partial s_k^h} = -\left(\sum_{l=1}^{N_o} \delta_l^o w_{kl}^o \right) S'(s_k^h)$$

$$\delta_k^h = -\frac{\partial E}{\partial s_k^h} = \left(\sum_{l=1}^{N_o} \delta_l^o w_{kl}^o \right) S'(s_k^h)$$

Hidden Layer III

Now, let's put it all together!

$$\frac{\partial E}{\partial s_k^h} = \frac{\partial E}{\partial y_k^h} \frac{\partial y_k^h}{\partial s_k^h} = -\left(\sum_{l=1}^{N_o} \delta_l^o w_{kl}^o \right) S'(s_k^h)$$

$$\delta_k^h = -\frac{\partial E}{\partial s_k^h} = \left(\sum_{l=1}^{N_o} \delta_l^o w_{kl}^o \right) S'(s_k^h)$$

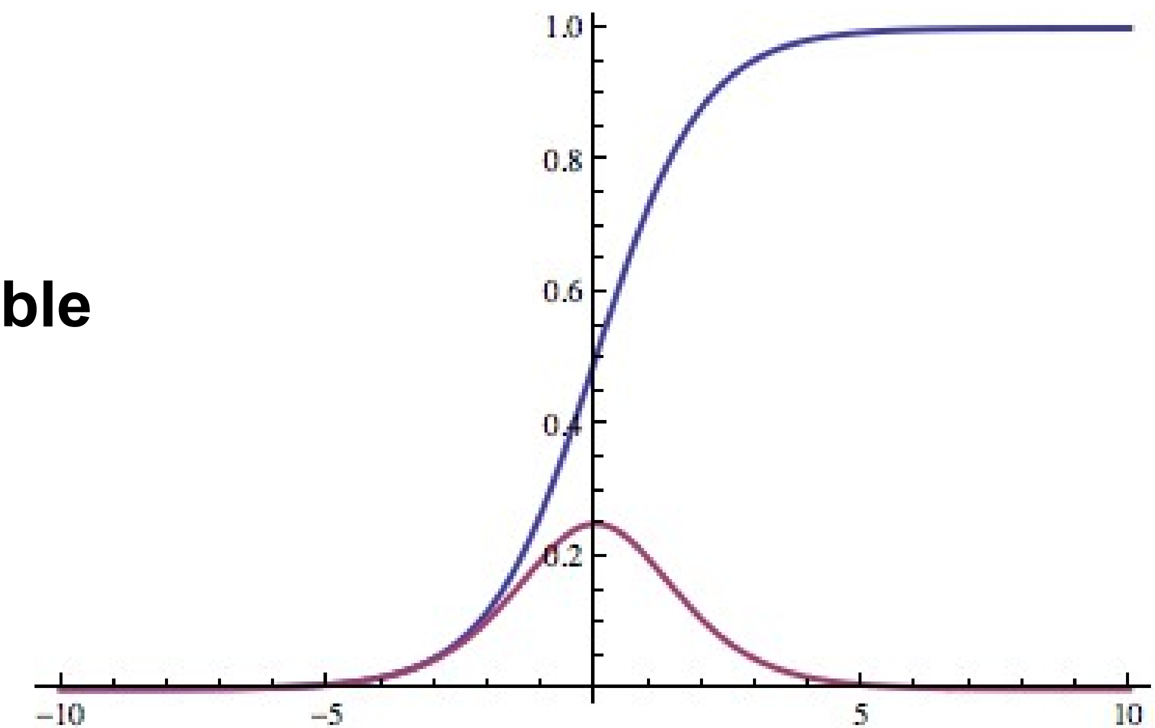
The derivation of the activation function is the last thing to deal with!

$$\Delta w_{jk}^h = \eta \delta_k^h x_j = \eta \left(\sum_{l=1}^{N_o} \delta_l^o w_{kl}^o \right) S'(s_k^h) x_j$$

Sigmoid Derivation

$$S'(s_k) = \left(\frac{1}{1+e^{-\gamma s_k}} \right)' = \frac{\gamma}{1+e^{-\gamma s_k}} \frac{e^{-\gamma s_k}}{1+e^{-\gamma s_k}} = \gamma \, y_k (1 - y_k)$$

That is why we needed continuous & differentiable activation functions!



BP Put All Together

Output layer:

$$\Delta w^o_{jk} = \eta \gamma y^o_k (1 - y^o_k)(d_k - y^o_k) y^h_j$$

This is equal to x_j when we get to inputs.

Hidden layer *m* (note that *h+1 = o*):

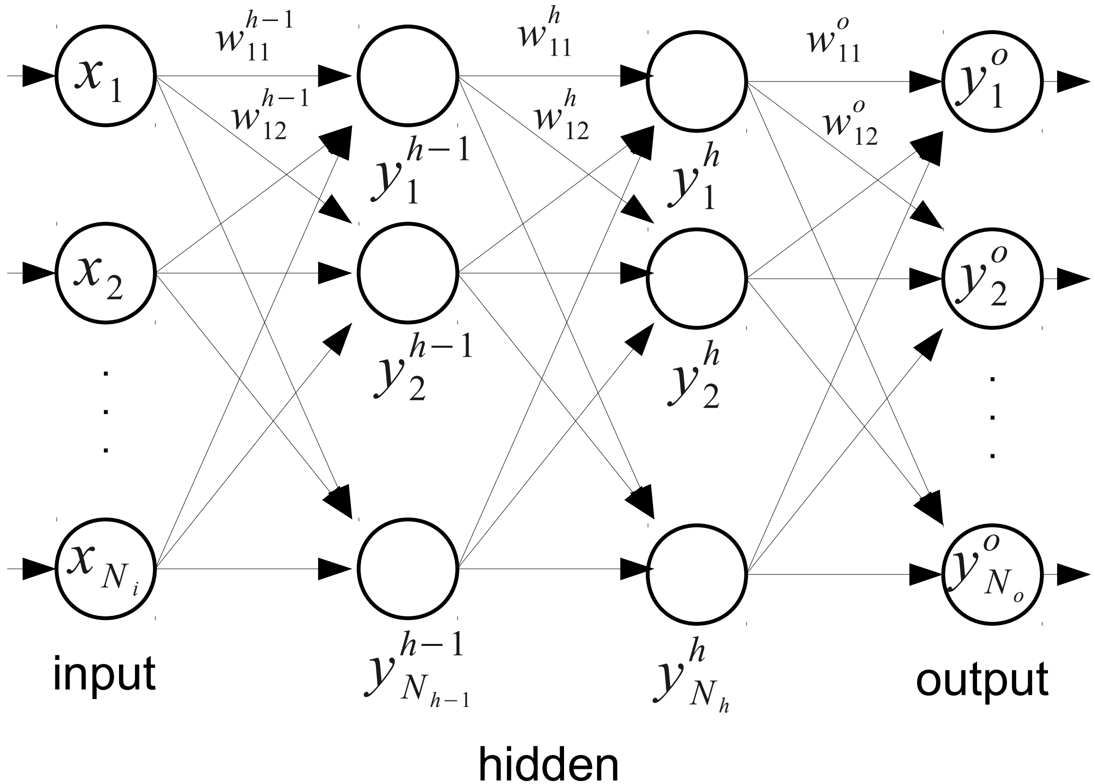
$$\Delta w^m_{jk} = \eta \delta^m_k y^{m-1}_j = \eta \gamma y^m_k (1 - y^m_k) \left(\sum_{l=1}^{N_{m+1}} \delta^{m+1}_l w^{m+1}_{kl} \right) y^{m-1}_j$$

Weight (threshold) updates:

$$w_{jk}(t+1) = w_{jk}(t) + \Delta w_{jk}(t)$$

How About General Case?

- Arbitrary number of hidden layers?



- It's the same: for layer *h-1* use δ_k^h.

Potential Problems

- High dimension of weight (threshold) space.
- Complexity of energy function.
- Different shape of energy function for different input vectors.

Modifications to Standard BP

- Momentum
- Simple, but greatly helps when avoiding local minima:

$$\Delta w_{ij}(t) = \eta \delta_j(t) y_i(t) + \alpha \Delta w_{ij}(t-1)$$

momentum constant: $\alpha \in [0,1)$

Modifications to Standard BP II

- Normalized cumulated delta,
  - all changes applied together,
- Delta-bar-delta rule,
  - using also previous gradient, individual learning rates for each weight,
- Extended,
  - both above together.

Other Approaches Based on Numerical Optimization

- Compute partial derivatives over the total energy:

$$\frac{\partial E_{TOTAL}}{\partial w_{jk}}$$

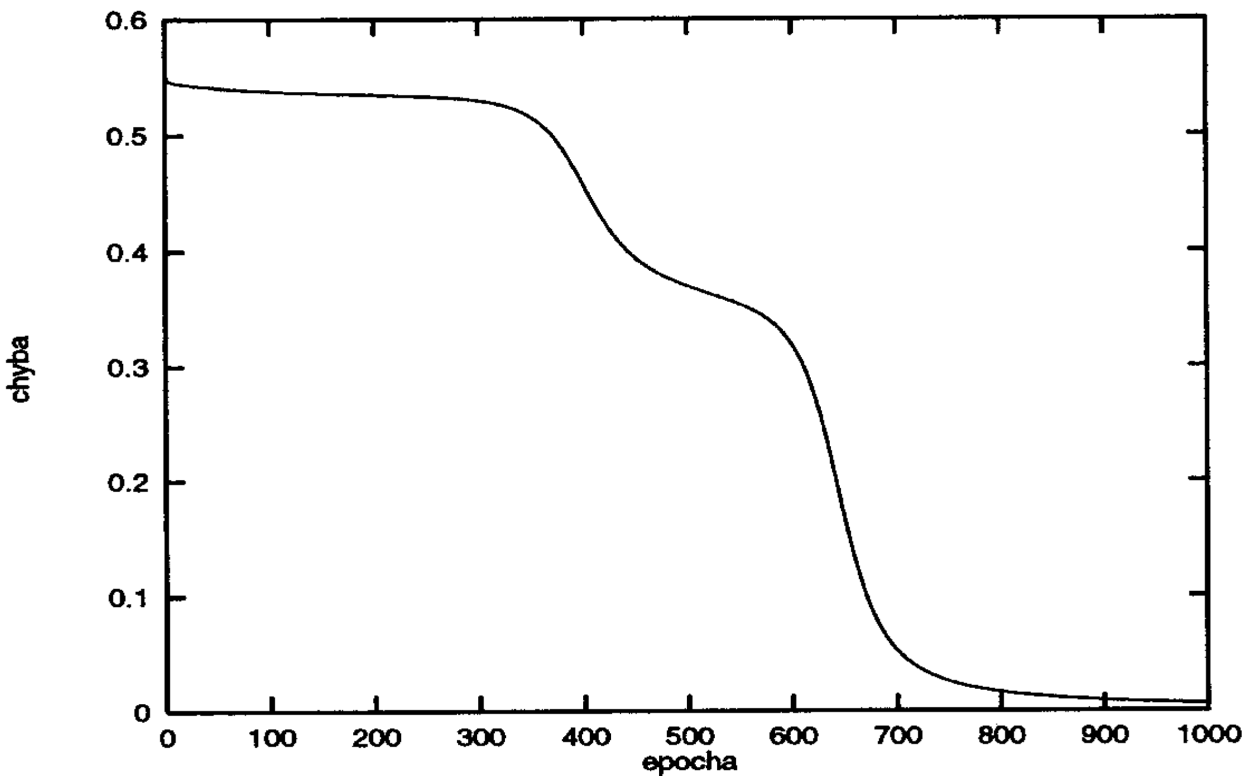
and use **any** numerical optimization method, i.e.:

  - Conjugated gradients,
  - Quasi-Newton methods,
  - Levenberg-Marquardt

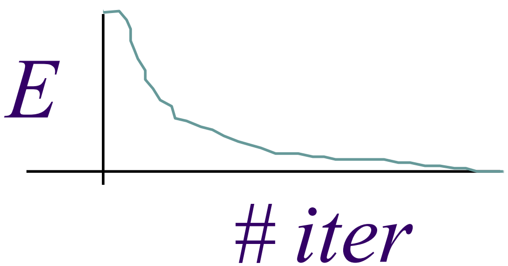
Other Methods

- Quick Propagation (QUICKPROP)
  - based on Newton's method
  - second-order approach.
- Resilient Propagation (RPROP)
  - does not use gradient value – the step sizefor each weight is adapted using its sign, only.
- Levenberg–Marquardt
  - non-linear least squares,
  - combines Gauss-Newton algorithm and Gradient Descent.

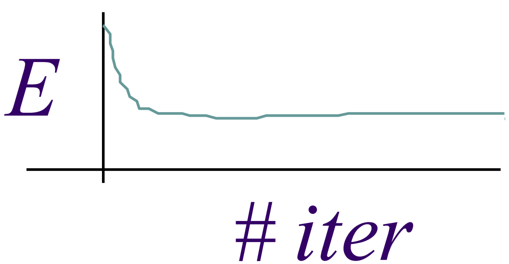
Typical Energy Behaviour During Learning



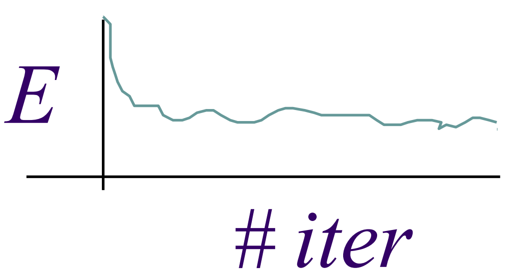
Typical Learning Runs



This is best! Constant and fast decrease of error.



Seems like local minimum. Change learning rate, momentum, ANN architecture, run again (random weight initialization)...



Noisy data.

Next Lecture

- Recurrent ANNs = RNNs