Artificial Neural Networks
MLP, RBF & GMDH

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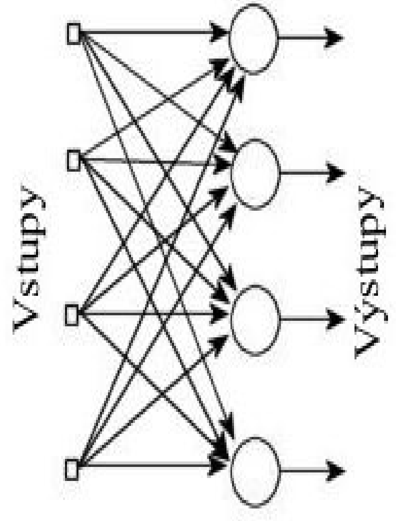
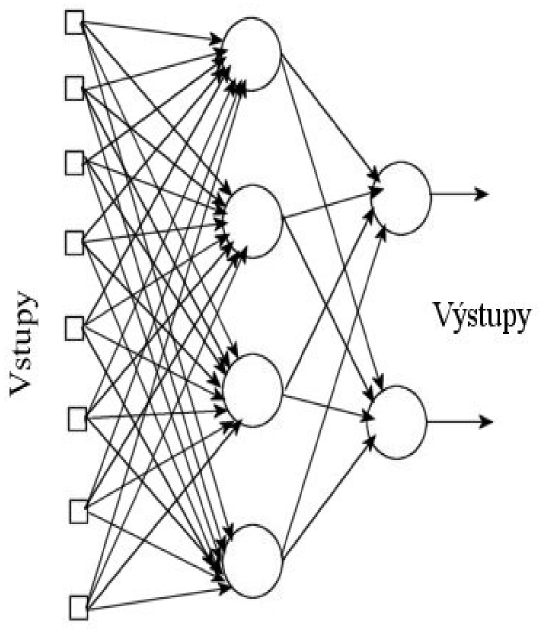
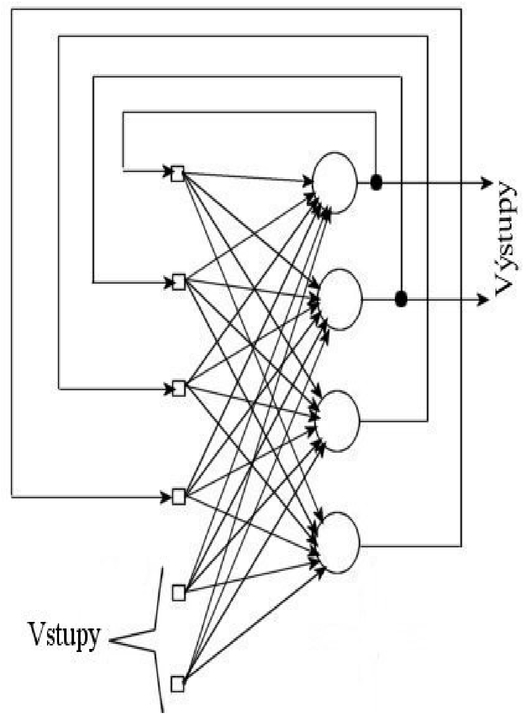
Outline

- MultiLayer Perceptron (MLP).
- How many layers and neurons?
- How to train ANNs and preprocess data?
- Radial Basis Function (RBF).
- Group Method of Data Handling (GMDH).

Layered ANNs





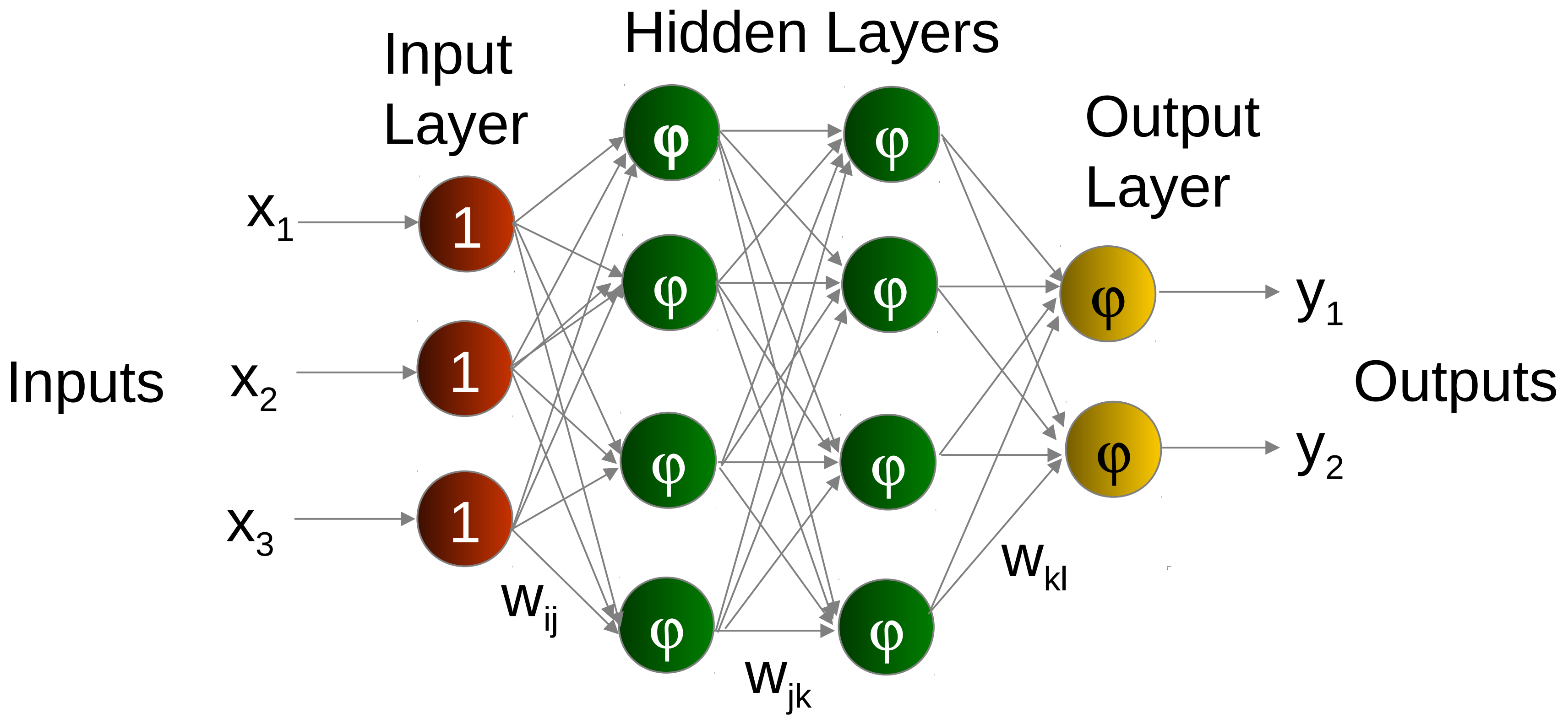


single layer **two layers**

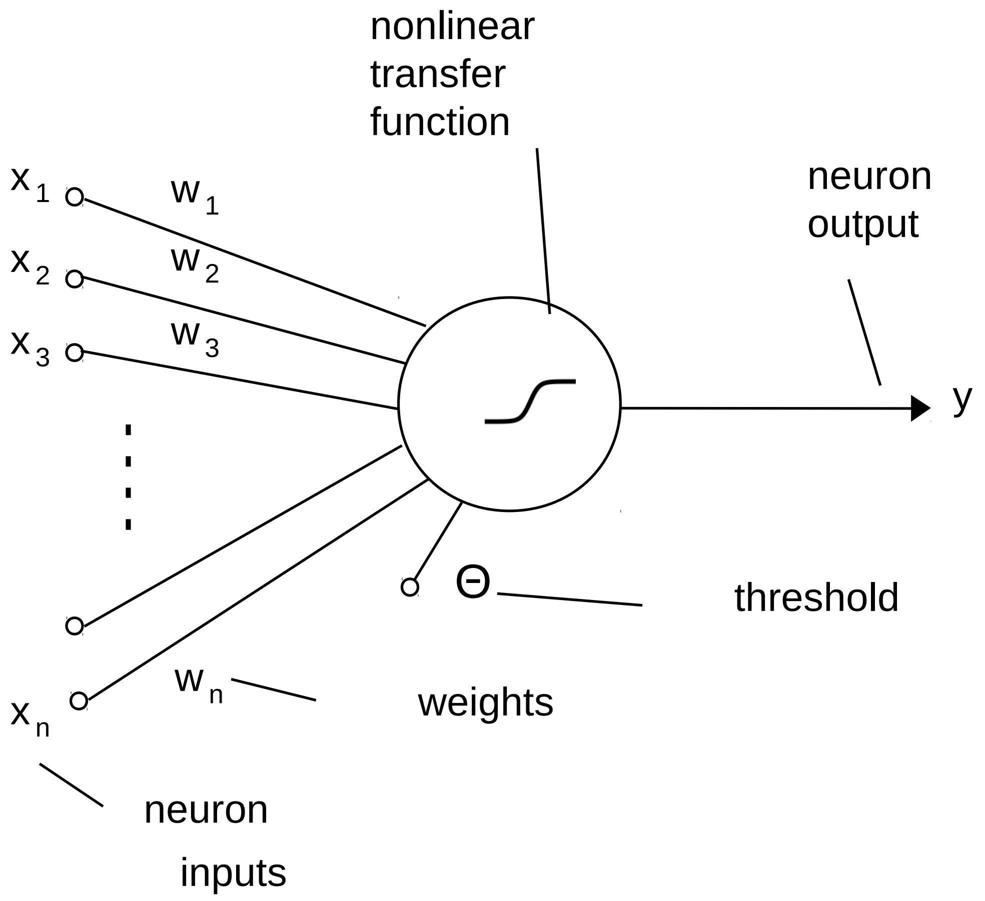
feed-forward networks

recurrent network

MultiLayer Perceptron (MLP)

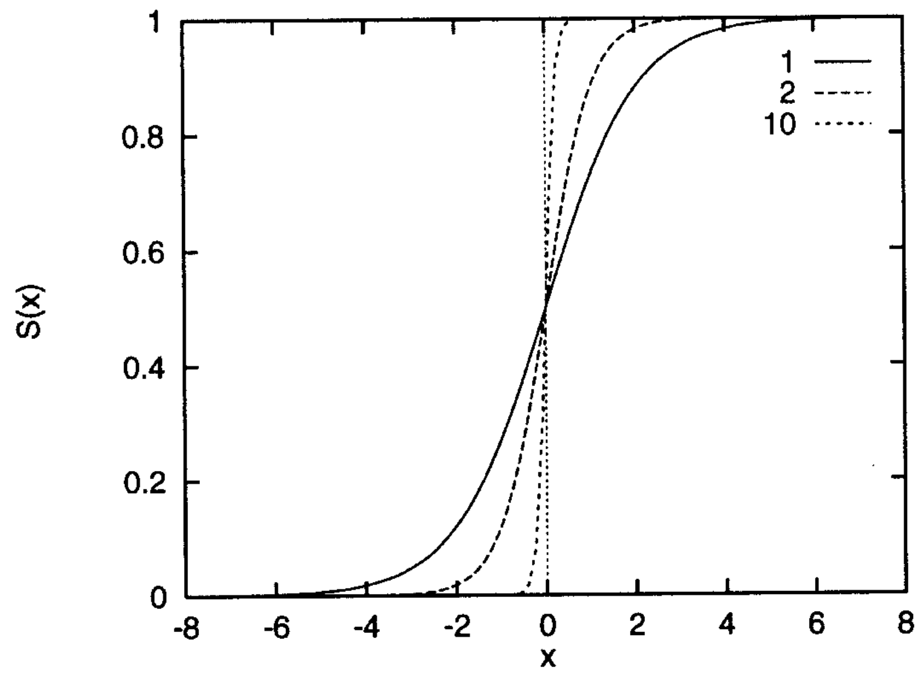


Neurons in MLPs



McCulloch-Pitts perceptron.

Logistic Sigmoid Function



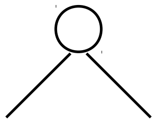
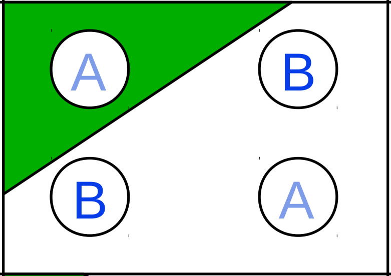
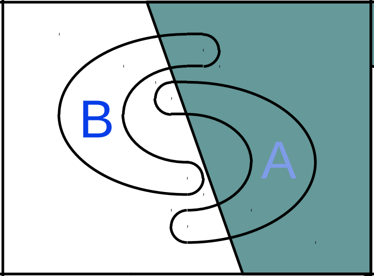
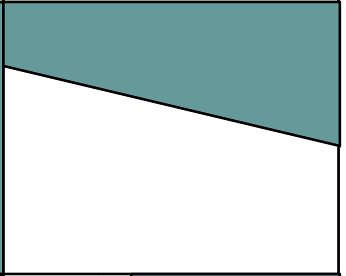
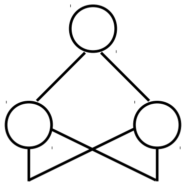
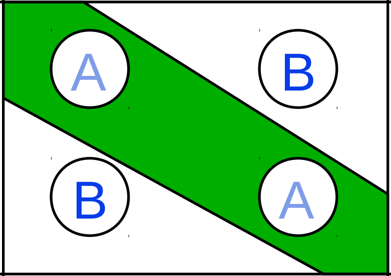
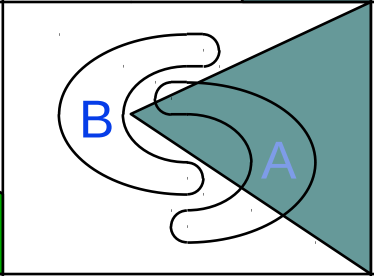
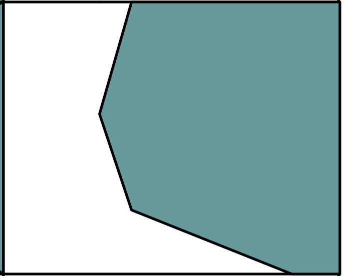
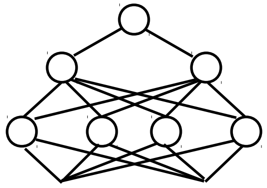
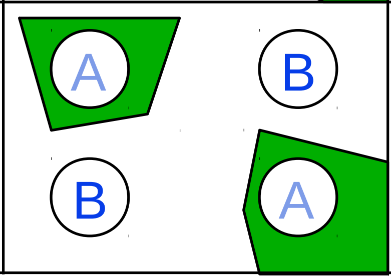
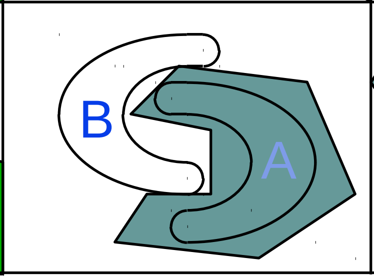
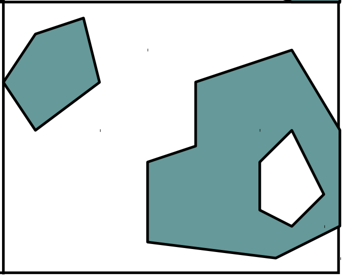
Sigmoid for different gain/slope parameter γ.

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

- 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.”
- Leshno, Lin, Pinkus & Schocken 1993: **non-polynomial activation function suffices**...

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**:

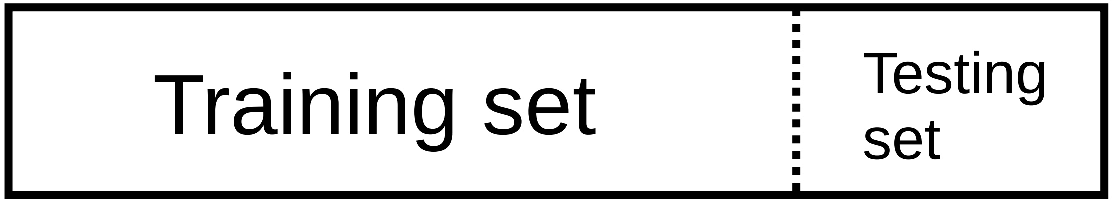
$$N_{\mathrm{hid}-1} = N_{\mathrm{out}} \cdot \left(\sqrt[3]{\frac{N_{\mathrm{in}}}{N_{\mathrm{out}}}} \right)^2 , \quad N_{\mathrm{hid}-2} = N_{\mathrm{out}} \cdot \left(\sqrt[3]{\frac{N_{\mathrm{in}}}{N_{\mathrm{out}}}} \right) .$$

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



Random samples.

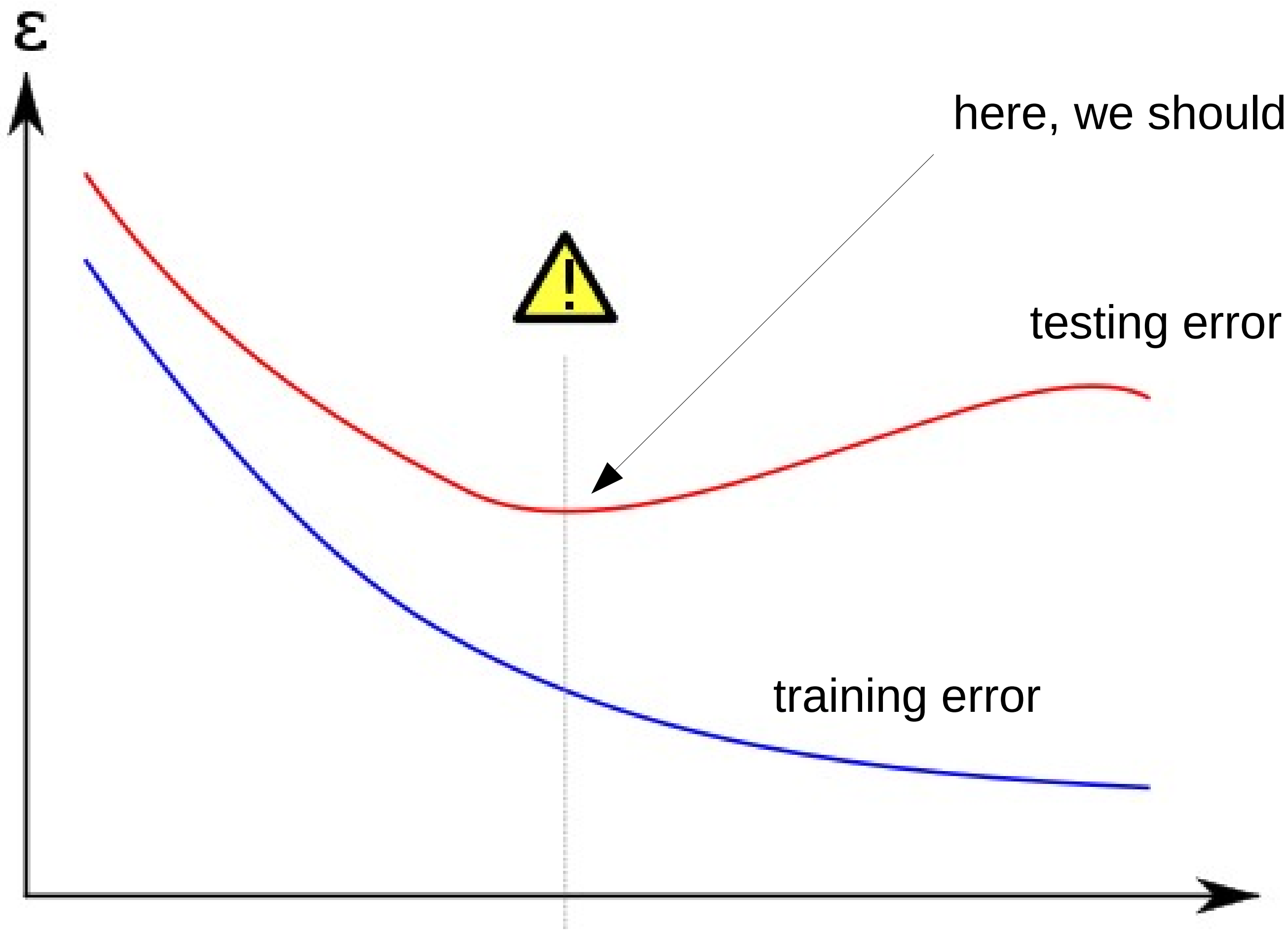
~70%

~30%

Used to train ANN model.

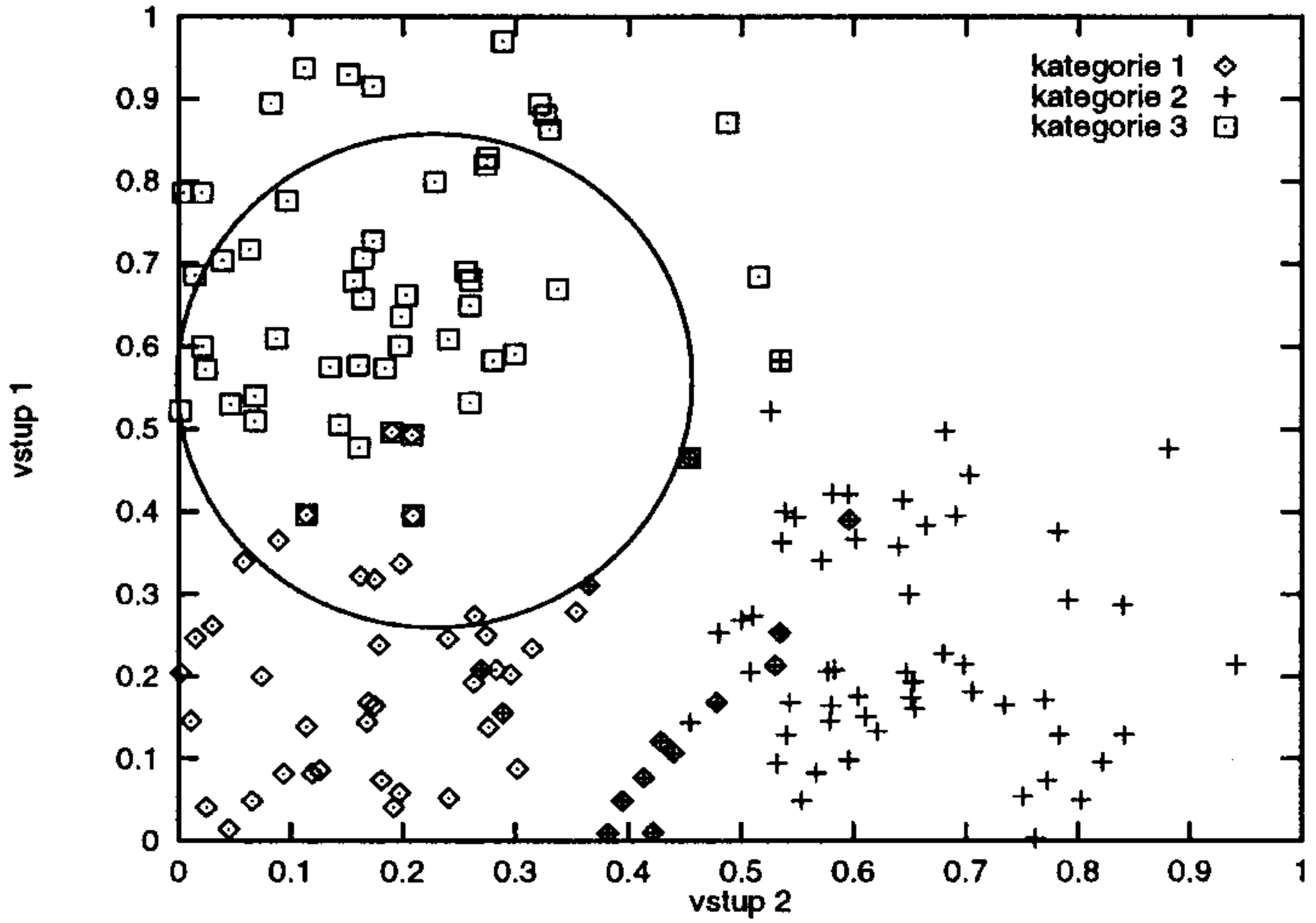
Testing set error
→ generalization

Overfitting Example



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

Example: Bad Choice of A Training Set

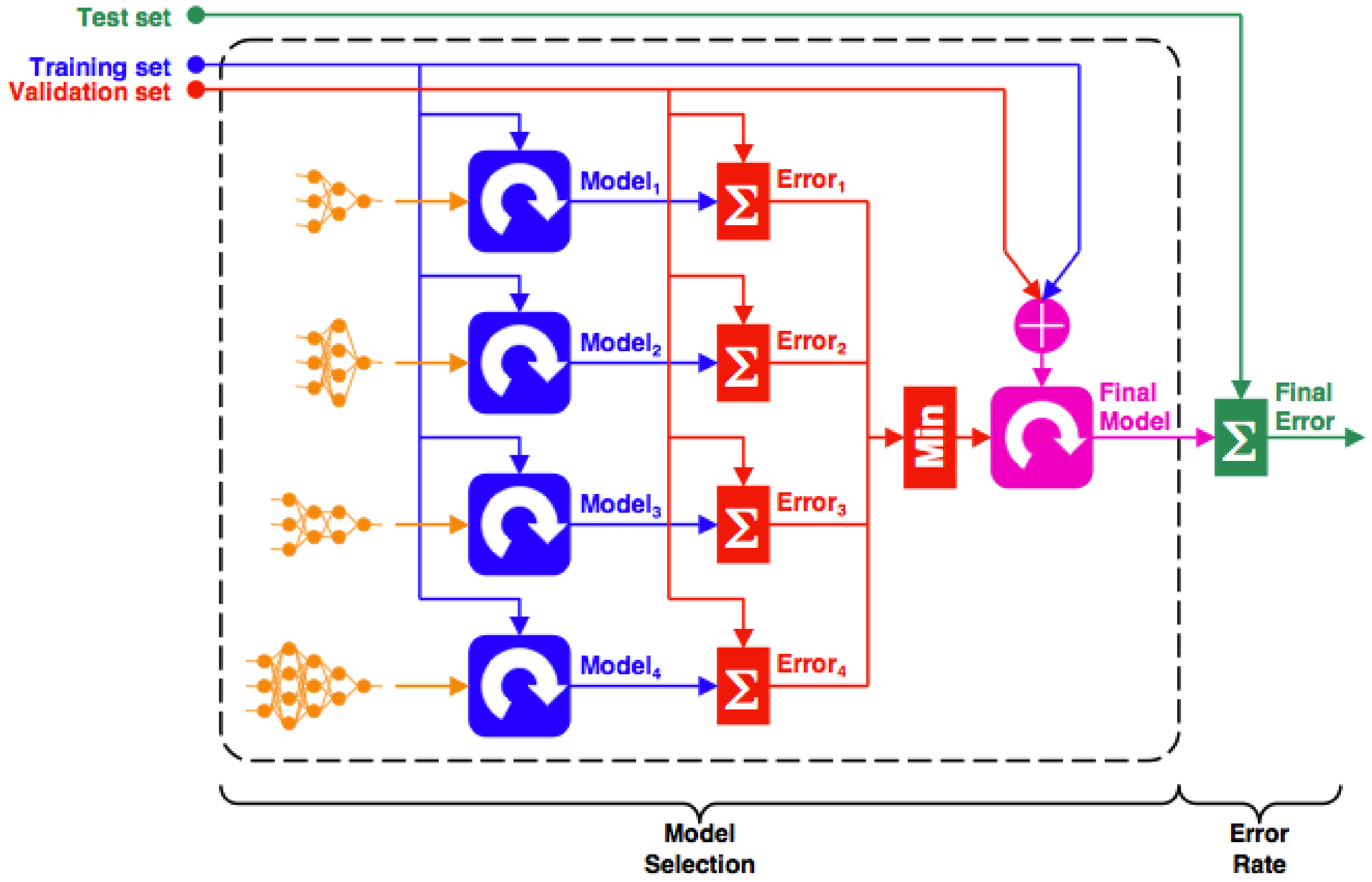


Training/Validation/Testing Sets

- 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

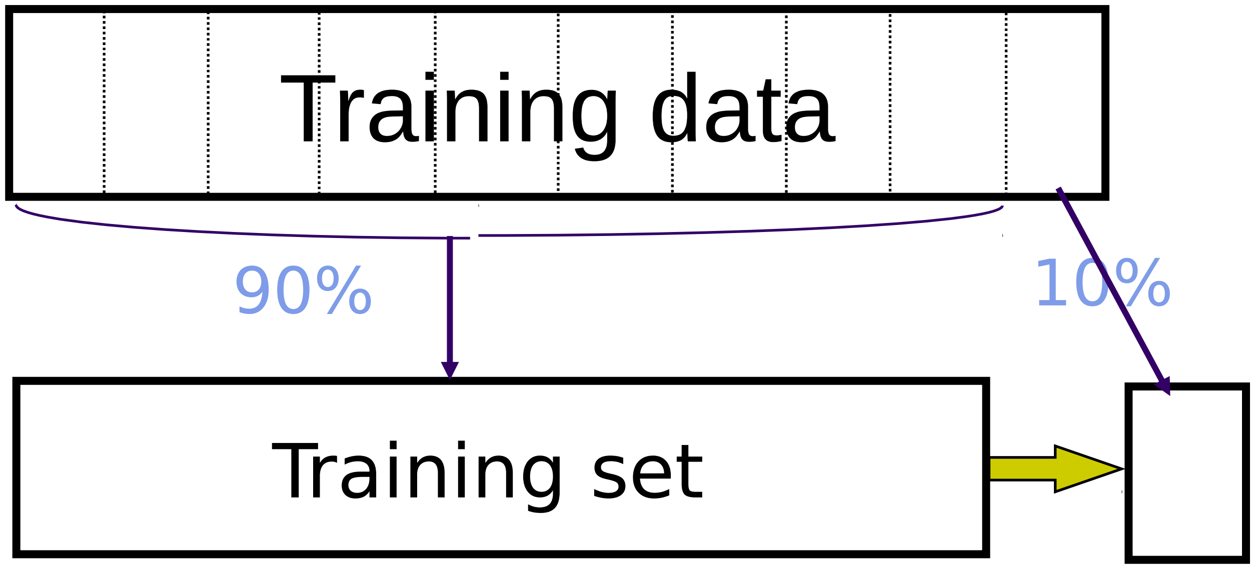


•Taken from Ricardo Gutierrez-Osuna's slides: http://courses.cs.tamu.edu/rgutier/ceg499_s02/l13.pdf

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

- Sometimes needed for too 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!**

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)**.

Weight Update

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

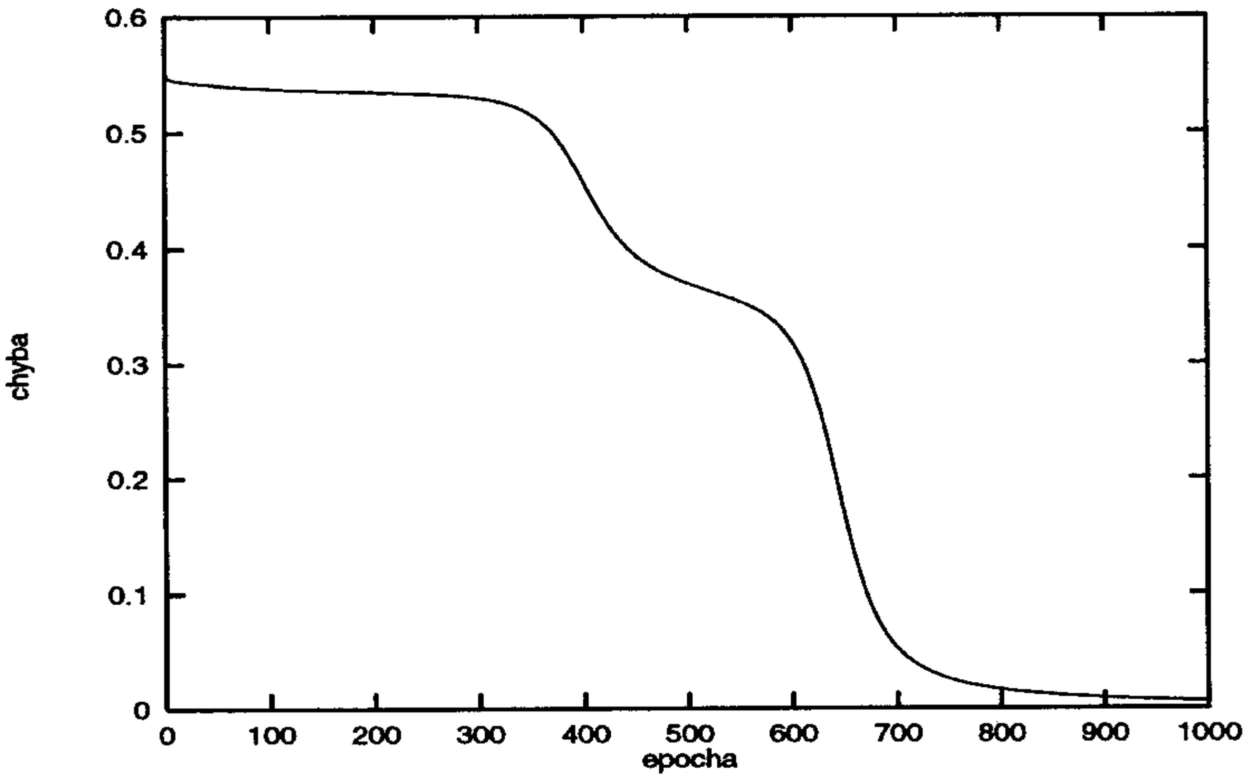
$$\Delta w_{jk} = -\eta \frac{\partial E}{\partial w_{jk}}$$

weight "delta"

learning rate

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

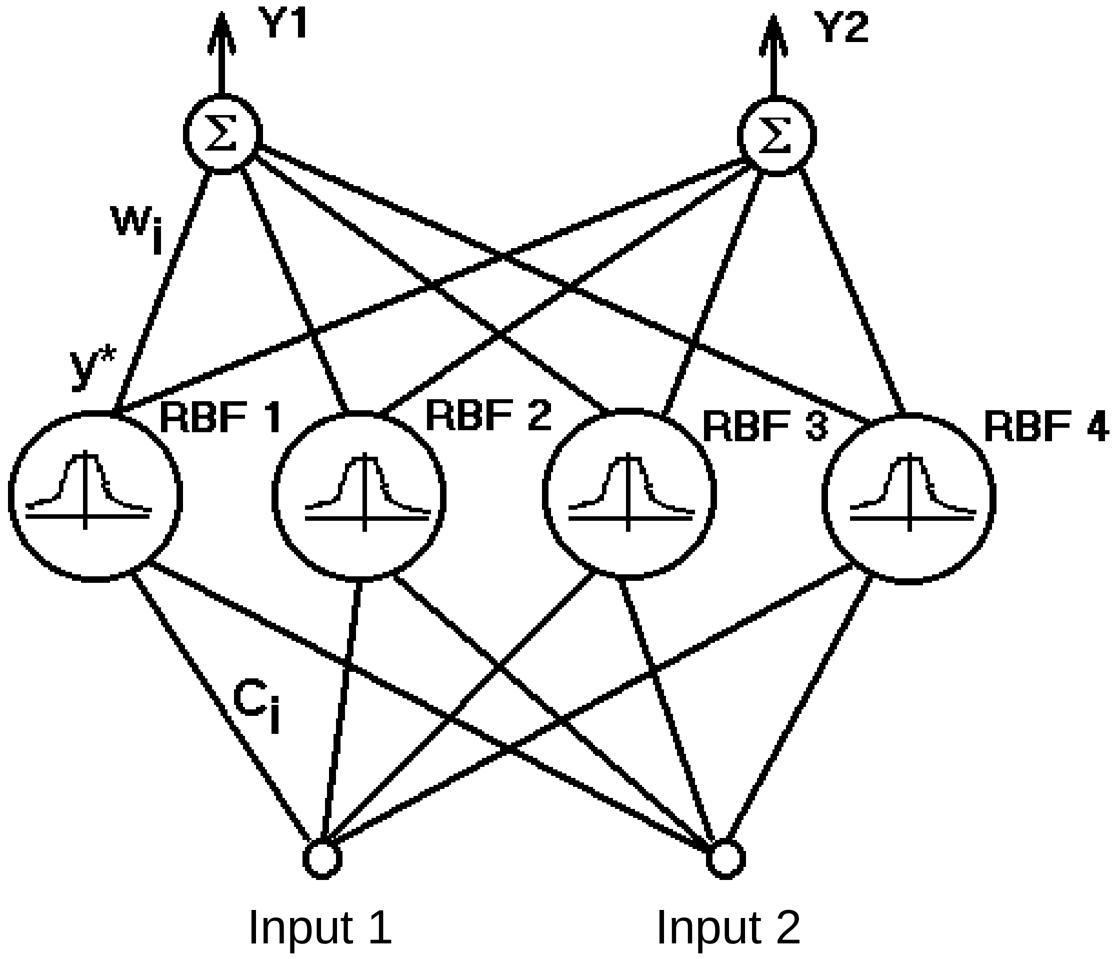
Typical Energy Behaviour During Learning



Radial Basis Function (RBF) Networks

- Two layers, different types of neurons in each layer.
- Feed-forward.
- Supervised Learning.
- Broomhead, Lowe (1988).
- Universal approximator.

RBF Architecture



RBF Neurons

- **Hidden layer:**
  - inner potential $$\phi = \sqrt{\sum_{i=1}^{n} (x_i - c_i)^2}$$
  - non-linear activation function

$$y^* = f(\Phi)$$

- **Output layer:**
  - linear perceptron

$$y = \sum_{i=1}^{n} w_i \, y_i^*$$

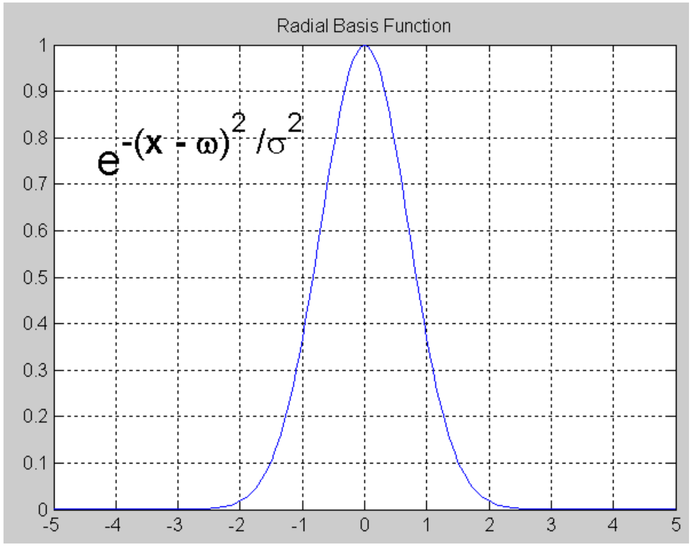
Typical RBF Activation Functions

$y^* = \varphi$

$y^* = \varphi^2 \log \varphi$

$y^* = (\varphi^2 + ß)^\alpha,\ ß \geq 0,\ 0 < \alpha < 1$

$$y^* = e^{-\frac{\varphi^2}{\sigma^2}}, \sigma > 0$$



Sphere of Influence

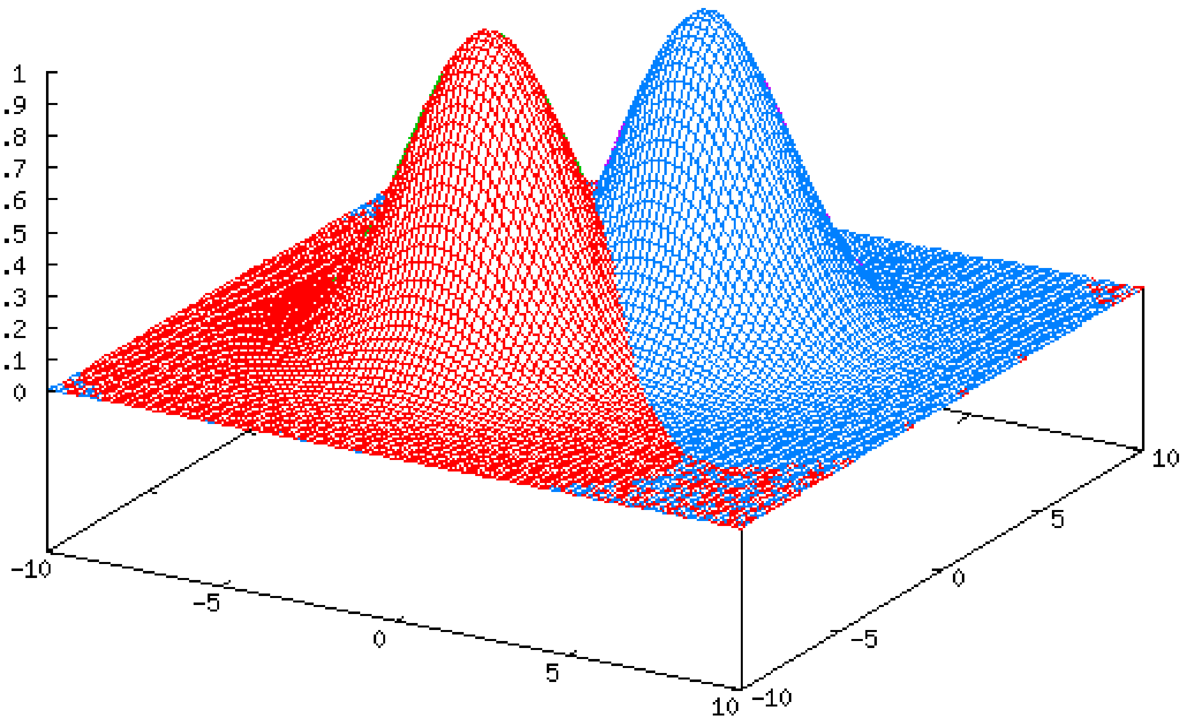
- Hypersphere with center *C* and radius *R*.
- Determined by euclidean metric.
- The center is called **the prototype**.

- The prototype represents a cluster of input data.

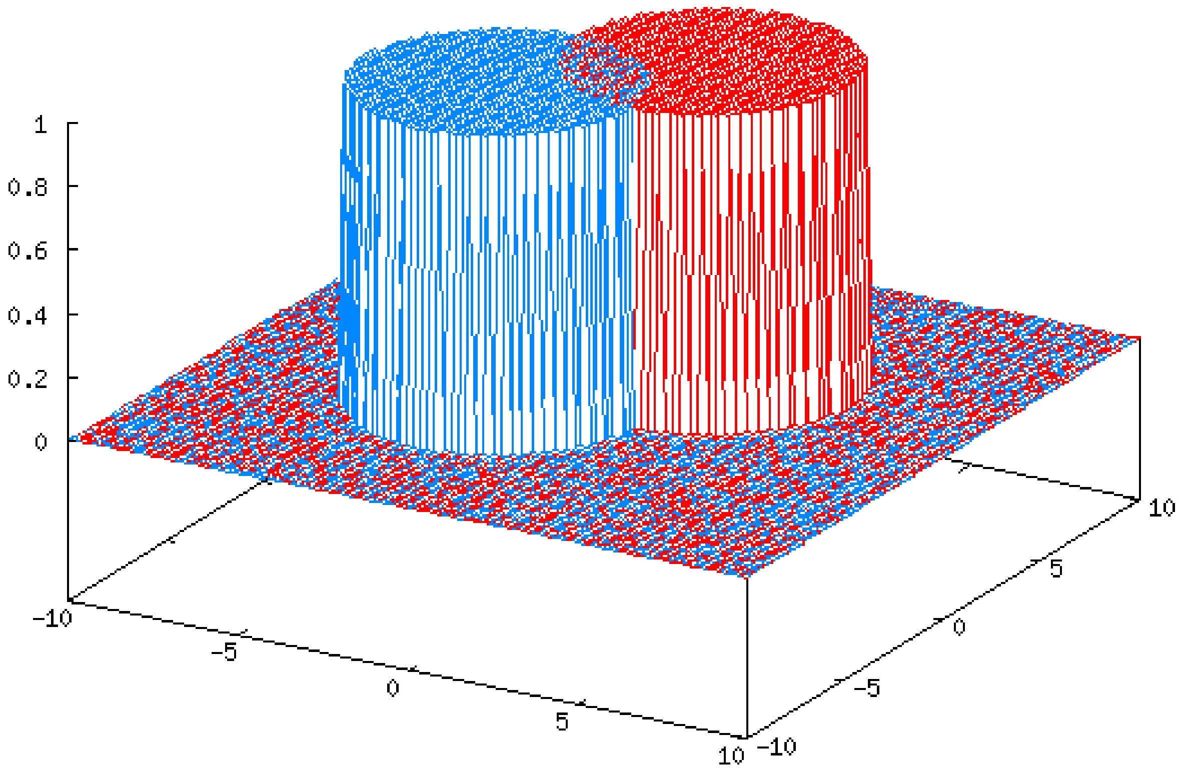
How to Determine the Sphere of Influence?

- Mostly we use Gauss function:
  - If an input vector has same weights as the prototype ($\varphi = 0$), the function gains maximum ($= 1$). This is also the maximum activation value of the neuron.
- With an increasing distance of input vector from the prototype the activity of neuron decreases.
- σ (which corresponds to a variance of normal distribution) determines a gain (width) of the activation function.
-

Sphere of Influence: Example



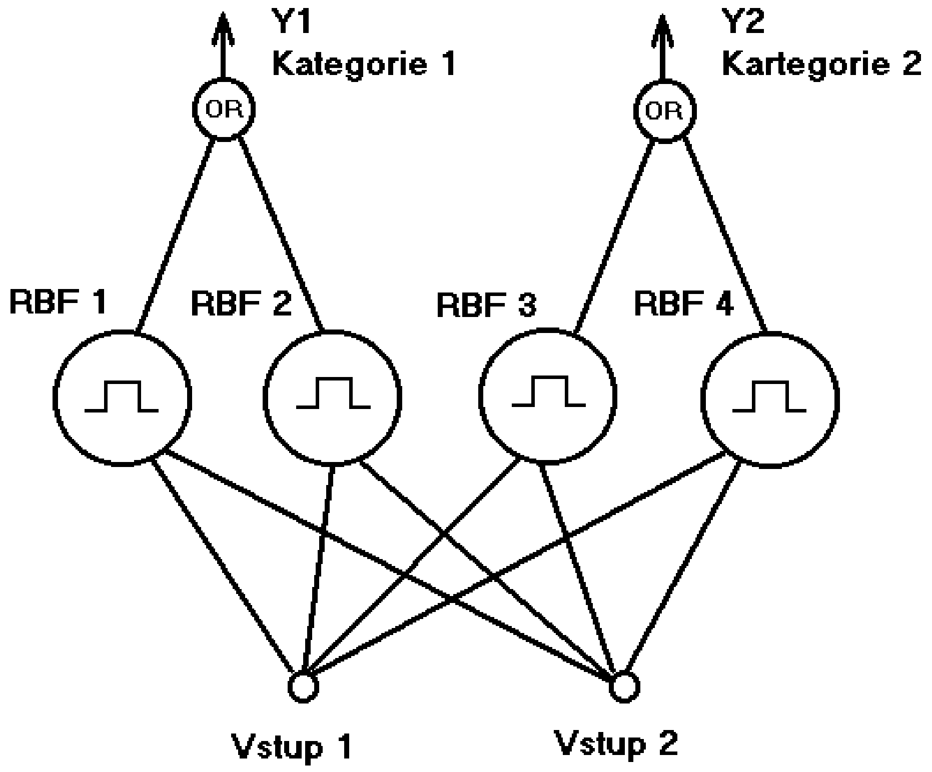
Sphere of Influence for Hardware Implementations

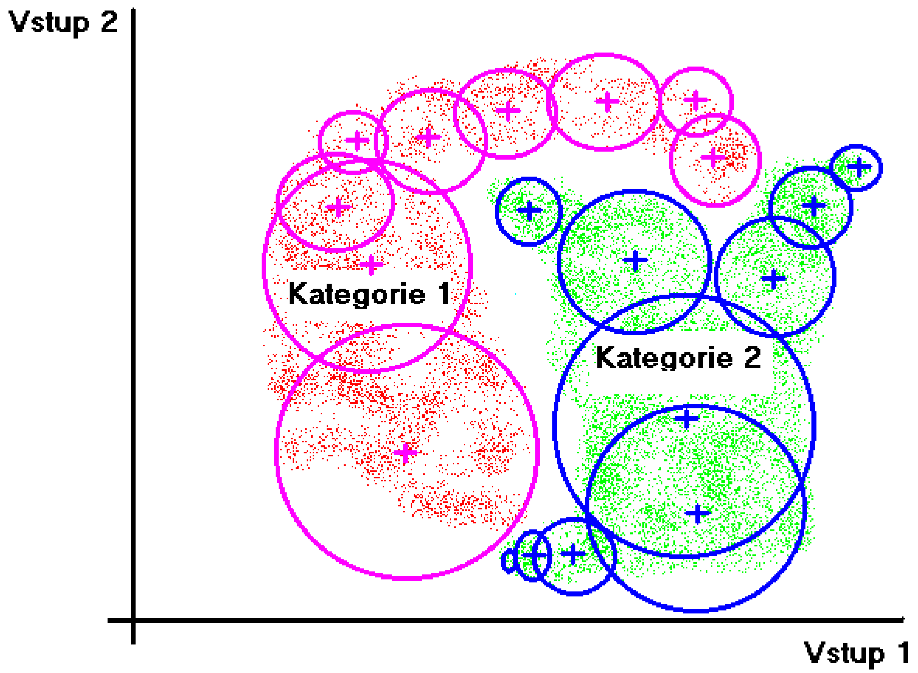


Neuron Types Discussion

- RBF neurons:
  - inner potential is a measure of distance between input vector and the prototype (represented by the weights),
  - activation function delimits the sphere of influence.
- Output neurons:
  - accumulate RBF neurons' outputs to achieve accurate approximation, OR
  - perform union of sets for classification.

RBF as a Classifier



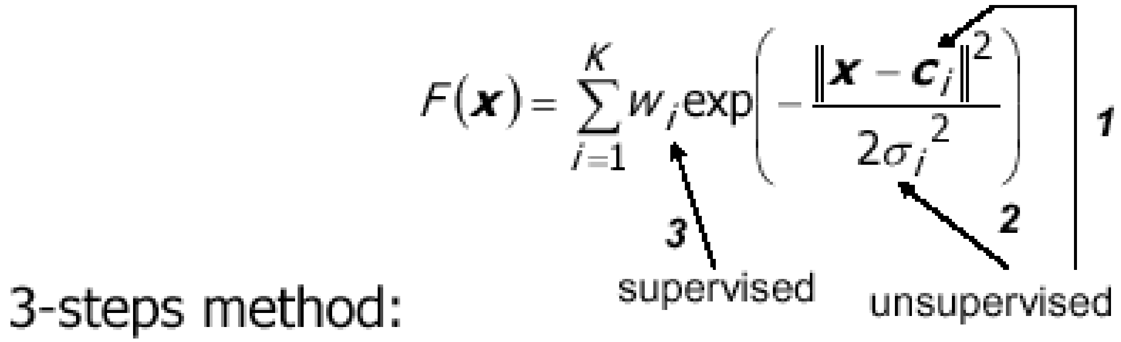


Application Areas

- Same as MLPs.
- Universal approximator (1991: Park, Sandberg).

Training RBF Networks

- Two phases:
  - training prototypes,
  - training output neurons.
- Training prototypes:
  - Unsupervised: Cluster Analysis.
- Training output neurons:
  - Supervised.



$$F(\mathbf{x}) = \sum_{i=1}^{K} w_i \exp\left(-\frac{\|\mathbf{x}-\mathbf{c}_i\|^2}{2\sigma_i^2}\right)$$

Training Prototypes I

- Estimate the number of clusters in input data :(
- Define a *membership function* ***m(x)***:
  - determines whether an input pattern belongs to a certain cluster,
  - choose cluster by the closest prototype.
- Estimate coordinates of all vectors $\mathbf{C}_p$ which correspond to cluster centers:
  → we use a well-known K-means algorithm.

Training Prototypes II: K-means

- **Steps of K-means algorithm**:
  - randomly initialize centers $\boldsymbol{C_i}$ of RBF neurons,
  - *) evaluate ***m()*** for all input patterns,
  - determine a new center $\boldsymbol{C_k}$ as an average of all patterns which belong to cluster ***k*** according to ***m()***.
  - stop when ***m()*** does not change anymore, otherwise go to *)

Training Prototypes III

- There exists also an *adaptive version* of the previous algorithm:
  - reminds perceptron learning algorithms (i.e. delta rule),
  - moves a center closer to input vectors.

Training Prototypes IV: Adaptive K-means

- **Steps of adaptive K-means**:
  - randomly initialize centers $\boldsymbol{C_i}$,
  - *) take input pattern $\boldsymbol{X}$,
  - determine closest center $\boldsymbol{C_k}$ and change its coordinates according to:

    $$\bar{C}_k^{(t+1)} = \bar{C}_k^{t} + \eta\left(\bar{X}^{(t)} - \bar{C}_k^{t}\right)$$

    where η denotes adaptation rate, which decreases with successive iterations.
  - stop when $\eta = 0$ or after certain # of iterations. Otherwise continue with *).

Training Prototypes V: Estimate # of Clusters

- Start with zero number of clusters,
- *) take input pattern ***X***,
- Find the closest cluster ***k***, If the distance between ***C_k*** and ***X*** < some constant ***r***, modify:

$$\bar{C}_k^{(t+1)} = \bar{C}_k^t + \eta\left(\bar{X}^{(t)} - \bar{C}_k^t\right)$$

- If the distance > ***r***, create a new center with coordinates of ***X***:

$$\bar{C}_k^{t+1} = \bar{X}^{(t)}$$

stop when $\eta = 0$ or after certain # of iterations. Otherwise continue with *).

- How to choose ***r*** ?

Training Prototypes V: Determine σ

- Parameter σ is determined by a root mean squared error (RMSE) of distance between patterns and cluster center:

$$\sigma_k = \sqrt{\frac{1}{Q} \sum_{q=1}^{Q} \| \bar{C}_k - \bar{X}_q \|^2}$$

- where $\boldsymbol{X_q}$ is *q*-th pattern which belongs to cluster with center $\boldsymbol{C_k}$.

Other approach uses fixed σ.

Training Output Neurons

- Find weights by minimization of this energy function:

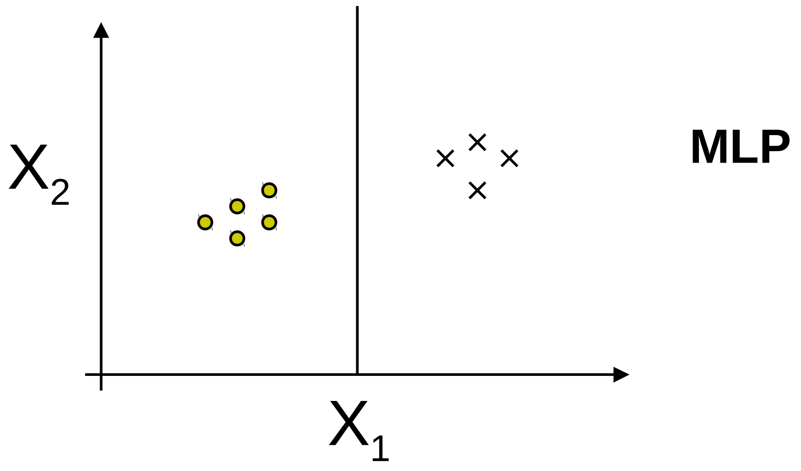
$$\Delta \bar{w}^{(t)} = -\eta \nabla E^{(t)} = \eta \left(D^{(t)} - Y^{(t)} \right) Y^{*(t)}$$

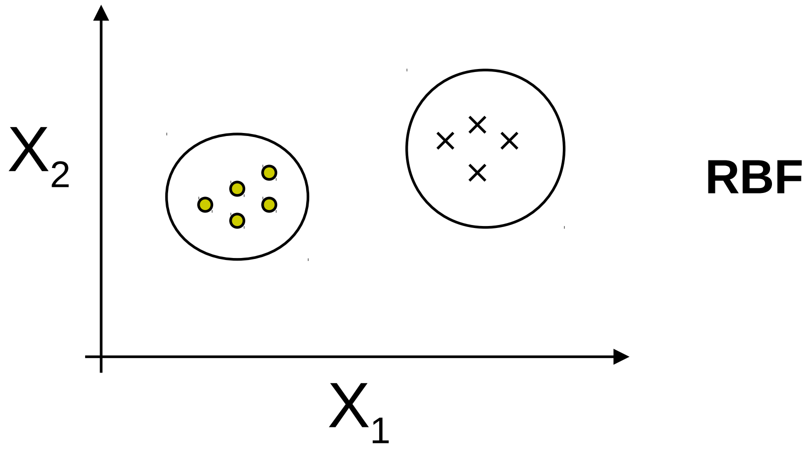
- Is it familiar?

$$E = \frac{1}{2} \sum_{t=1}^{m} \sum_{i=1}^{n} \left(d_i^{(t)} - y_i^{(t)} \right)^2$$

MLP vs. RBF

- **Learning**
  - RBF learns faster.
- **Applications**
  - MLP/RBF usable for regression & classification
- **Properties**
  - both are universal approximators.
- **As classifiers:**
  - MLPs - hyperplanes,
  - RBFs - hyperspheres.

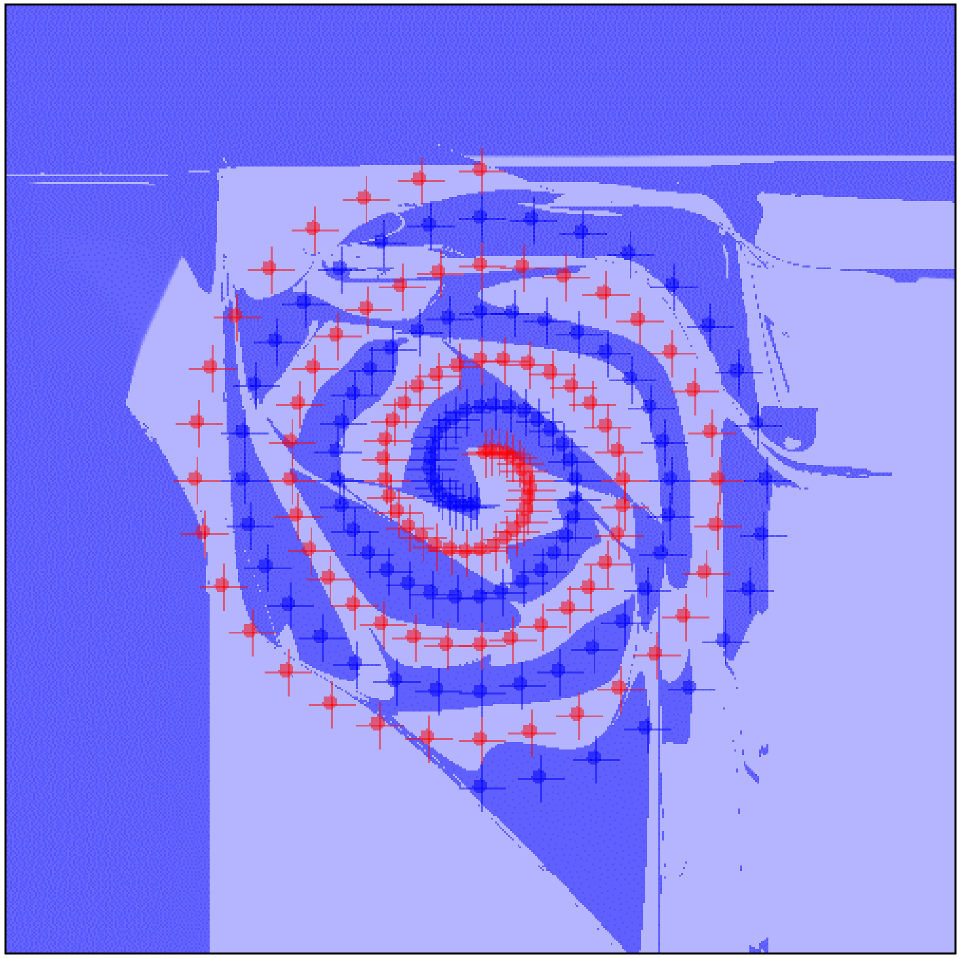




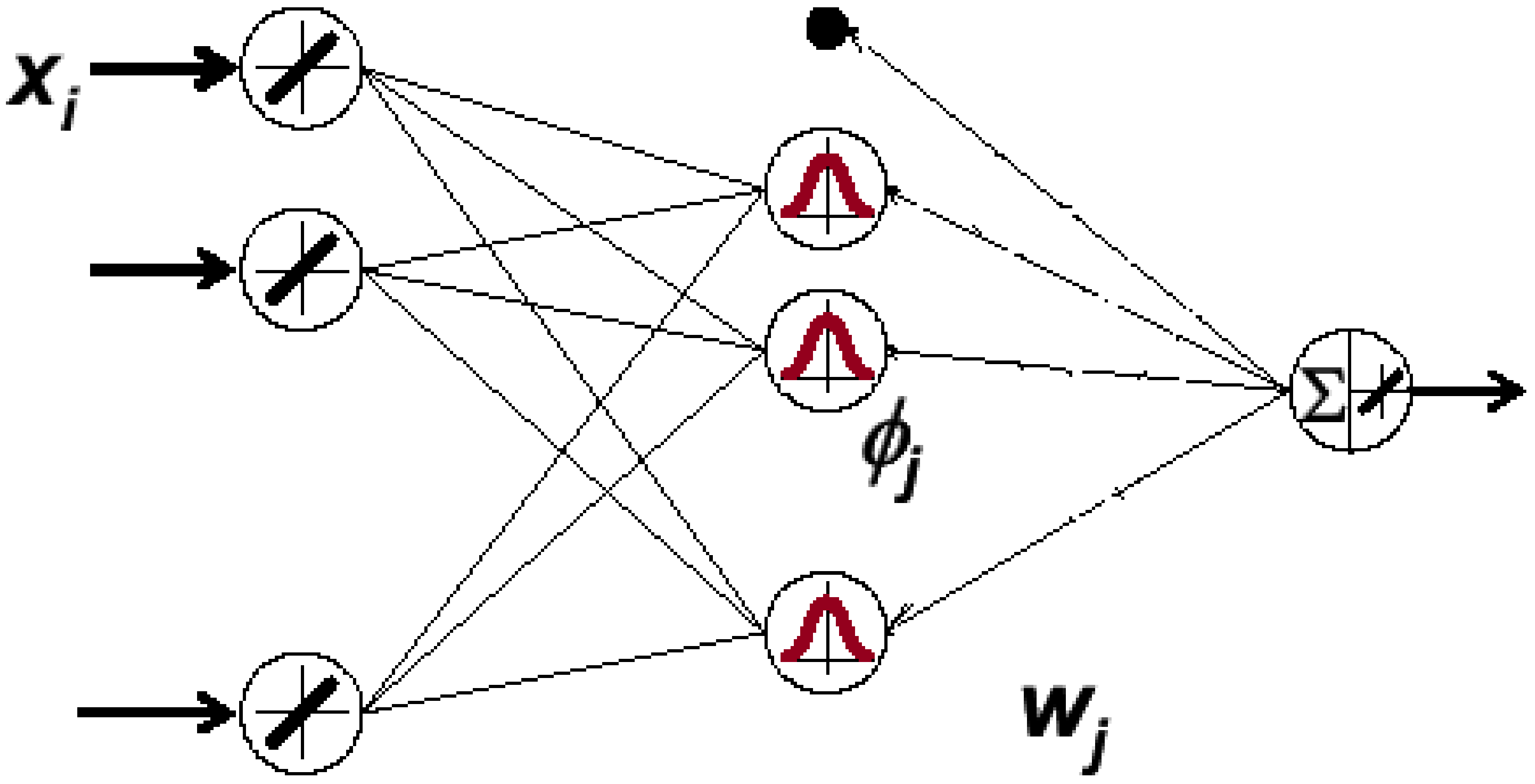
The Spiral problem

One of the most challenging artificial benchmarks: separate two inter-winded spirals.

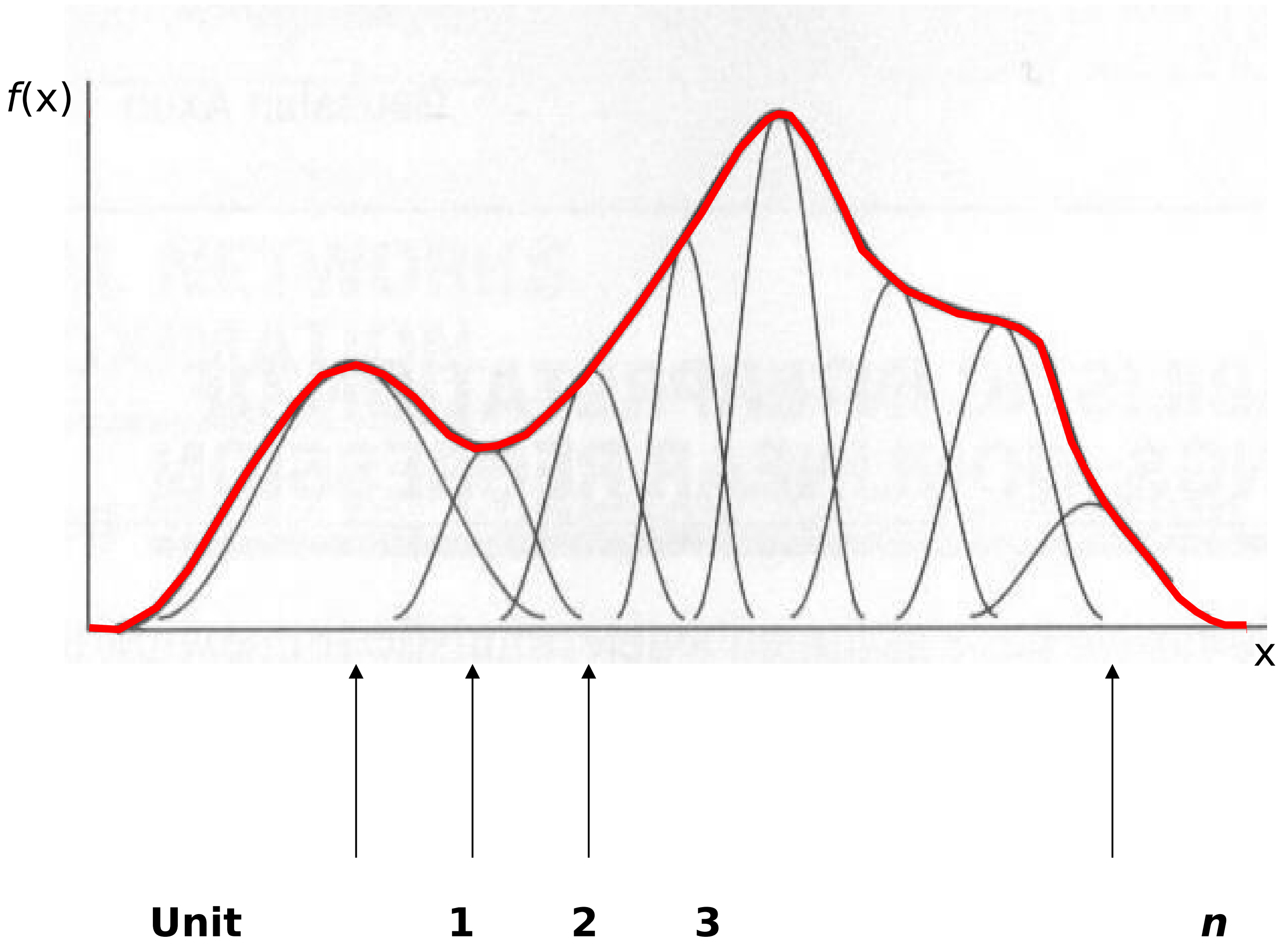
How can MLP solve it?
How about RBF?



RBF for Approximation



Approximation by RBF: Example



GMDH

- **G**roup **M**ethod of **D**ata **H**andling.
- By A.G. Ivakhnenko, 1968.
- Network is constructed by **induction**.
- Multiple layers.
- Feed-forward.
- Supervised.
- See http://www.gmdh.net ...

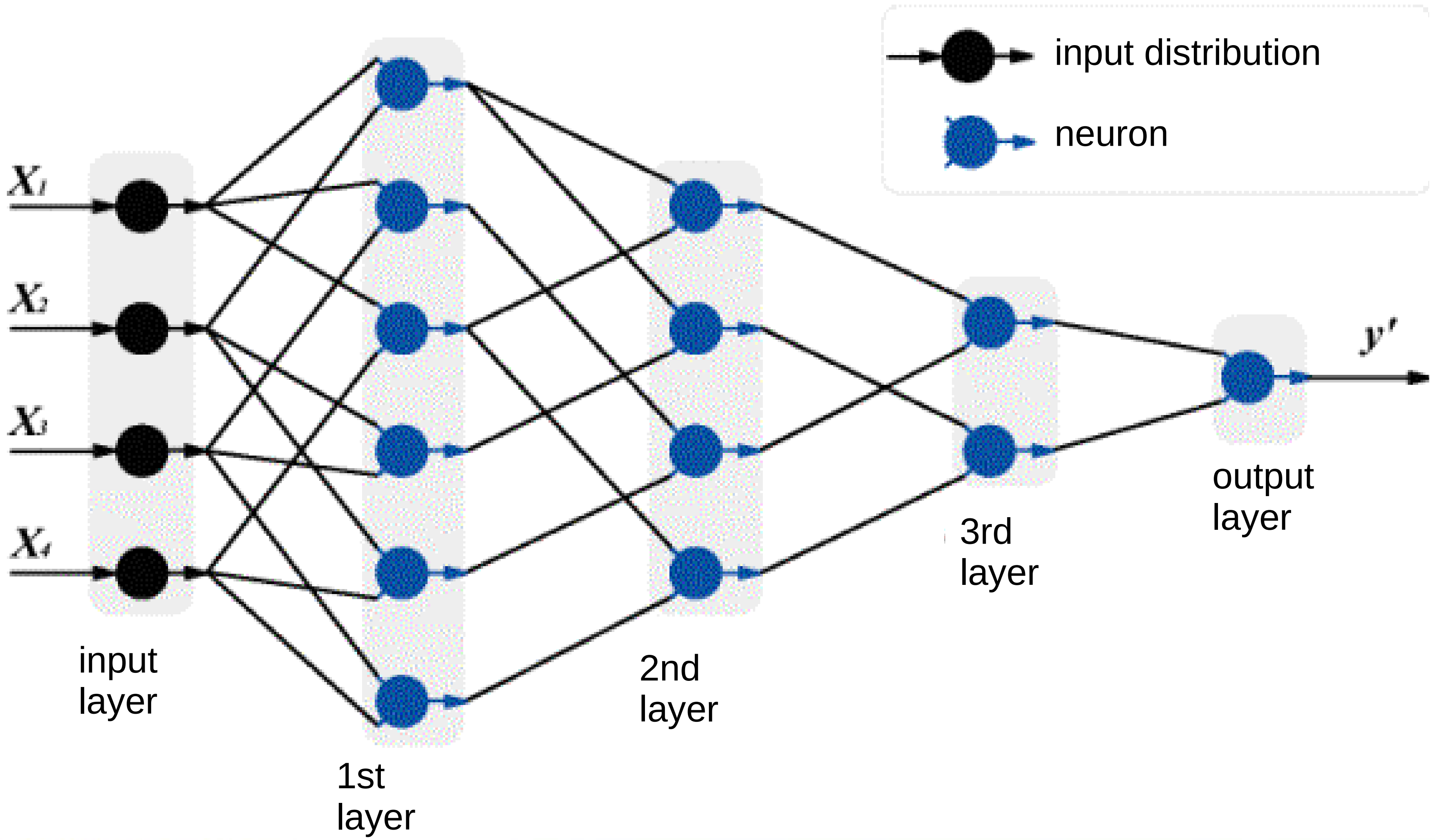
Induction vs. Deduction

- There are two approaches to create a model of a system:
  - **data-driven**: based on observations of a real system. The task is to infer general rule from specific cases → this the way GMDH model is built → **induction**,
  - **theory-driven**: based on theoretical knowledge of system functionality → the way to create mathematical models → **deduction**.

GMDH Types

- Parametric
  - parameters are set during training,
  - MIA (Multilayer Iterative Algorithm) → partial induction
  - COMBI (Combinatorial Algorithm) → full induction
- Other variants are non-parametric.

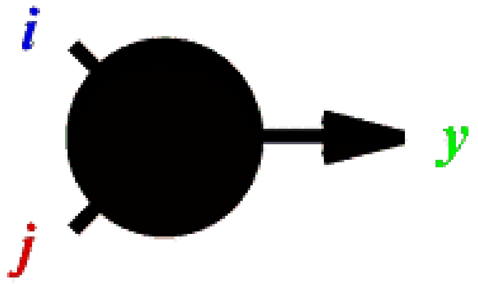
GMDH MIA Architecture



Remarks

- The structure (topology) of this network forms itself during learning process.
- # of neurons and even # of hidden layers changes during learning,
  → network self-organizes (but in a different way than SOM)

GMDH MIA Neuron



$$y = ai^2 + bij + cj^2 + di + ej + f$$

Ivakhnenko's polynomial.

Example of other Ivakhnenko's polynomials:

$$y = a + bi + cj \ ,$$
$$y = ai + bjk \ .$$

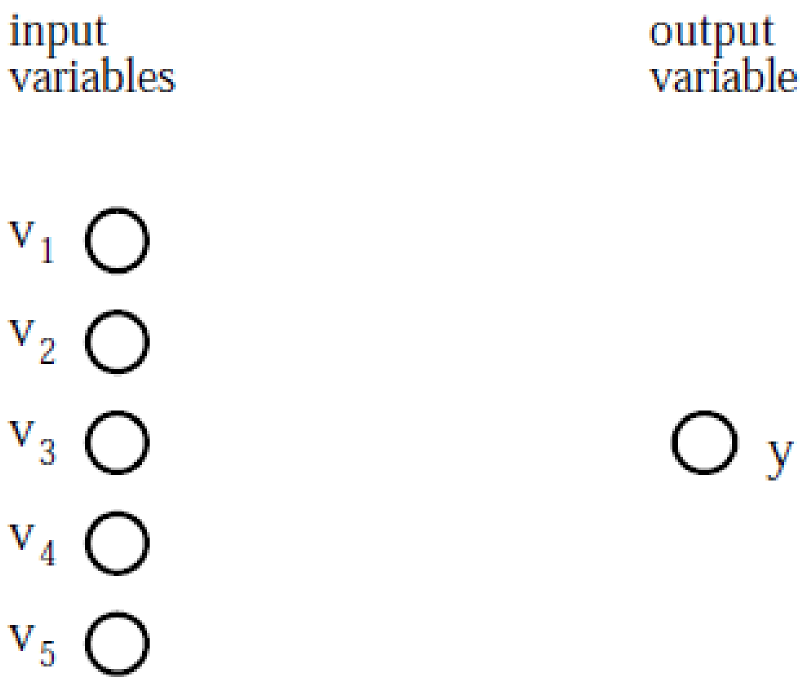
MIA Characteristics

- MIA network uses supervised learning.
- MIA uses single type of neurons (unlike other GMDH variants).
- Training:
    - network is built layer by layer,
    - layers are added until some error criterion is met.
- Network evaluation is simple:
    - feed-forward, only single output.

MIA Training

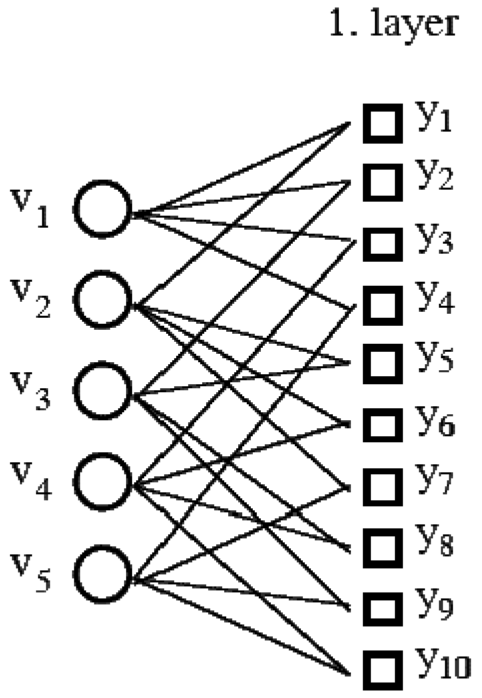
- **Configure k-th layer** (*k* denotes actual layer)
  - create new neurons in the layer,
  - compute all six coefficients of polynomial.
- **Selection of neurons in k-th layer**
  - elimination of unsuccessful neurons.
- Repeat or **finish training.**

MIA Training II



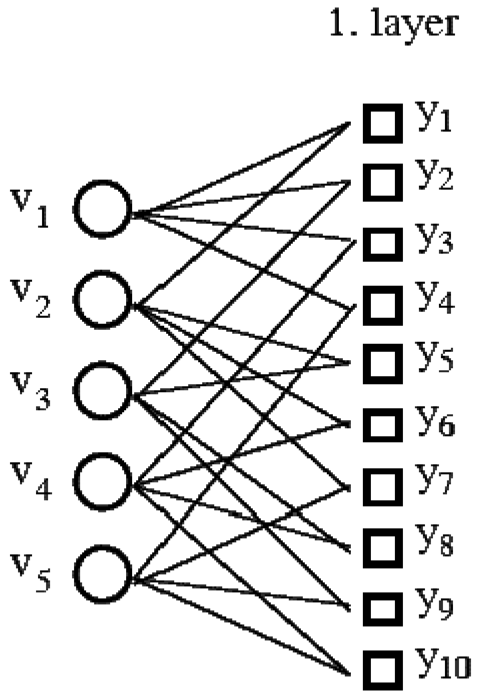
Lemke,Müller:SELF-ORGANIZING DATA MINING BASED ON GMDH PRINCIPLE

MIA Training III



- 1st layer creation:
- Active neurons with **optimized** transfer function $y_k=f_k(v_i,v_j)$.
- Two inputs only!
- They form “initial population”.
- How many neurons?

MIA Training III



- 1st layer creation:
- Active neurons with **optimized** transfer function $y_k = f_k(v_i, v_j)$.
- Two inputs only!
- They form "initial population".
- How many neurons?

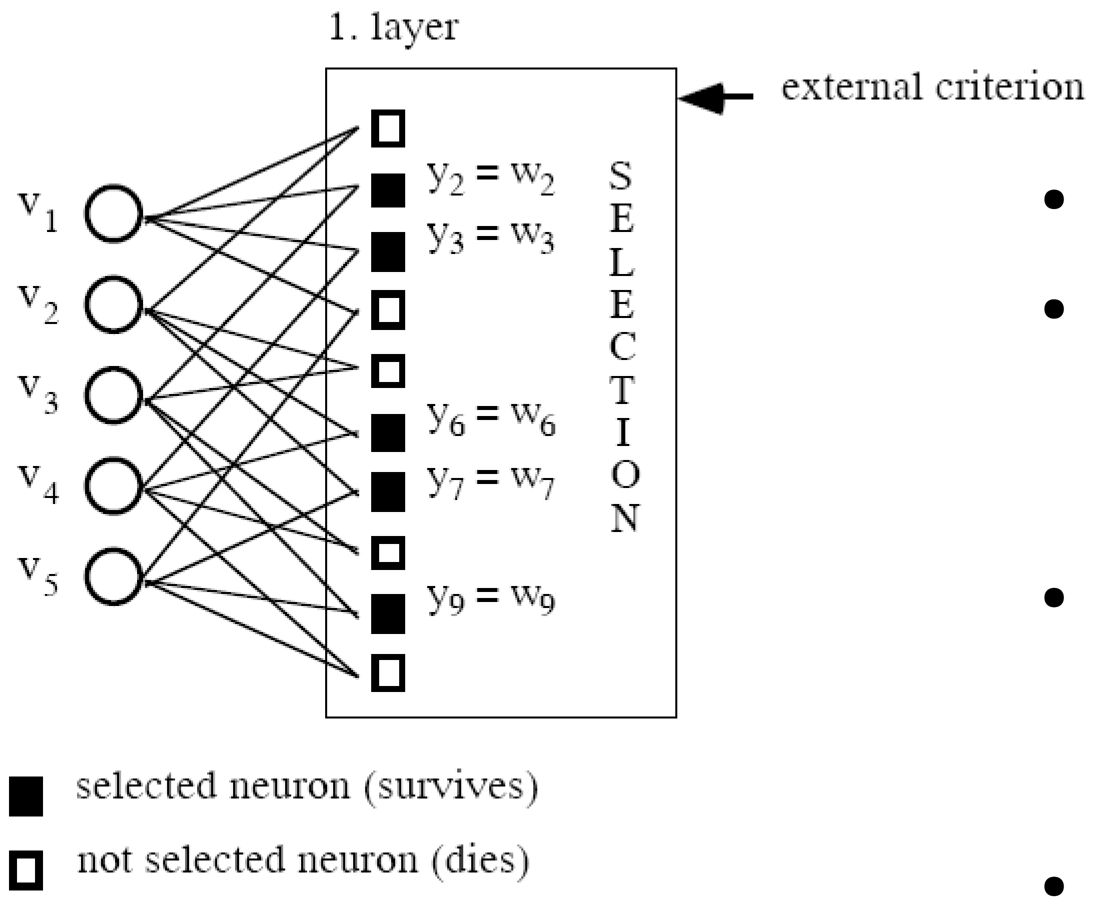
$$\binom{N}{2} = \frac{N(N-1)}{2}$$

MIA Training IV

- How to optimize neuron's coefficients?
  - Least Mean Squares (LMS),
  - we have to optimize six coefficients
    → choose 6 random input vectors
    → solve system of 6 linear equations

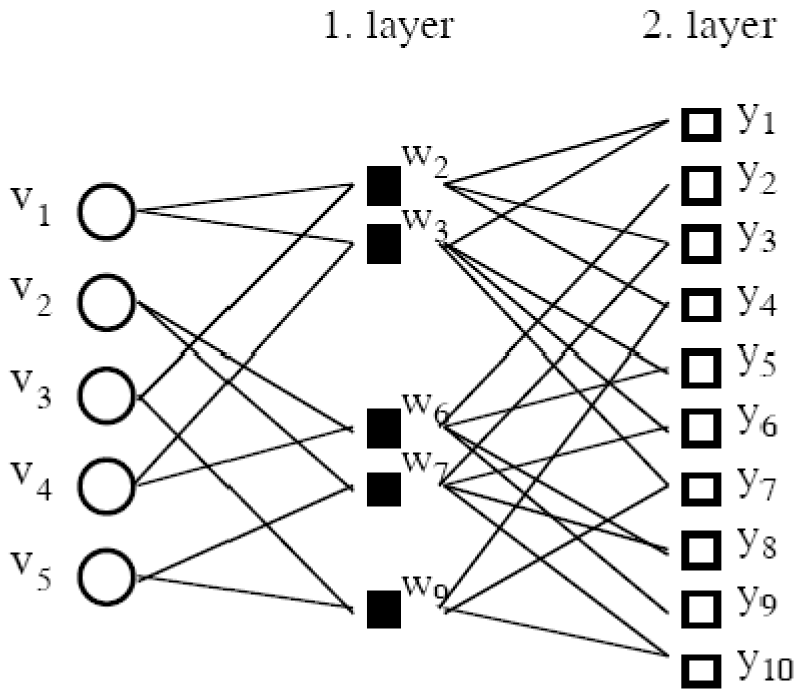
$$y = ai^2 + bij + cj^2 + di + ej + f$$

MIA Training V



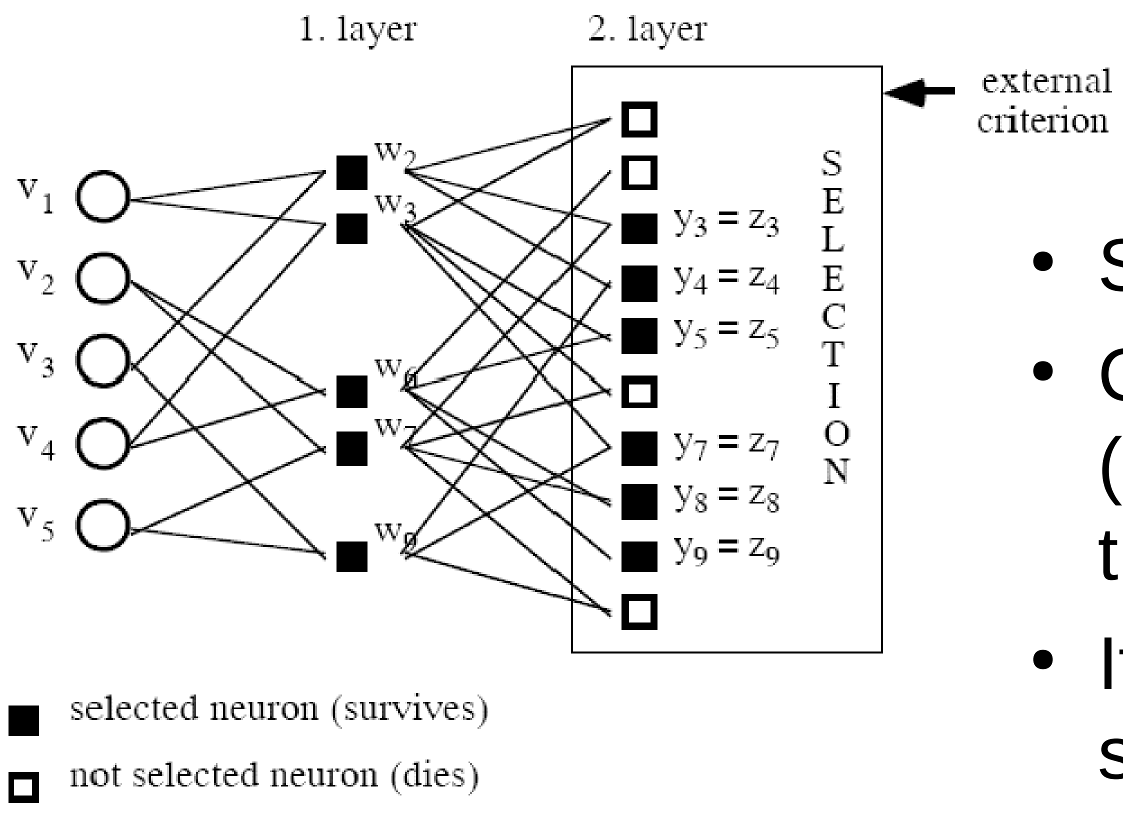
- Next step: Selection.
- According to a criterion (see later) some neurons survive, others not...
- If we are satisfied with the output (low error) → stop.
- Similar to evolutionary algorithms...

MIA Training VI



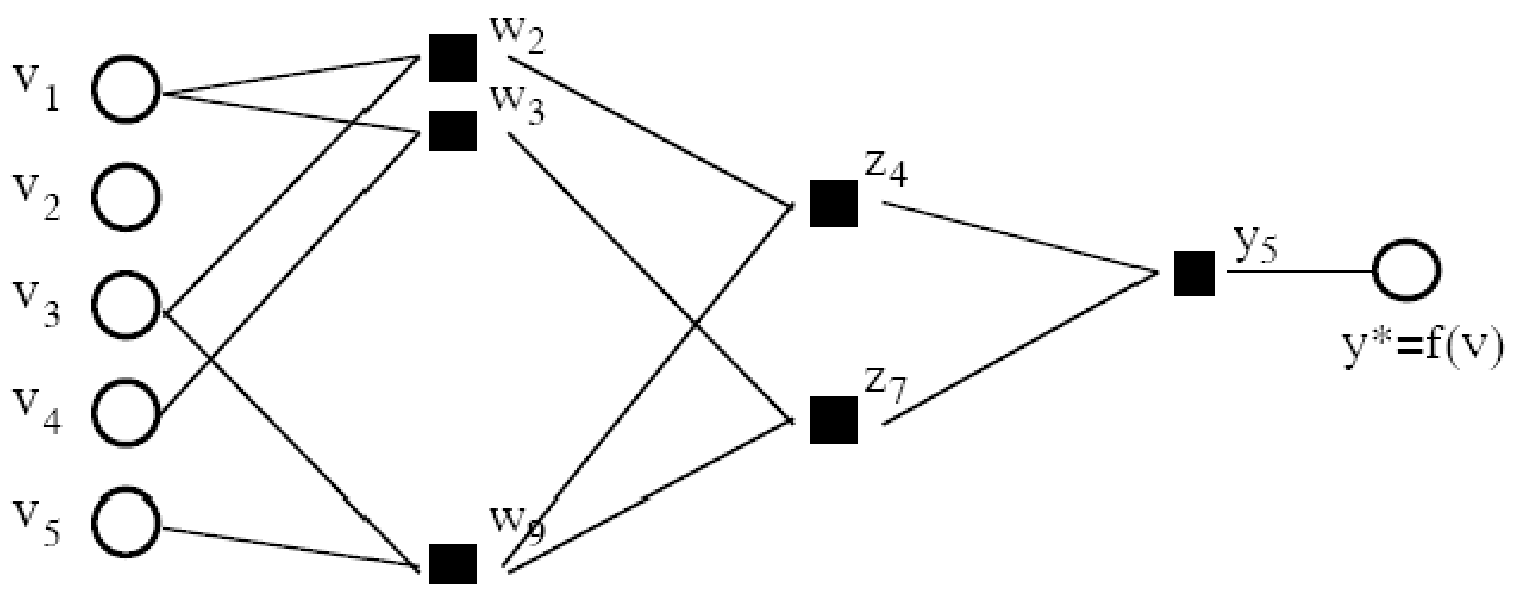
- 2nd layer:
- Again, initial population has to be created.
- Active neurons form the possible network output.
- Next step?

MIA Training VII



- Selection again.
- Competing neurons (survive and die) are of the same complexity.
- If we are still not satisfied with them → next layer is created.

MIA Training VII

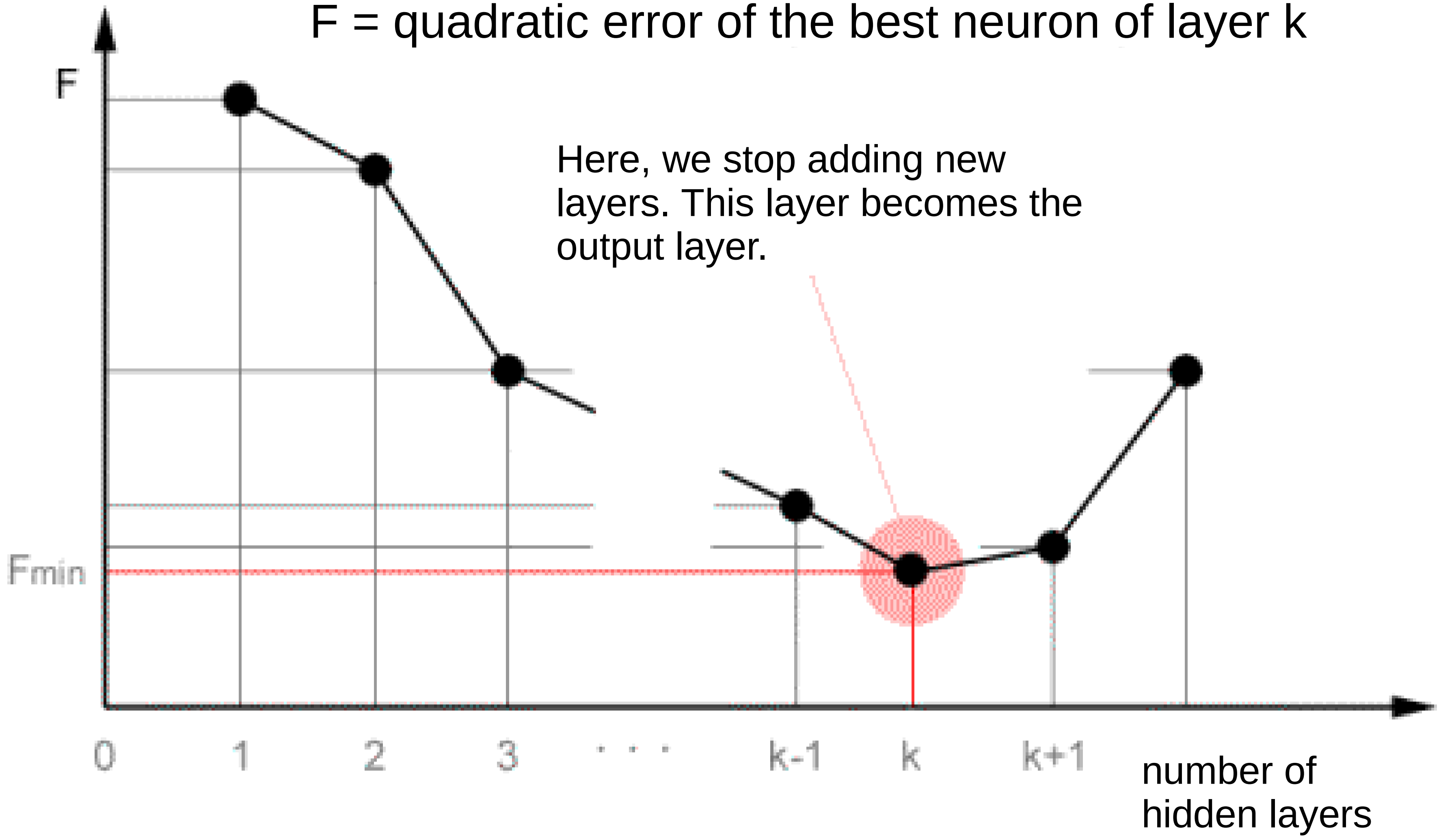


explicit analytically available optimal complex model.

network status:
order of regression model y*: ≤ 8
number of variables v in model y*: 4 (from initially 5 variables)

When to End Training?

F = quadratic error of the best neuron of layer k



Possibilities to Determine Fmin :)

$\frac{N}{N-p} s_e^2$ $s_{e,p}^2$

$s_e^2 + s_y^2 \ln N \frac{p}{N}$ *Schwarz*

Regularity criterion

$$AB = \frac{1}{N_B} \sum_{i=1}^{N_B} \left[y_i - \hat{y}_i(A) \right]^2 \to \min.$$

$\frac{N+p}{N-p} s_e^2$ *FPE*

$N \ln s_e^2 + p \ln N$ *Rissanen*

Discrimination criterion

$$\delta^2 = \frac{\sum_{i=1}^{N} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{N} (y_i - \bar{y})^2} < 1.0$$

$s_e^2 + 2\sigma_p^2 \frac{p}{N}$ *PSE*

$\frac{2ps_e^2}{N-p} - Ns_{y^m}^2$ *Kocerka*

$\frac{Ns_e^2}{\sigma_c^2} + 2p - N$ *Mallow C_p*

$\frac{\sum_{t=1}^{N} (\bar{y}_t^m - y_t)^2}{\sum_{t=1}^{N} y_t^2}$ *$i^2(N)$*

Validation criterion

$$R_{ij} = 1 - \sqrt{\frac{\frac{1}{N-P_i} \sum_{t=1}^{N} (y_t - y_t^i)^2}{\frac{1}{N-P_j} \sum_{t=1}^{N} (y_t - y_t^j)^2}}$$

$N \ln s_e^2 + 2p + c$ *AIC*

$N \ln s_{e,p}^2 + p \ln \left(\frac{s_{y^m}^2}{s_{e,p}^2} \quad \frac{N}{p} \right)$ *BIC*

$$\frac{s_e^2}{\left[1 - \lambda \sqrt{\frac{k(\ln(\frac{N}{k}) + 1) - \ln\alpha}{N}} \quad \left(1 - \frac{1}{4} \quad \frac{\ln(\frac{N}{k}) + 1) - \ln\alpha}{N} \right) \right]}$$ *Vapnik*

$$s_e^2 = \frac{1}{N} \sum_{t=1}^{N} (y_t - y_t^m)^2 = \frac{1}{N} \sum_{t=1}^{N} e_t^2; \quad s_y^2 = \frac{1}{N} \sum_{t=1}^{N} (y_t - \bar{y})^2; \quad s_{y^m}^2 = \frac{1}{N} \sum_{t=1}^{N} (y_t^m)^2$$

Most Common

Regularity Criterion:

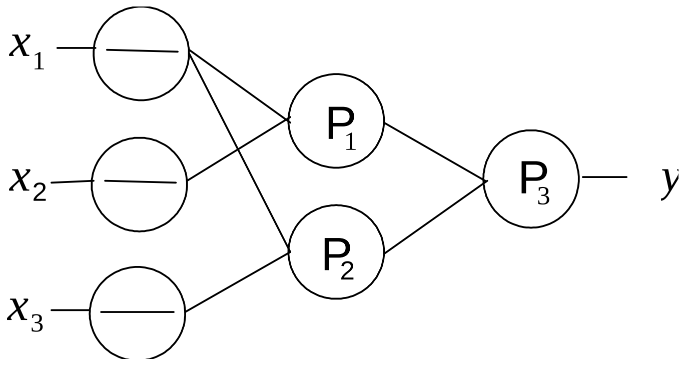
$$AB = \frac{1}{N_B} \sum_{i=1}^{N_B} \left[y_i - \hat{y}_i(A) \right]^2 \rightarrow \min.$$

$\hat{y}_i(A)$ … neuron‘s output trained on the A-subset.

Neurons are then ordered according to their error on validation data B-subset.

GMDH $\rightarrow$ Mathematical Model

- Example:



P_i are linear

$$y = P_3\left(P_2(x_1, x_3), P_1(x_1, x_2)\right) = a_{31}(a_{11}x_1 + a_{12}x_3 + a_{13}) + a_{32}(a_{21}x_1 + a_{22}x_2 + a_{23}) + a_{33} =$$
$$(a_{31}a_{11} + a_{32}a_{21})x_1 + (a_{32}a_{22})x_2 + (a_{31}a_{21})x_3 + a_{31}a_{13} + a_{32}a_{23} + a_{33}$$

COMBI vs. MIA

- What's the difference between partial and full induction?
- COMBI uses supervised learning, too.
- COMBI employs different types of neurons, but:
  - same in a single layer,
  - “more complex” in following layers,
  - not connected to a previous layer, but to network inputs
  - always combine “the most fit”.

Notes

- The full induction network (COMBI) works with a full input space all the time.
- It tries to apply successively complex transformations.
- The partial induction network (MIA) applies only a single transformation to most promising input subspaces.
  → It is a heuristic which speeds up the algorithm.

Other Inductive Approaches

- Cascade Correlation:
  diploma thesis by Minh Duc Do:
  https://dip.felk.cvut.cz/browse/details.php?f=F3&d=K13136&y=2009&a=dom1&t=dipl
- NEAT and other TWEANNs (Topology and Weight Evolving Neural Networks)
  → we will see later...

Next Lecture

- Backpropagation & Deep Neural Networks