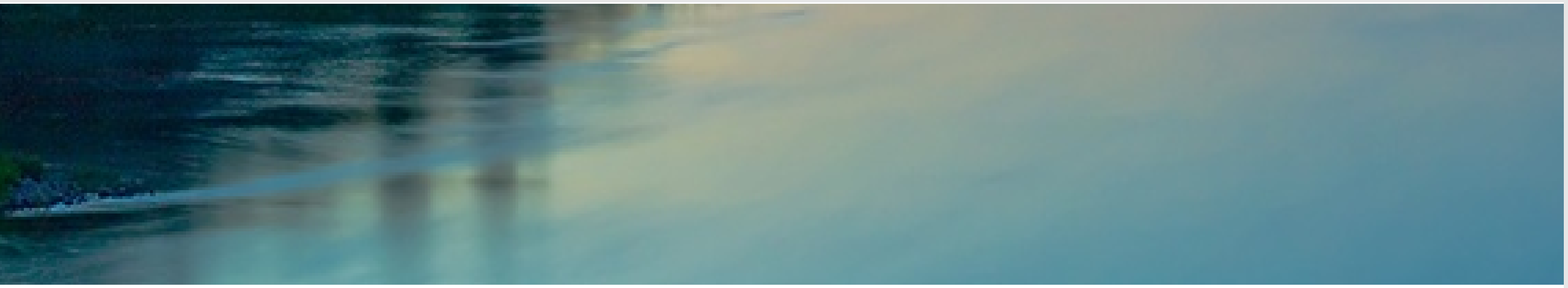

Neural Networks

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Radial Basis Function Networks

Radial Basis Funktion Networks

Properties of Radial Basis Funktion Networks (RBF-Networks)

- RBF-Networks are strictly layered feed-forward neural networks consisting of exactly 1 hidden layer.
- Radial Basis Functions are used for input and activation function.
- This way a “catchment area“ is assigned to every neuron.
- The weights of every connection between the input layer to a hidden neuron indicate the center of this „cathment area“.

Radial Basis Function Networks

A **radial basis function network (RBFN)** is a neural network with a graph $G = (U, C)$ that satisfies the following conditions

(i) $U_{\text{in}} \cap U_{\text{out}} = \emptyset$,

(ii) $C = (U_{\text{in}} \times U_{\text{hidden}}) \cup C', \quad C' \subseteq (U_{\text{hidden}} \times U_{\text{out}})$

The network input function of each hidden neuron is a **distance function** of the input vector and the weight vector, i.e.

$$\forall u \in U_{\text{hidden}} : \qquad f_{\text{net}}^{(u)}(\vec{w}_u, \vec{\text{in}}_u) = d(\vec{w}_u, \vec{\text{in}}_u),$$

where $d : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}_0^+$ is a function satisfying $\forall \vec{x}, \vec{y}, \vec{z} \in \mathbb{R}^n :$

$$\begin{aligned}
(i) \quad & d(\vec{x}, \vec{y}) = 0 \quad \Leftrightarrow \quad \vec{x} = \vec{y}, \\
(ii) \quad & d(\vec{x}, \vec{y}) = d(\vec{y}, \vec{x}) && \text{(symmetry)}, \\
(iii) \quad & d(\vec{x}, \vec{z}) \leq d(\vec{x}, \vec{y}) + d(\vec{y}, \vec{z}) && \text{(triangle inequality)}.
\end{aligned}$$

Distance Functions

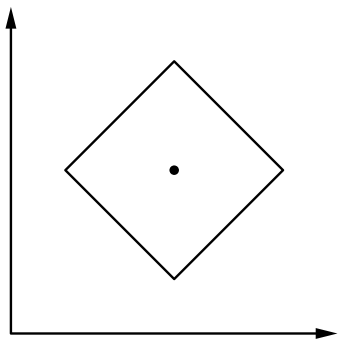
Illustration of distance functions

$$d_k(\vec{x}, \vec{y}) = \left(\sum_{i=1}^{n} (x_i - y_i)^k \right)^{\frac{1}{k}}$$

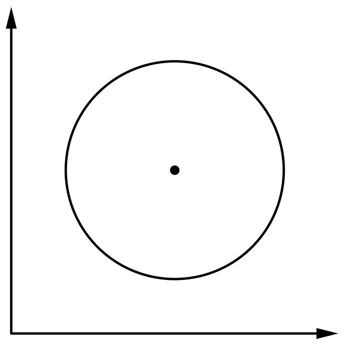
Well-known special cases from this family are:

$k = 1:$	Manhattan or city block distance,
$k = 2:$	Euclidean distance,
$k \to \infty:$	maximum distance, i.e. $d_\infty(\vec{x}, \vec{y}) = \max_{i=1}^{n} \lvert x_i - y_i \rvert$.

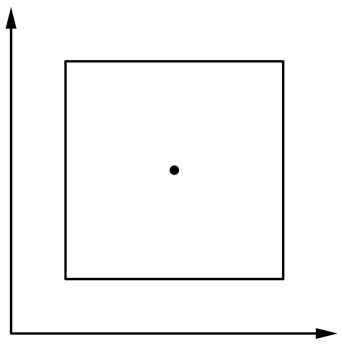
$k = 1$



$k = 2$



$k \to \infty$



Radial Basis Function Networks

The network input function of the output neurons is the weighted sum of their inputs, i.e.

$$\forall u \in U_{\text{out}}: \qquad f_{\text{net}}^{(u)}(\vec{w}_u, \vec{\text{in}}_u) = \vec{w}_u \vec{\text{in}}_u = \sum_{v \in \text{pred}\,(u)} w_{uv} \, \text{out}_v \,.$$

The activation function of each hidden neuron is a so-called **radial function**, i.e. a monotonously decreasing function

$$f : \mathbb{R}_0^+ \to [0,1] \quad \text{with} \quad f(0) = 1 \quad \text{and} \quad \lim_{x \to \infty} f(x) = 0.$$

The activation function of each output neuron is a linear function, namely

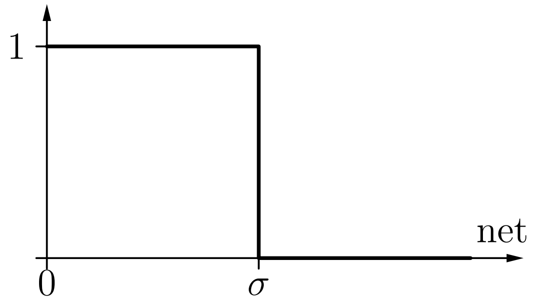
$$f_{\text{act}}^{(u)}(\text{net}_u, \theta_u) = \text{net}_u - \theta_u.$$

(The linear activation function is important for the initialization.)

Radial Activation Functions

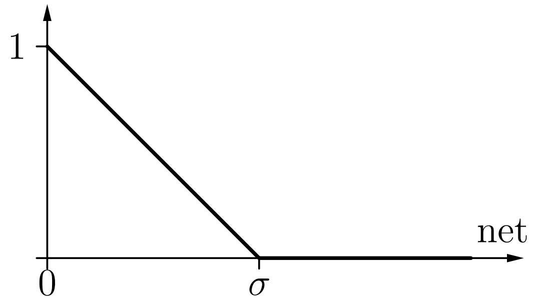
rectangle function:

$$f_{\text{act}}(\text{net}, \sigma) = \begin{cases} 0, & \text{if net} > \sigma, \\ 1, & \text{otherwise.} \end{cases}$$



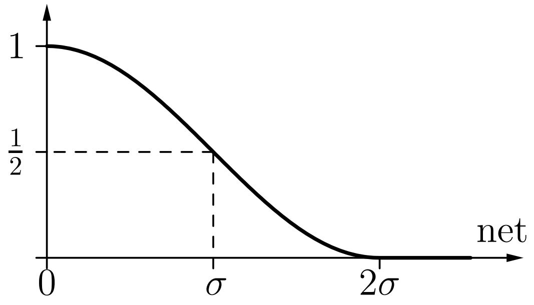
triangle function:

$$f_{\text{act}}(\text{net}, \sigma) = \begin{cases} 0, & \text{if net} > \sigma, \\ 1 - \frac{\text{net}}{\sigma}, & \text{otherwise.} \end{cases}$$



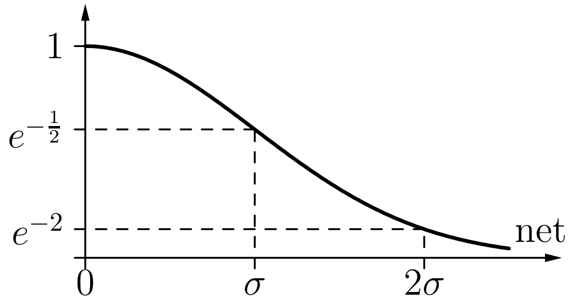
cosine until zero:

$$f_{\text{act}}(\text{net}, \sigma) = \begin{cases} 0, & \text{if net} > 2\sigma, \\ \frac{\cos\left(\frac{\pi}{2\sigma}\text{net}\right)+1}{2}, & \text{otherwise.} \end{cases}$$



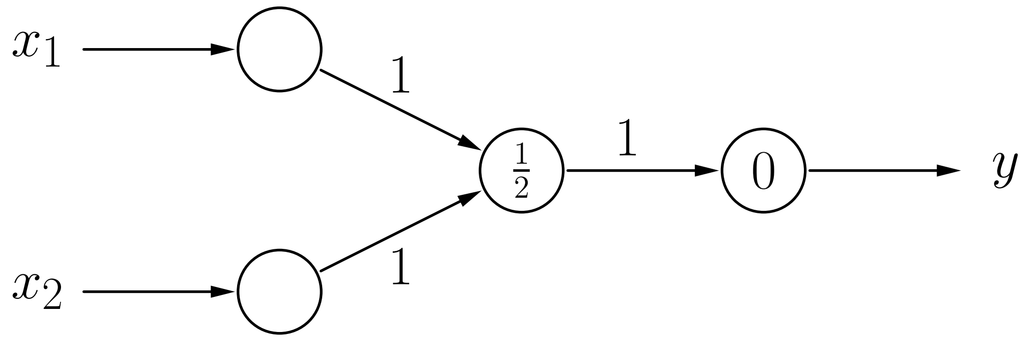
Gaussian function:

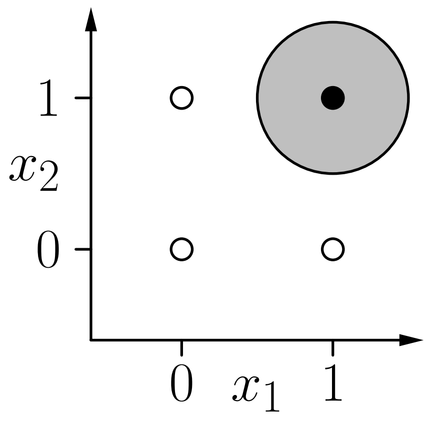
$$f_{\text{act}}(\text{net}, \sigma) = e^{-\frac{\text{net}^2}{2\sigma^2}}$$



Radial Basis Function Networks: Examples

Radial basis function networks for the conjunction $x_1 \wedge x_2$

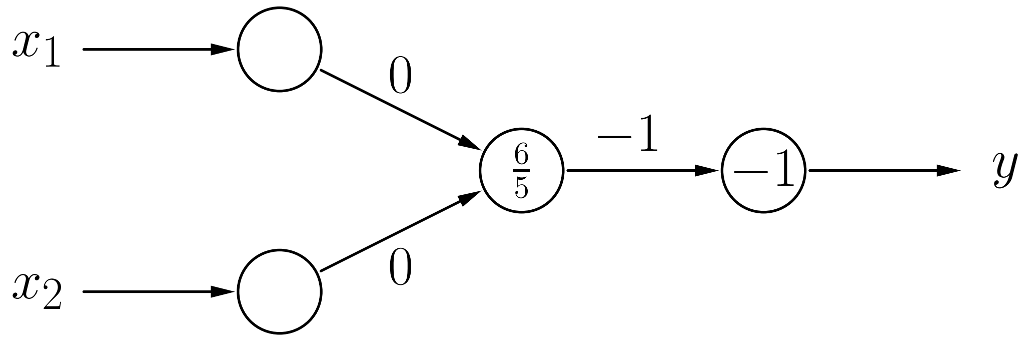


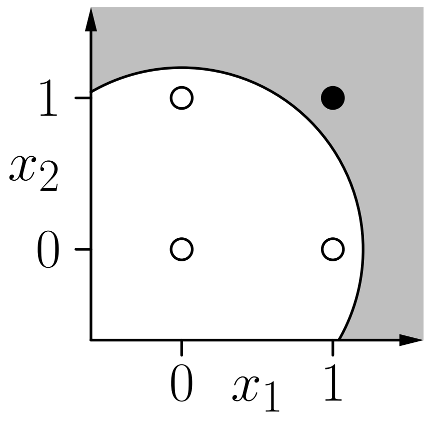


- (1,1) is the center
- $\frac{1}{2}$ is the reference radius
- Euclidean distance
- rectengular function as the activation function
- bias of 0 in the output neuron

Radial Basis Function Networks: Examples

Radial basis function networks for the conjunction $x_1 \wedge x_2$





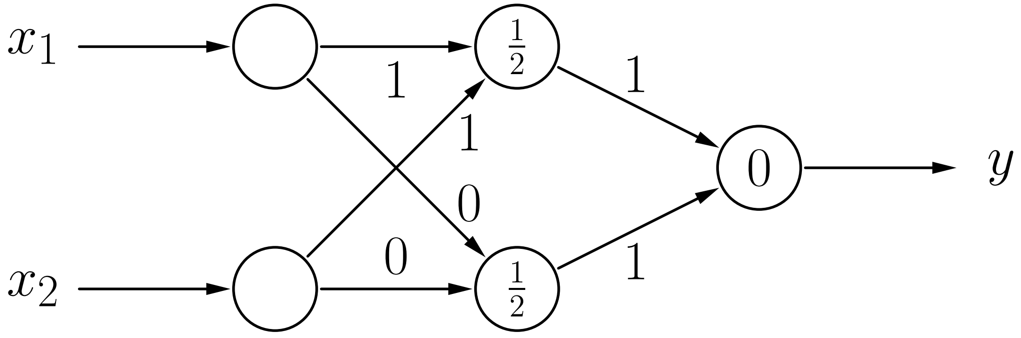
- (0,0) is the center
- $\frac{6}{5}$ is the reference radius
- Euclidean distance
- rectengular function as the activation function
- bias of -1 in the output neuron

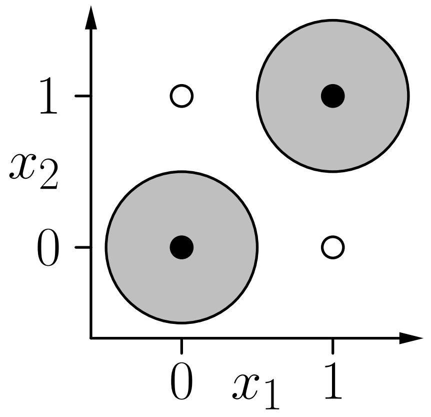
Radial Basis Function Networks: Examples

Radial basis function networks for the biimplication $x_1 \leftrightarrow x_2$

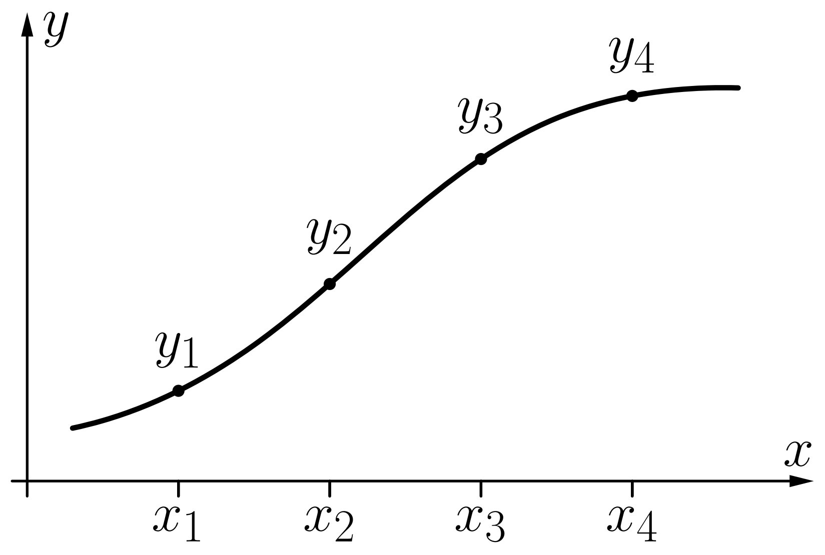
Idea: logical decomposition

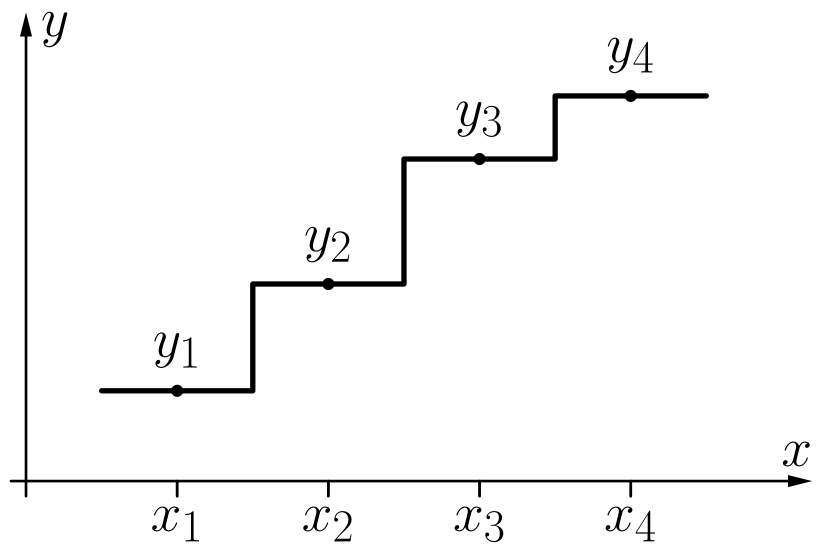
$$x_1 \leftrightarrow x_2 \quad \equiv \quad (x_1 \wedge x_2) \vee \neg(x_1 \vee x_2)$$

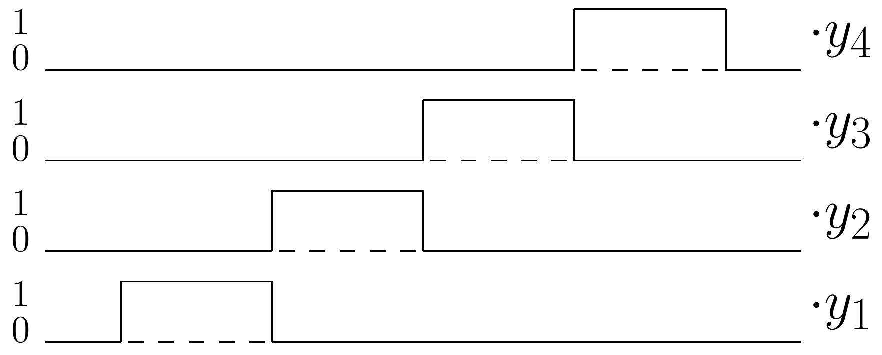




Radial Basis Function Networks: Function Approximation

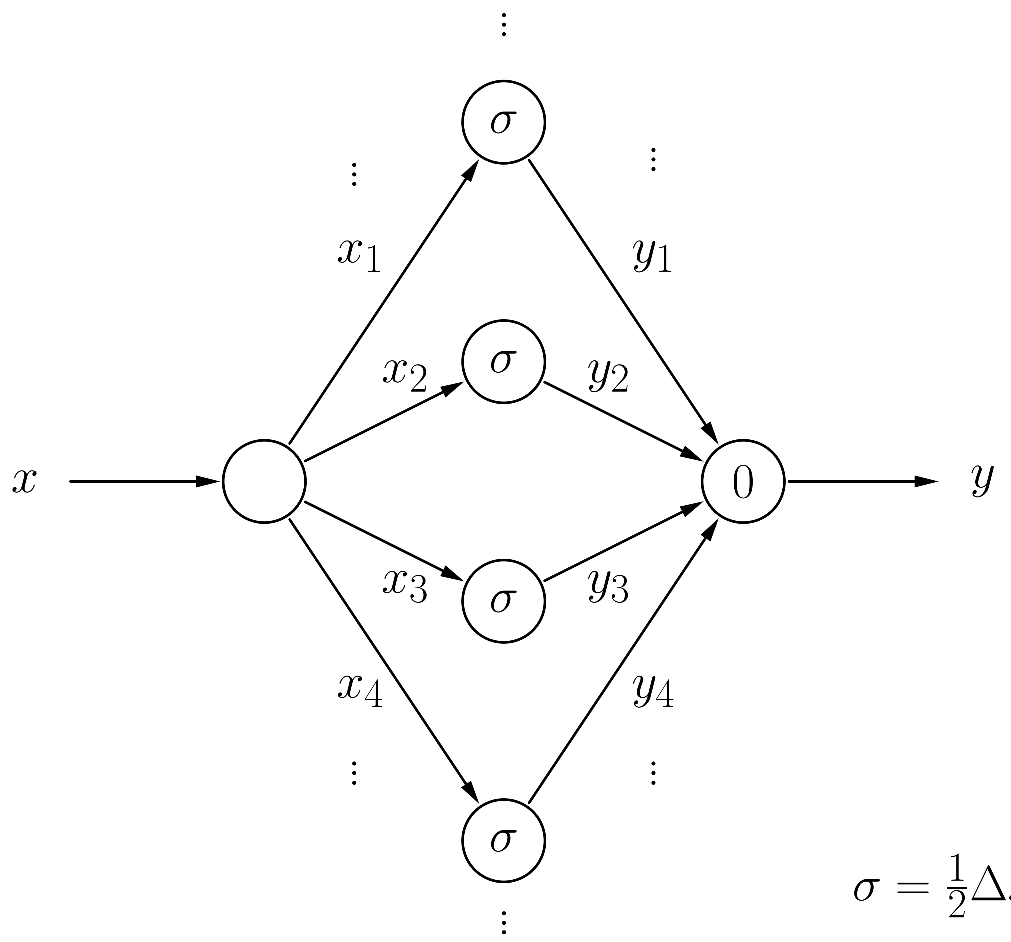






Approximation of the original function by a step function with each step being resembled by one of the RBF-Network's neurons. (compare MLPs)

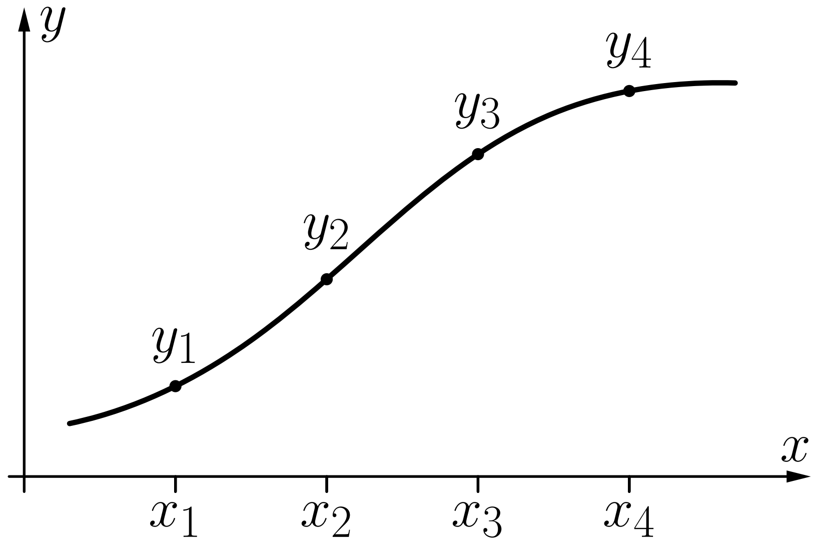
Radial Basis Function Networks: Function Approximation

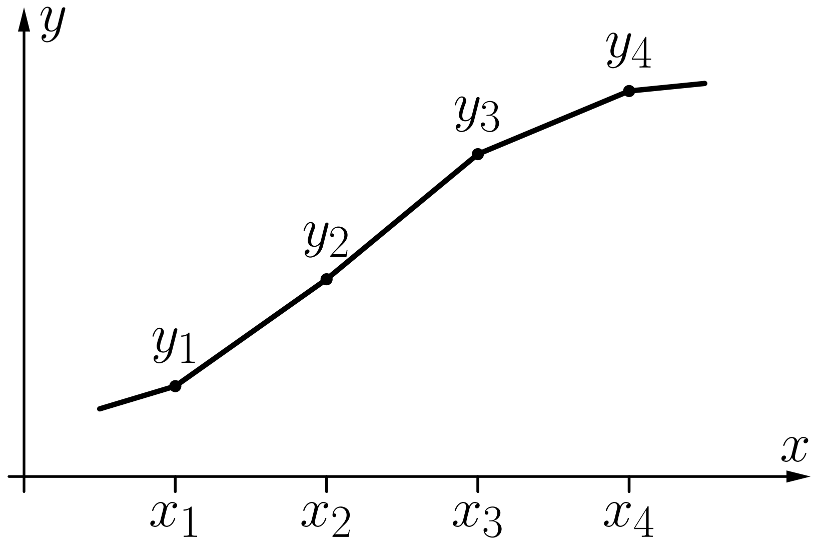


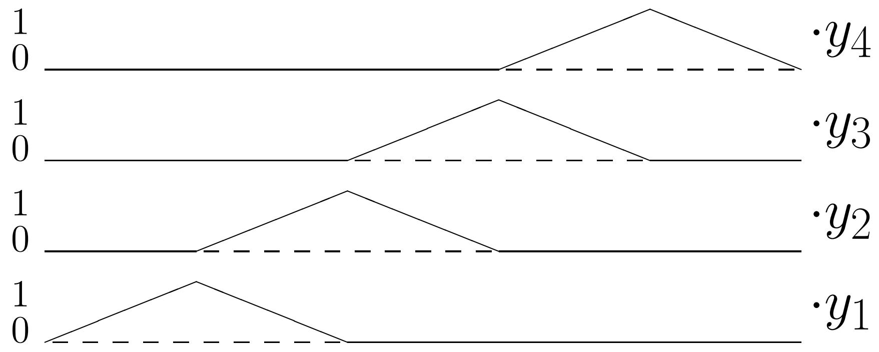
$$\sigma = \frac{1}{2}\Delta x = \frac{1}{2}(x_{i+1} - x_i)$$

RBF-Network calculating the step function shown on the previous slide and the partially linear function on the following slide. The only change is made to the activation function of the hidden neurons.

Radial Basis Function Networks: Function Approximation

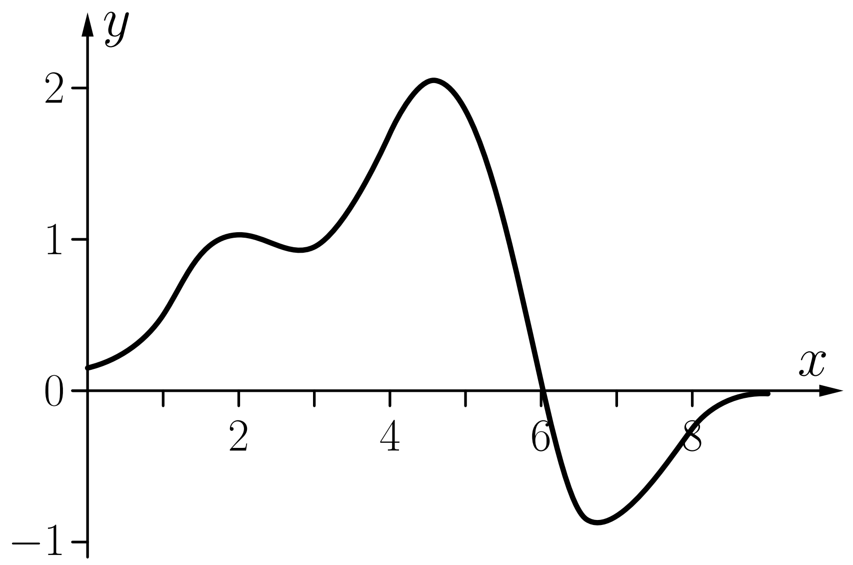


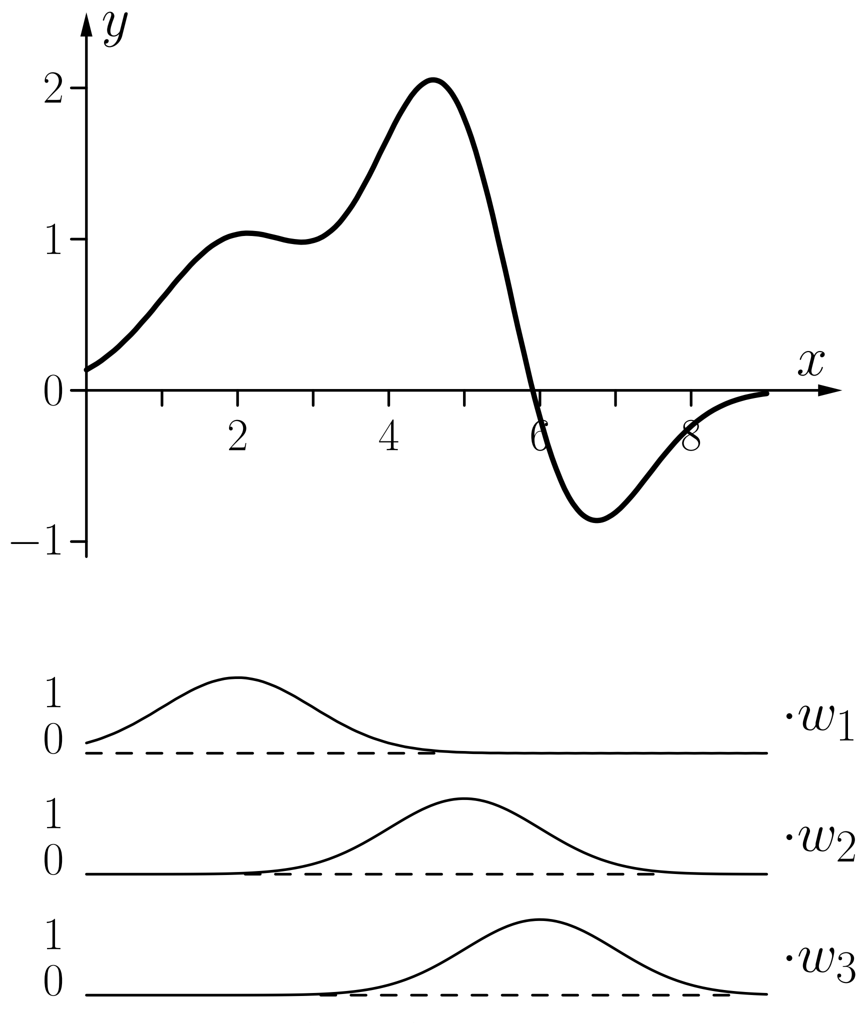




Representation of a partially linear function by the weighted sum of a triangular function with centers x_i.

Radial Basis Function Networks: Function Approximation

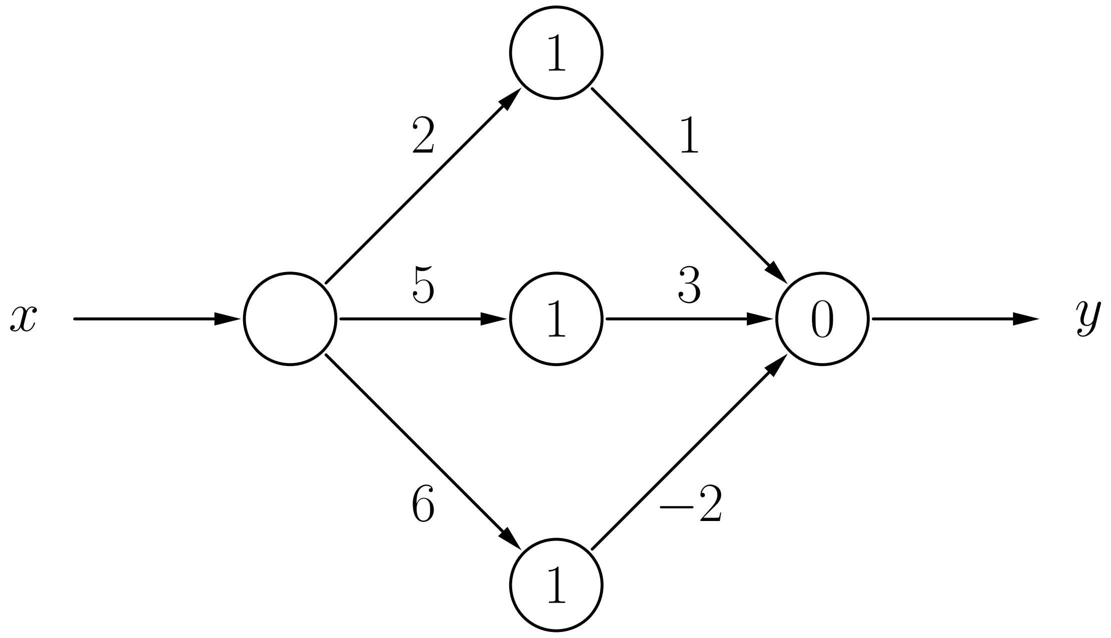




Approximation of a function by the sum of gaussians with radius $\sigma = 1$.
$w_1 = 2$, $w_2 = 3$ and $w_3 = -2$.

Radial Basis Function Networks: Function Approximation

Radial basis function network for a sum of three Gaussian functions



Training Radial Basis Function Networks

Radial Basis Function Networks: Initialization

Let $L_{\text{fixed}} = \{l_1, \ldots, l_m\}$ be a fixed learning task, consisting of m training patterns $l = (\vec{\imath}^{\,(l)}, \vec{o}^{\,(l)})$.

Simple radial basis function network:
One hidden neuron v_k, $k = 1, \ldots, m$, for each training pattern:

$$\forall k \in \{1, \ldots, m\} : \qquad \vec{w}_{v_k} = \vec{\imath}^{\,(l_k)}.$$

If the activation function is the Gaussian function, the radii σ_k are chosen heuristically

$$\forall k \in \{1, \ldots, m\} : \qquad \sigma_k = \frac{d_{\max}}{\sqrt{2m}},$$

where

$$d_{\max} = \max_{l_j, l_k \in L_{\text{fixed}}} d\left(\vec{\imath}^{\,(l_j)}, \vec{\imath}^{\,(l_k)}\right).$$

Radial Basis Function Networks: Initialization

Initializing the connections from the hidden to the output neurons

$$\forall u: \sum_{k=1}^{m} w_{uv_m} \operatorname{out}_{v_m}^{(l)} - \theta_u = o_u^{(l)} \qquad \text{or abbreviated} \qquad \mathbf{A} \cdot \vec{w}_u = \vec{o}_u,$$

where $\vec{o}_u = (o_u^{(l_1)}, \ldots, o_u^{(l_m)})^\top$ is the vector of desired outputs, $\theta_u = 0$, and

$$\mathbf{A} = \begin{pmatrix} \operatorname{out}_{v_1}^{(l_1)} & \operatorname{out}_{v_2}^{(l_1)} & \ldots & \operatorname{out}_{v_m}^{(l_1)} \\ \operatorname{out}_{v_1}^{(l_2)} & \operatorname{out}_{v_2}^{(l_2)} & \ldots & \operatorname{out}_{v_m}^{(l_2)} \\ \vdots & \vdots & & \vdots \\ \operatorname{out}_{v_1}^{(l_m)} & \operatorname{out}_{v_2}^{(l_m)} & \ldots & \operatorname{out}_{v_m}^{(l_m)} \end{pmatrix}.$$

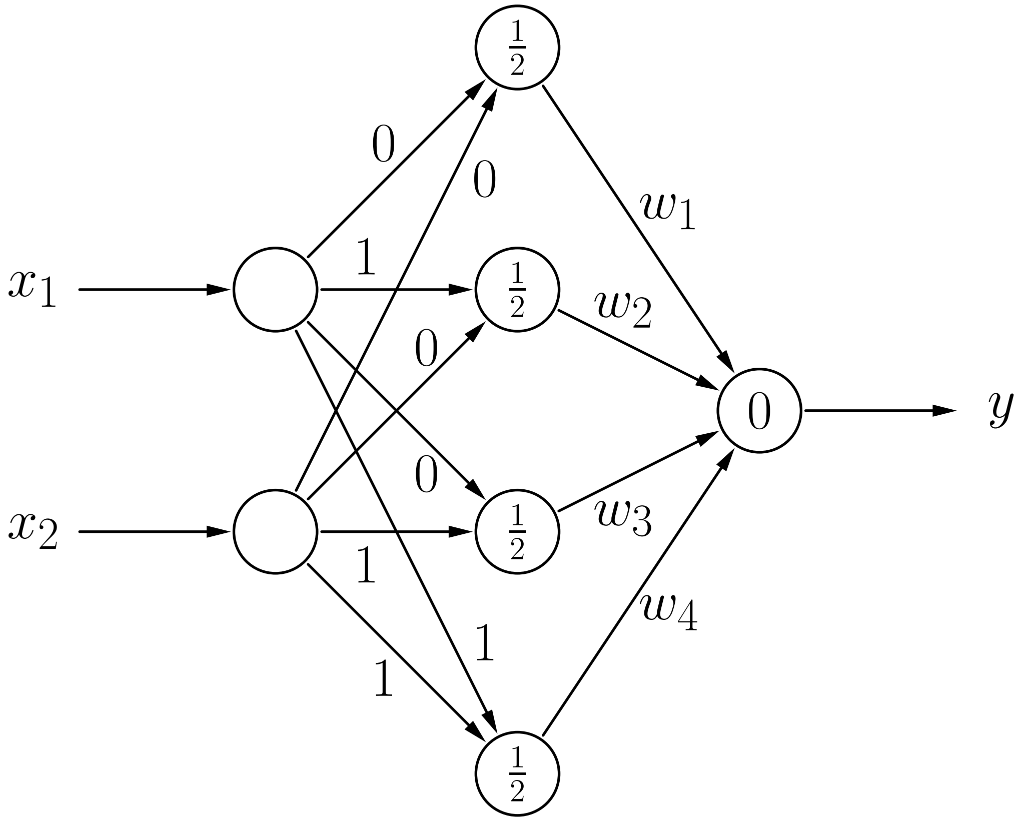
This is a linear equation system, that can be solved by inverting the matrix **A**:

$$\vec{w}_u = \mathbf{A}^{-1} \cdot \vec{o}_u.$$

RBFN Initialization: Example

Simple radial basis function network for the biimplication $x_1 \leftrightarrow x_2$

x_1	x_2	y
0	0	1
1	0	0
0	1	0
1	1	1



RBFN Initialization: Example

Simple radial basis function network for the biimplication $x_1 \leftrightarrow x_2$

$$\mathbf{A} = \begin{pmatrix} 1 & e^{-2} & e^{-2} & e^{-4} \\ e^{-2} & 1 & e^{-4} & e^{-2} \\ e^{-2} & e^{-4} & 1 & e^{-2} \\ e^{-4} & e^{-2} & e^{-2} & 1 \end{pmatrix} \qquad \mathbf{A}^{-1} = \begin{pmatrix} \frac{a}{D} & \frac{b}{D} & \frac{b}{D} & \frac{c}{D} \\ \frac{b}{D} & \frac{a}{D} & \frac{c}{D} & \frac{b}{D} \\ \frac{b}{D} & \frac{c}{D} & \frac{a}{D} & \frac{b}{D} \\ \frac{c}{D} & \frac{b}{D} & \frac{b}{D} & \frac{a}{D} \end{pmatrix}$$

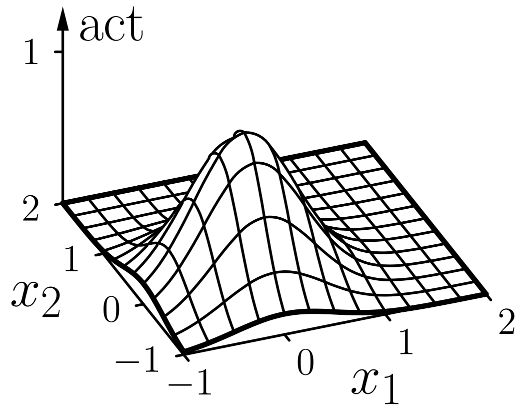
where

$$\begin{aligned} D &= 1 - 4e^{-4} + 6e^{-8} - 4e^{-12} + e^{-16} &\approx&\ \ 0.9287 \\ a &= \ 1 \quad - 2e^{-4} + e^{-8} &\approx&\ \ 0.9637 \\ b &= -e^{-2} + 2e^{-6} - e^{-10} &\approx&\ -0.1304 \\ c &= \ e^{-4} - 2e^{-8} + e^{-12} &\approx&\ \ 0.0177 \end{aligned}$$

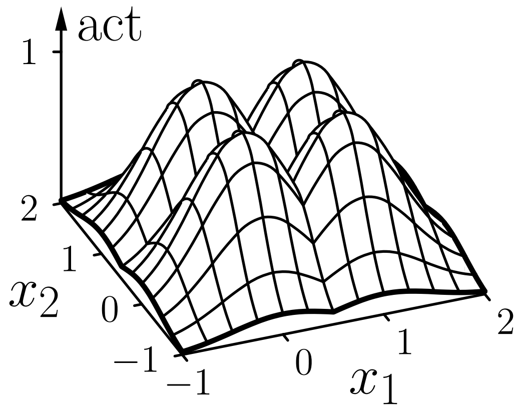
$$\vec{w}_u = \mathbf{A}^{-1} \cdot \vec{o}_u = \frac{1}{D} \begin{pmatrix} a+c \\ 2b \\ 2b \\ a+c \end{pmatrix} \approx \begin{pmatrix} 1.0567 \\ -0.2809 \\ -0.2809 \\ 1.0567 \end{pmatrix}$$

RBFN Initialization: Example

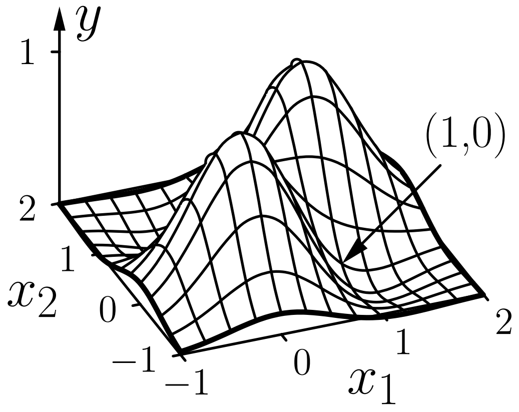
Simple radial basis function network for the biimplication $x_1 \leftrightarrow x_2$



single basis function



all basis functions



output

- Initialization leads already to a perfect solution of the learning task.
- Subsequent training is not necessary.

Radial Basis Function Networks: Initialization

Normal radial basis function networks:
Select subset of k training patterns as centers.

$$\mathbf{A} = \begin{pmatrix} 1 & \text{out}_{v_1}^{(l_1)} & \text{out}_{v_2}^{(l_1)} & \ldots & \text{out}_{v_k}^{(l_1)} \\ 1 & \text{out}_{v_1}^{(l_2)} & \text{out}_{v_2}^{(l_2)} & \ldots & \text{out}_{v_k}^{(l_2)} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & \text{out}_{v_1}^{(l_m)} & \text{out}_{v_2}^{(l_m)} & \ldots & \text{out}_{v_k}^{(l_m)} \end{pmatrix} \qquad \mathbf{A} \cdot \vec{w}_u = \vec{o}_u$$

Compute (Moore–Penrose) pseudo inverse:

$$\mathbf{A}^+ = (\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top.$$

The weights can then be computed by

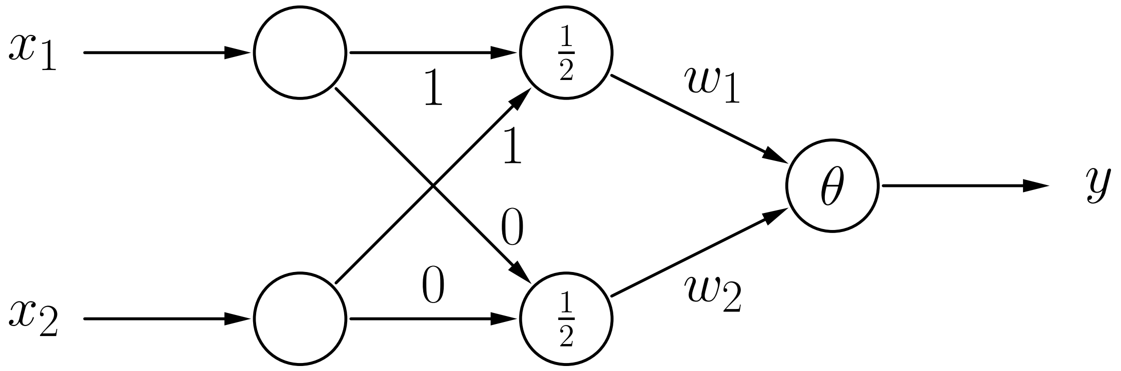
$$\vec{w}_u = \mathbf{A}^+ \cdot \vec{o}_u = (\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top \cdot \vec{o}_u$$

RBFN Initialization: Example

Normal radial basis function network for the biimplication $x_1 \leftrightarrow x_2$

Select two training patterns:

- $l_1 = (\vec{\imath}^{\,(l_1)}, \vec{o}^{\,(l_1)}) = ((0,0),(1))$
- $l_4 = (\vec{\imath}^{\,(l_4)}, \vec{o}^{\,(l_4)}) = ((1,1),(1))$



RBFN Initialization: Example

Normal radial basis function network for the biimplication $x_1 \leftrightarrow x_2$

$$\mathbf{A} = \begin{pmatrix} 1 & 1 & e^{-4} \\ 1 & e^{-2} & e^{-2} \\ 1 & e^{-2} & e^{-2} \\ 1 & e^{-4} & 1 \end{pmatrix} \qquad \mathbf{A}^+ = (\mathbf{A}^\top \mathbf{A})^{-1}\mathbf{A}^\top = \begin{pmatrix} a & b & b & a \\ c & d & d & e \\ e & d & d & c \end{pmatrix}$$

where

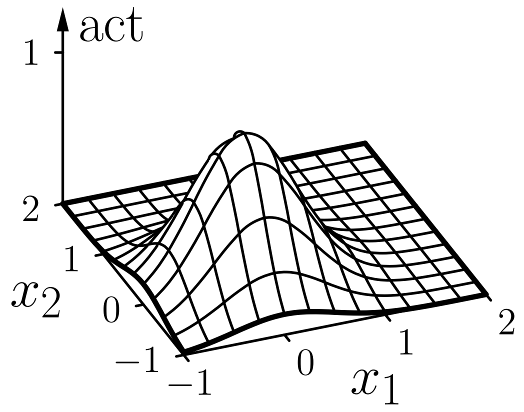
$$\begin{aligned} a &\approx -0.1810, & b &\approx 0.6810, & & \\ c &\approx 1.1781, & d &\approx -0.6688, & e &\approx 0.1594. \end{aligned}$$

Resulting weights:

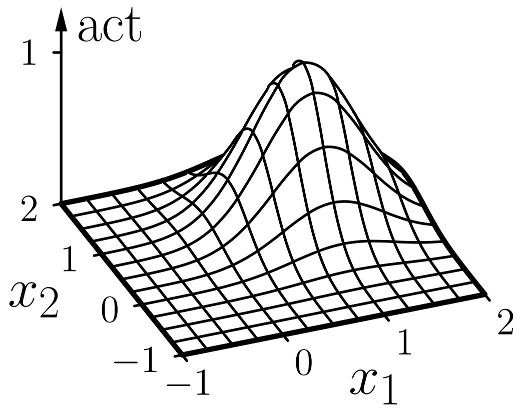
$$\vec{w}_u = \begin{pmatrix} -\theta \\ w_1 \\ w_2 \end{pmatrix} = \mathbf{A}^+ \cdot \vec{o}_u \approx \begin{pmatrix} -0.3620 \\ 1.3375 \\ 1.3375 \end{pmatrix}.$$

RBFN Initialization: Example

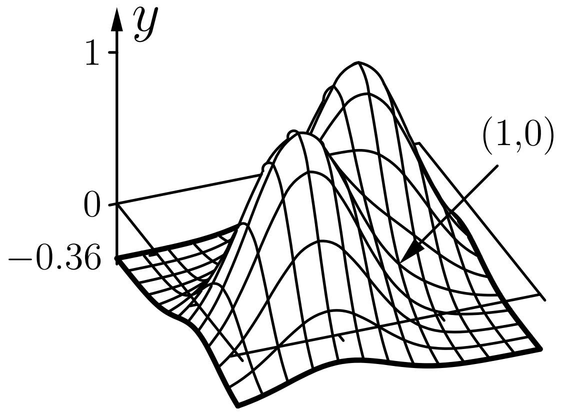
Normal radial basis function network for the biimplication $x_1 \leftrightarrow x_2$



basis function (0,0)



basis function (1,1)



output

- Initialization leads already to a perfect solution of the learning task.
- This is an accident, because the linear equation system is not over-determined, due to linearly dependent equations.

Radial Basis Function Networks: Initialization

Finding appropriate centers for the radial basis functions

One approach: **k-means clustering**

- Select randomly k training patterns as centers.
- Assign to each center those training patterns that are closest to it.
- Compute new centers as the center of gravity of the assigned training patterns
- Repeat previous two steps until convergence,
  i.e., until the centers do not change anymore.
- Use resulting centers for the weight vectors of the hidden neurons.

Alternative approach: **learning vector quantization**

Radial Basis Function Networks: Training

Training radial basis function networks:
Derivation of update rules is analogous to that of multilayer perceptrons.

Weights from the hidden to the output neurons.

Gradient:

$$\vec{\nabla}_{\vec{w}_u} e_u^{(l)} = \frac{\partial e_u^{(l)}}{\partial \vec{w}_u} = -2(o_u^{(l)} - \mathrm{out}_u^{(l)})\, \vec{\mathrm{in}}_u^{(l)},$$

Weight update rule:

$$\Delta \vec{w}_u^{(l)} = -\frac{\eta_3}{2} \vec{\nabla}_{\vec{w}_u} e_u^{(l)} = \eta_3(o_u^{(l)} - \mathrm{out}_u^{(l)})\, \vec{\mathrm{in}}_u^{(l)}$$

(Two more learning rates are needed for the center coordinates and the radii.)

Radial Basis Function Networks: Training

Training radial basis function networks:
Center coordinates (weights from the input to the hidden neurons).

Gradient:

$$\vec{\nabla}_{\vec{w}_v} e^{(l)} = \frac{\partial e^{(l)}}{\partial \vec{w}_v} = -2 \sum_{s \in \mathrm{succ}(v)} (o_s^{(l)} - \mathrm{out}_s^{(l)}) w_{su} \frac{\partial\, \mathrm{out}_v^{(l)}}{\partial\, \mathrm{net}_v^{(l)}} \frac{\partial\, \mathrm{net}_v^{(l)}}{\partial \vec{w}_v}$$

Weight update rule:

$$\Delta \vec{w}_v^{(l)} = -\frac{\eta_1}{2} \vec{\nabla}_{\vec{w}_v} e^{(l)} = \eta_1 \sum_{s \in \mathrm{succ}(v)} (o_s^{(l)} - \mathrm{out}_s^{(l)}) w_{sv} \frac{\partial\, \mathrm{out}_v^{(l)}}{\partial\, \mathrm{net}_v^{(l)}} \frac{\partial\, \mathrm{net}_v^{(l)}}{\partial \vec{w}_v}$$

Radial Basis Function Networks: Training

Training radial basis function networks:
Center coordinates (weights from the input to the hidden neurons).

Special case: **Euclidean distance**

$$\frac{\partial \operatorname{net}_v^{(l)}}{\partial \vec{w}_v} = \left(\sum_{i=1}^{n} (w_{vp_i} - \operatorname{out}_{p_i}^{(l)})^2 \right)^{-\frac{1}{2}} (\vec{w}_v - \vec{\operatorname{in}}_v^{(l)}).$$

Special case: **Gaussian activation function**

$$\frac{\partial \operatorname{out}_v^{(l)}}{\partial \operatorname{net}_v^{(l)}} = \frac{\partial f_{\text{act}}(\operatorname{net}_v^{(l)}, \sigma_v)}{\partial \operatorname{net}_v^{(l)}} = \frac{\partial}{\partial \operatorname{net}_v^{(l)}} \, e^{-\frac{\left(\operatorname{net}_v^{(l)}\right)^2}{2\sigma_v^2}} = -\frac{\operatorname{net}_v^{(l)}}{\sigma_v^2} \, e^{-\frac{\left(\operatorname{net}_v^{(l)}\right)^2}{2\sigma_v^2}}.$$

Radial Basis Function Networks: Training

Training radial basis function networks:
Radii of radial basis functions.

Gradient:

$$\frac{\partial e^{(l)}}{\partial \sigma_v} = -2 \sum_{s \in \text{succ}(v)} (o_s^{(l)} - \text{out}_s^{(l)}) w_{su} \frac{\partial\, \text{out}_v^{(l)}}{\partial \sigma_v}.$$

Weight update rule:

$$\Delta \sigma_v^{(l)} = -\frac{\eta_2}{2} \frac{\partial e^{(l)}}{\partial \sigma_v} = \eta_2 \sum_{s \in \text{succ}(v)} (o_s^{(l)} - \text{out}_s^{(l)}) w_{sv} \frac{\partial\, \text{out}_v^{(l)}}{\partial \sigma_v}.$$

Special case: **Gaussian activation function**

$$\frac{\partial\, \text{out}_v^{(l)}}{\partial \sigma_v} = \frac{\partial}{\partial \sigma_v} e^{-\frac{\left(\text{net}_v^{(l)}\right)^2}{2\sigma_v^2}} = \frac{\left(\text{net}_v^{(l)}\right)^2}{\sigma_v^3} e^{-\frac{\left(\text{net}_v^{(l)}\right)^2}{2\sigma_v^2}}.$$

Radial Basis Function Networks: Generalization

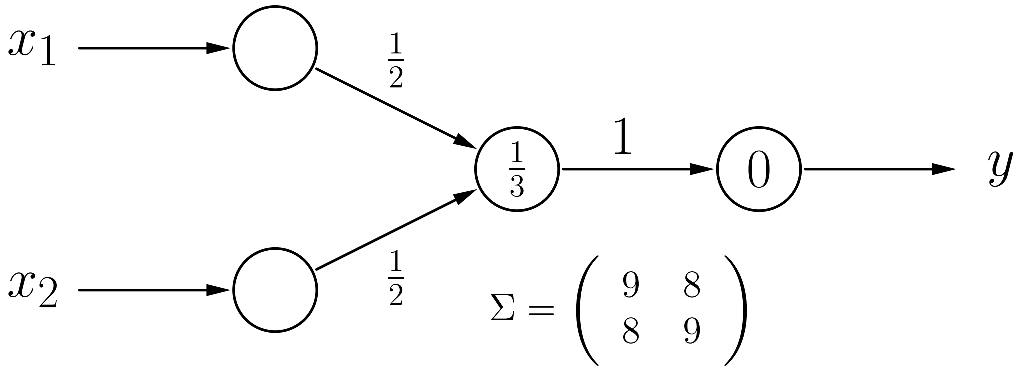
Generalization of the distance function

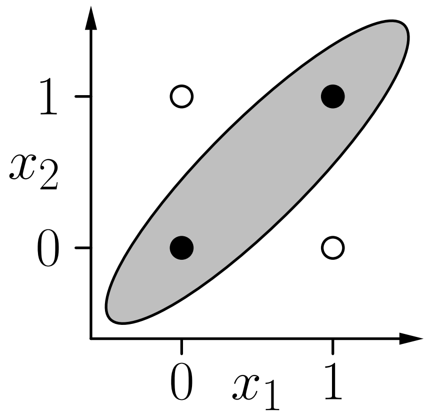
Idea: Use anisotropic distance function.

Example: **Mahalanobis distance**

$$d(\vec{x}, \vec{y}) = \sqrt{(\vec{x} - \vec{y})^\top \Sigma^{-1} (\vec{x} - \vec{y})}.$$

Example: **biimplication**





Radial Basis Function Networks: Application

Advantages

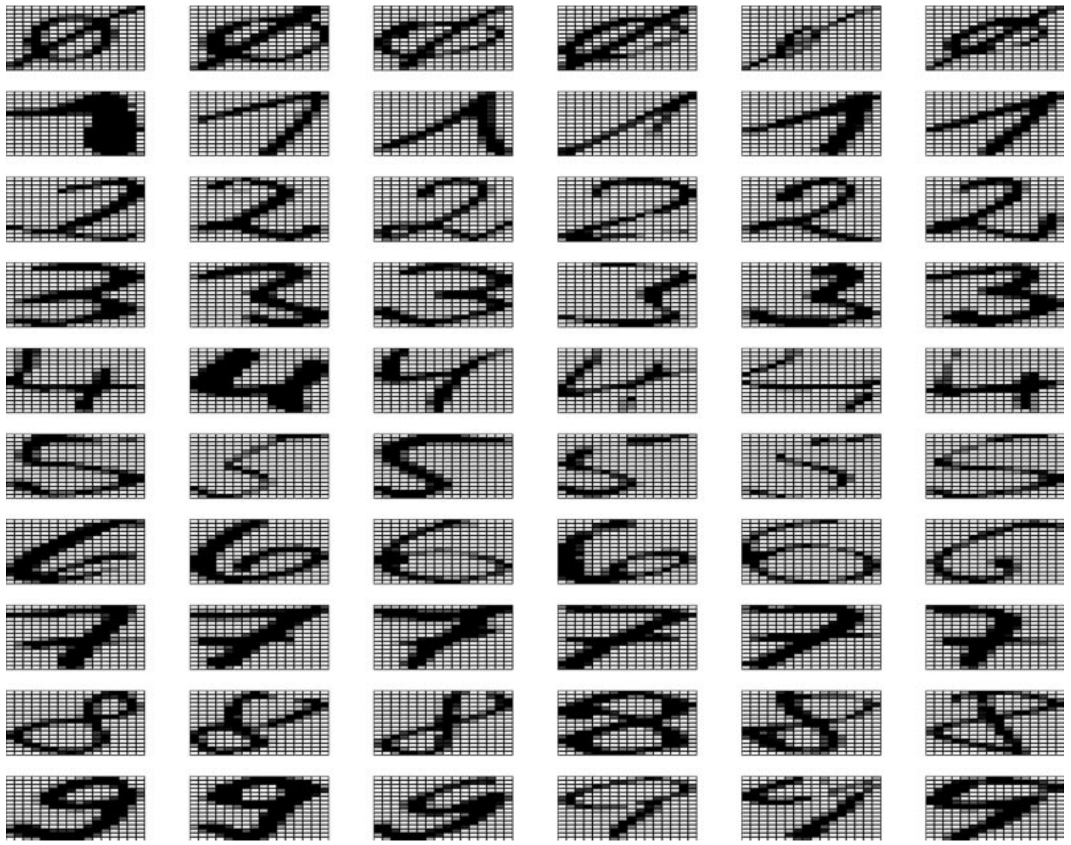
- simple feed-forward architecture
- easy adaption
- $\Rightarrow$ quick optimization and calculations

Application

- continuous processes adapting to changes rapidly
- Approximation
- Pattern Recognition
- Control Engineering

Below: Examples from [Schwenker *et al.* 2001]

Example: Handwriting Recognition of digits



- dataset: 20.000 handwritten digits (2.000 samples of each class)
- normalized in height and width
- represented by 16×16 greyscale values $G_{ij} \in \{0, \ldots, 255\}$
- data source: EU-project *StatLog* [Michie *et al.* 1994]

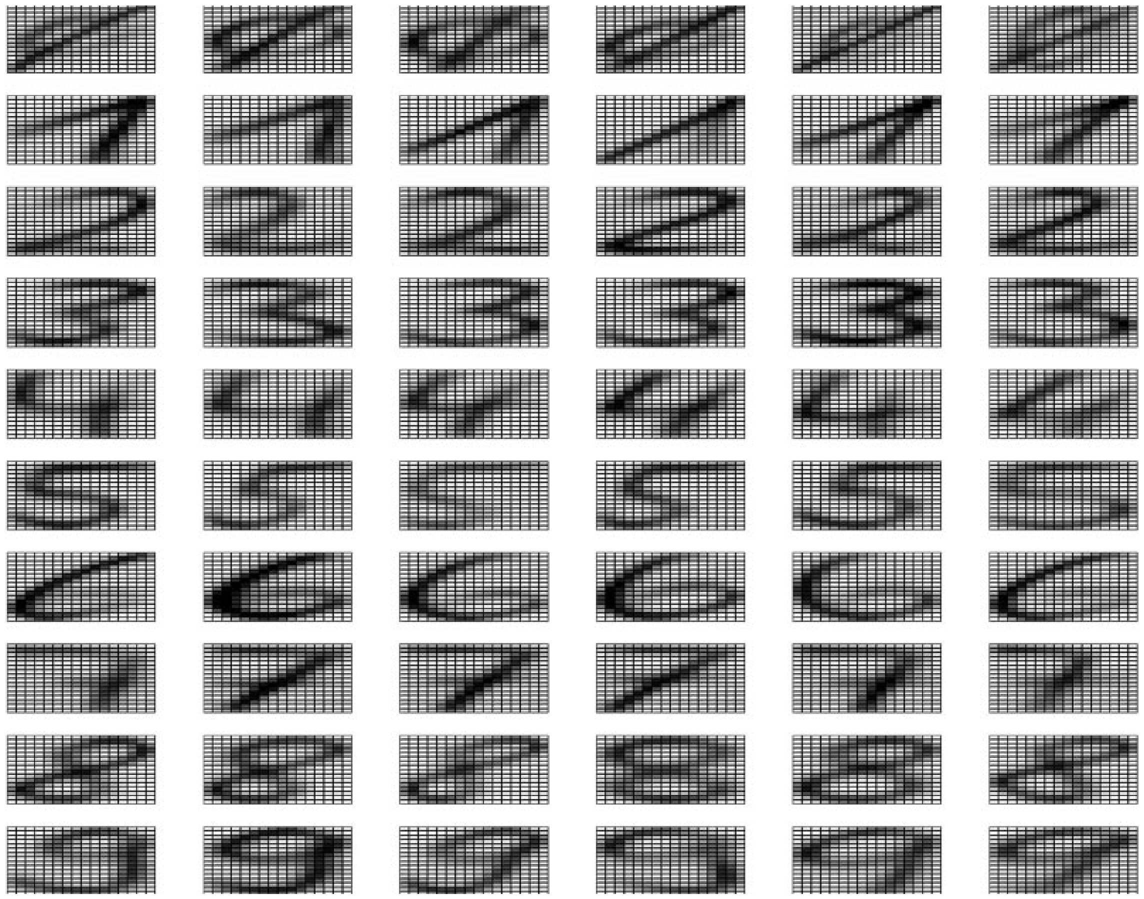
Example: Results of RBF-Networks

- 10.000 training samples and 10.000 validation samples (1.000 for each class)
- training data for learning of classificators, validation data for evaluation
- initialization by k-means-clustering with 200 prototypes (20 for each class)

Method	Explanation	Test accuracy
C4.5	Decision Tree	91.12%
RBF	k-means for RBF-centers	96.94%
MLP	1 hidden layer with 200 neurons	97.59%

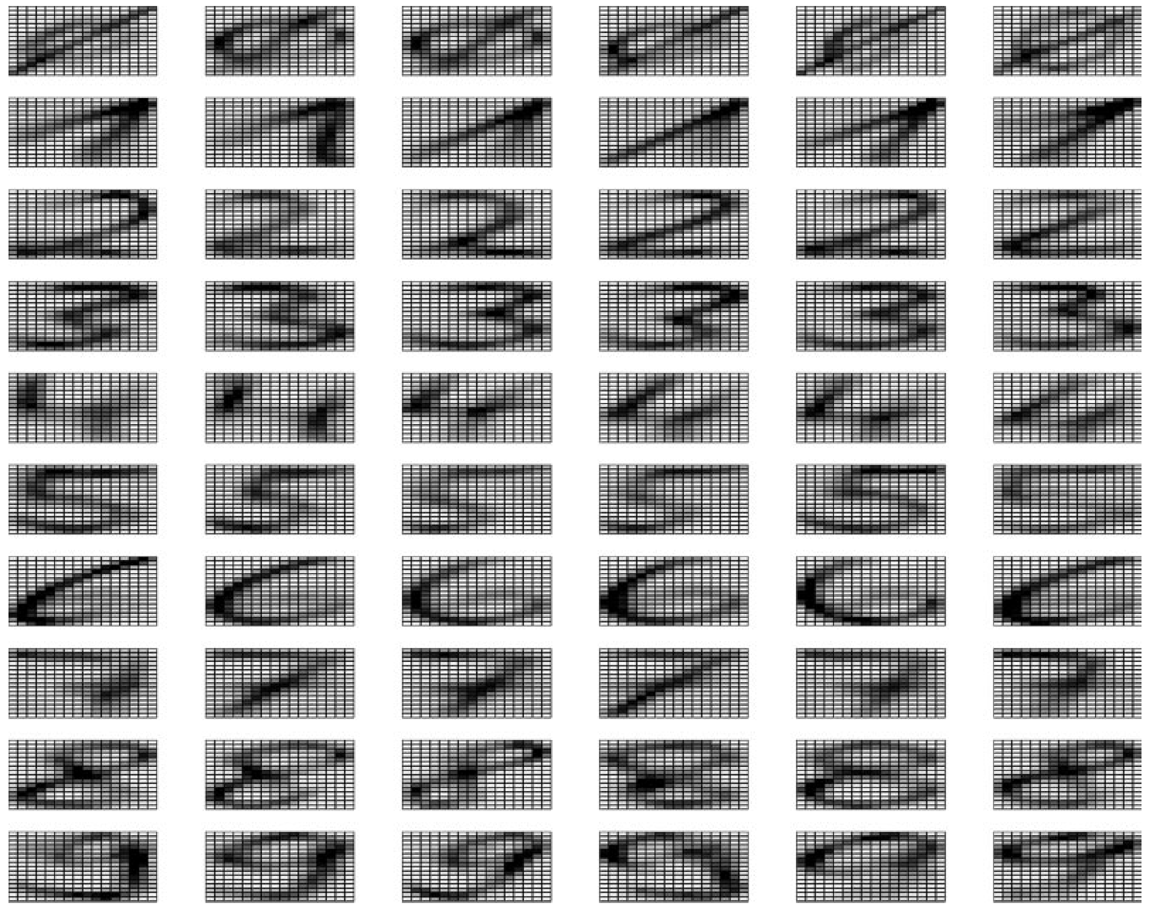
- here: median of test accuracy for three training and validation runs

Example: k-means-Clustering for RBF-initialization



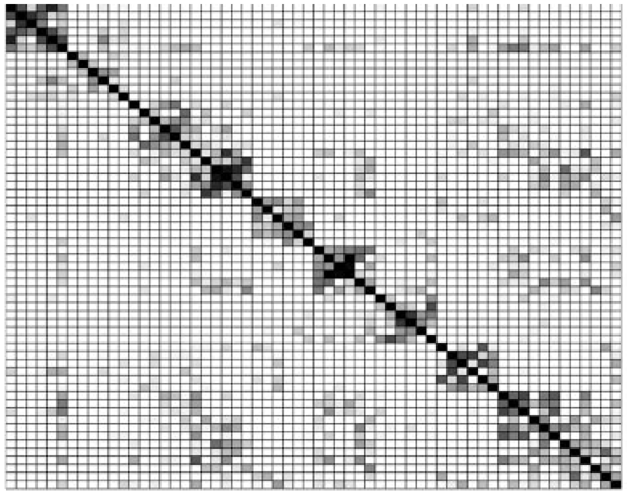
- shown: 60 cluster-centers of the digits after k-means-clustering
- separate run of the algorithm for every digit, with $k = 6$
- centers were initialized by samples chosen from the training data set randomly

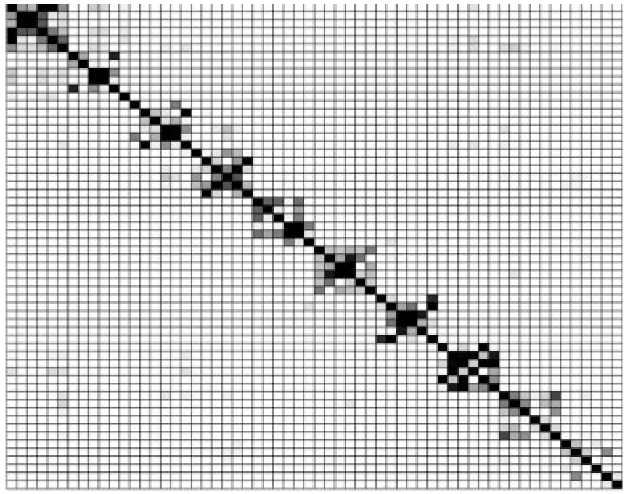
Example: found RBF-centers after 3 runs



- shown: 60 RBF-centers of the digits after 3 backpropagation runs of the RBF-Network
- hardly a difference can be seen in comparison to k-means, but...

Example: Comparison of k-means and RBF-Network





- here: Eucledian distance of the 60 RBF-centers before and after training
- Centers are sorted by class with the first 6 columns/rows representing the digit 0, the next 6 rows/digits representing the digit 1 etc.
- Distances are coded as greyscale values: The smaller, the darker.
- left: a lot of small distances between centers of different classes (e.g. 2–3 and 8–9)
- these small distance cause misclassifications
- right: after training there are no small distances anymore.