technische universität
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Computational Intelligence

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- Application Fields of ANNs
  - Classification
  - Prediction
  - Function Approximation
- Recurrent MLP
  - Elman Nets
  - Jordan Nets
- Radial Basis Function Nets (RBF Nets)
  - Model
  - Training

Classification

<u>given</u>: set of training patterns (input / output)

$\tilde{x}_i \quad \tilde{y}_i$

output = label
(e.g. class A, class B, ...)

$$f(x;\overbrace{\underbrace{(\tilde{x}_1,\tilde{y}_1),\ldots,(\tilde{x}_m,\tilde{y}_m)}_{\text{training patterns (known)}},\underbrace{w_1,\ldots,w_n}_{\text{weights (learnt)}}}^{\text{parameters}}) \to \hat{y}$$

input
(unknown)

output
(guessed)

phase I:

train network

phase II:

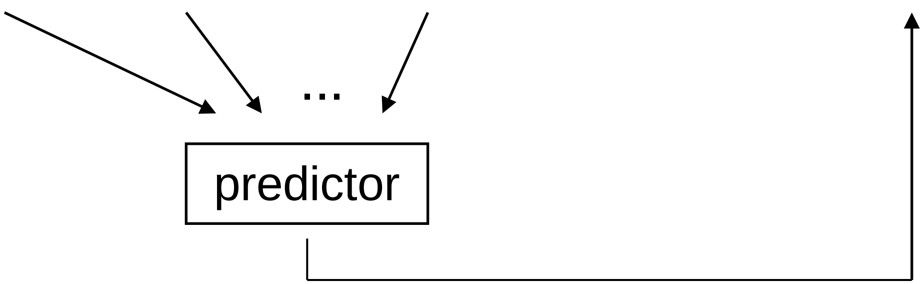
apply network to unkown inputs for classification

Prediction of Time Series

time series $x_1, x_2, x_3, \ldots$ (e.g. temperatures, exchange rates, ...)

task: given a subset of historical data, predict the future

$$f(x_{t-k}, x_{t-k+1}, \ldots, x_t; w_1, \ldots, w_n) \rightarrow \hat{x}_{t+\tau}$$



training patterns:

historical data where true output is known;

error per pattern = $(\hat{x}_{t+\tau} - x_{t+\tau})^2$

phase I:

train network

phase II:

apply network to historical inputs for predicting <u>unkown</u> outputs

Prediction of Time Series: Example for Creating Training Data

given: time series 10.5, 3.4, 5.6, 2.4, 5.9, 8.4, 3.9, 4.4, 1.7

time window: k=3

(10.5, 3.4, 5.6) 2.4 first input / output pair

known input known output

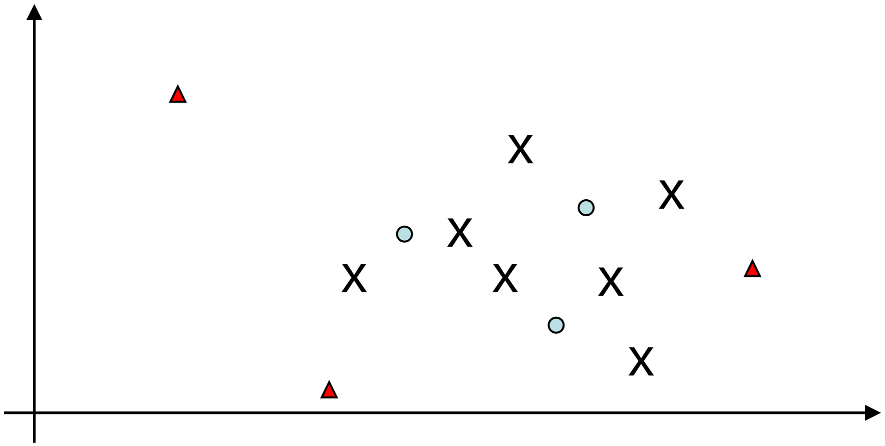
further input / output pairs:
(3.4, 5.6, 2.4) 5.9
(5.6, 2.4, 5.9) 8.4
(2.4, 5.9, 8.4) 3.9
(5.9, 8.4, 3.9) 4.4
(8.4, 3.9, 4.4) 1.7

Function Approximation (the general case)

task: given training patterns (input / output), approximate unkown function

→ should give outputs close to true unkown function for arbitrary inputs

- values between training patterns are **interpolated**
- values outside convex hull of training patterns are **extrapolated**



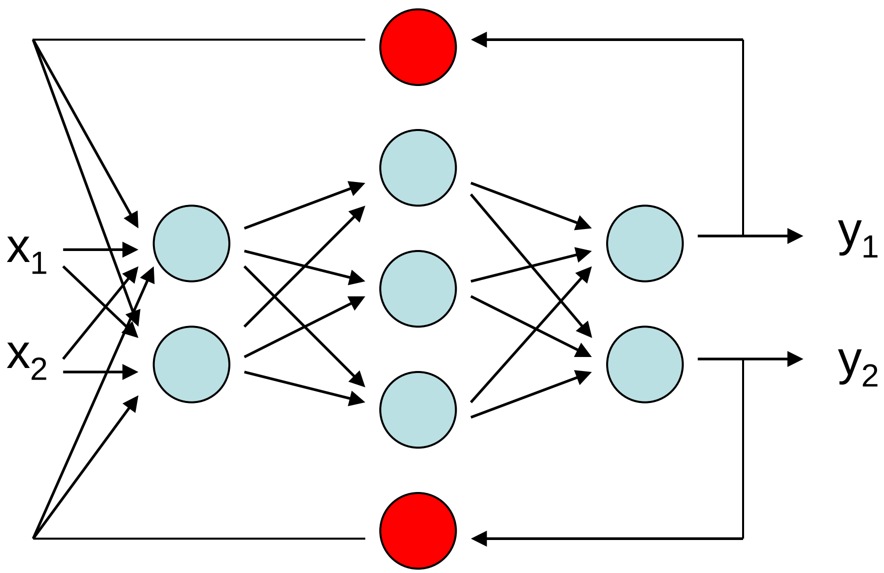
x : input training pattern

○ : input pattern where output to be interpolated

▲ : input pattern where output to be extrapolated

Jordan nets (1986)

• **context neuron**:
reads output from some neuron at step t and feeds value into net at step t+1



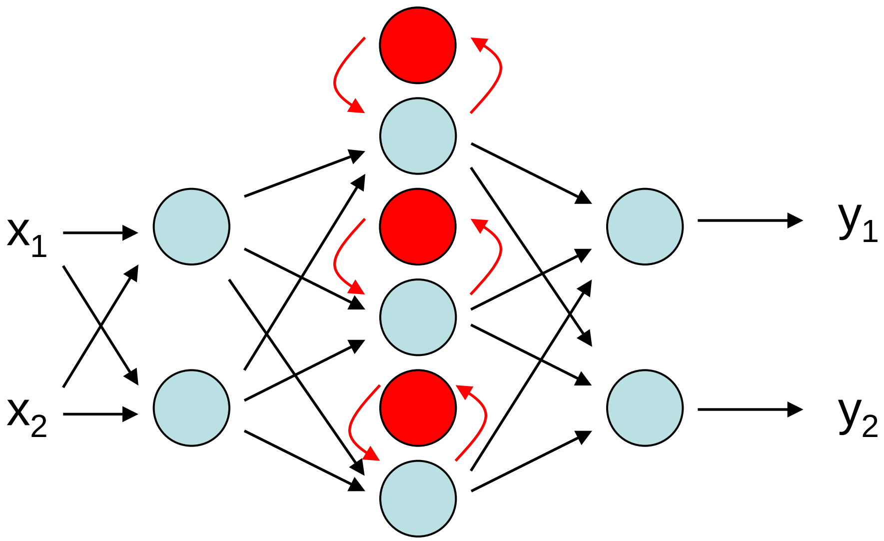
Jordan net =

MLP + context neuron
for each output,
context neurons fully
connected to input layer

Elman nets (1990)

Elman net =

MLP + context neuron for each hidden layer neuron‘s output of MLP,
context neurons fully connected to emitting MLP layer



Training?

⇒ unfolding in time (“loop unrolling“)

- identical MLPs serially connected (finitely often)
- results in a large MLP with many hidden (inner) layers
- backpropagation may take a long time
- but reasonable if most recent past more important than layers far away

Why using backpropagation?

⇒ use *Evolutionary Algorithms* directly on recurrent MLP!

later!

Definition:

A function $\phi : \mathbb{R}^n \to \mathbb{R}$ is termed **radial basis function**

iff $\exists \varphi : \mathbb{R} \to \mathbb{R} : \forall x \in \mathbb{R}^n : \phi(x;\, c) = \varphi(\, \|x - c\|\,).$ □

Definition:

RBF **local** iff

$\varphi(r) \to 0$ as $r \to \infty$ □

typically, || x || denotes Euclidean norm of vector x

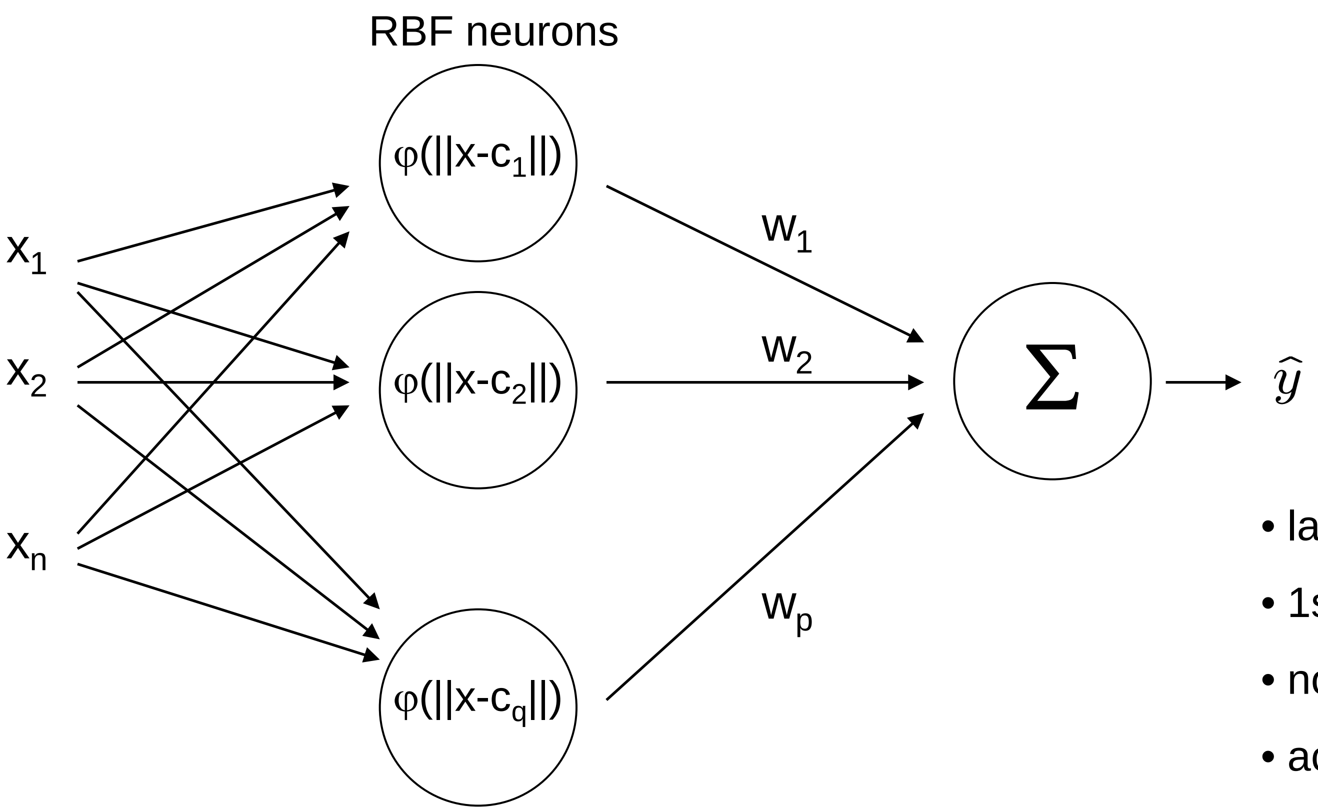
examples:

$\varphi(r) = \exp\left(-\frac{r^2}{\sigma^2}\right)$	Gaussian	unbounded	local
$\varphi(r) = \frac{3}{4}(1 - r^2) \cdot 1_{\{r \le 1\}}$	Epanechnikov	bounded	local
$\varphi(r) = \frac{\pi}{4} \cos\left(\frac{\pi}{2} r\right) \cdot 1_{\{r \le 1\}}$	Cosine	bounded	local

Definition:

A function f: $\mathbb{R}^n \to \mathbb{R}$ is termed **radial basis function net (RBF net)**

iff $f(x) = w_1\, \varphi(\|\, x - c_1 \,\|) + w_2\, \varphi(\|\, x - c_2 \,\|) + \ldots + w_p\, \varphi(\|\, x - c_q \,\|)$ □



- layered net
- 1st layer fully connected
- no weights in 1st layer
- activation functions differ

given : N training patterns (x_i, y_i) and q RBF neurons

find : weights $w_1, \ldots, w_q$ with minimal error

solution:

we know that $f(x_i) = y_i$ for i = 1, ..., N and therefore we insist that

$$\sum_{k=1}^{q} \underbrace{w_k}_{\text{unknown}} \cdot \underbrace{\varphi(\|x_i - c_k\|)}_{p_{ik}\text{ known value}} = \underbrace{y_i}_{\text{known value}}$$

$$\Rightarrow \quad \sum_{k=1}^{q} w_k \cdot p_{ik} = y_i$$

$\Rightarrow$ N linear equations with q unknowns

in matrix form: $P\,w = y$ with $P = (p_{ik})$ and P: N x q, y: N x 1, w: q x 1,

case N = q: $w = P^{-1}\,y$ if P has full rank

case N < q: many solutions but of no practical relevance

case N > q: $w = P^{+}\,y$ where P^{+} is Moore-Penrose pseudo inverse

$P\,w = y$ | · P‘ from left hand side (P‘ is transpose of P)

$P'P\,w = P'\,y$ | · $(P'P)^{-1}$ from left hand side

$\underbrace{(P'P)^{-1}\,P'P}_{\text{unit matrix}}\,w = \underbrace{(P'P)^{-1}\,P'}_{P^{+}}\,y$ | simplify

- existence of $(P'P)^{-1}$?
- numerical stability ?

Tikhonov Regularization (1963)

idea:
choose $(P'P + h\,I_q)^{-1}$ instead of $(P'P)^{-1}$ ($h > 0$, I_q is q-dim. unit matrix)

excursion to linear algebra:

Def : matrix A positive semidefinite (p.s.d) iff $\forall x \in \mathbb{R}^n : x'Ax \geq 0$
Def : matrix A positive definite (p.d.) iff $\forall x \in \mathbb{R}^n \setminus \{0\} : x'Ax > 0$
Thm : matrix $A : n \times n$ regular $\Leftrightarrow$ rank$(A) = n \Leftrightarrow A^{-1}$ exists $\Leftarrow A$ is p.d.

Lemma : $a, b > 0,\ A, B : n \times n,\ A$ p.d. and B p.s.d. $\Rightarrow a \cdot A + b \cdot B$ p.d.

Proof : $\forall x \in \mathbb{R}^n \setminus \{0\} : x'(a \cdot A + b \cdot B)x = \underbrace{a}_{>0} \cdot \underbrace{x'Ax}_{>0} + \underbrace{b}_{>0} \cdot \underbrace{x'Bx}_{\geq 0} > 0$ q.e.d.

Lemma : $P : n \times q \Rightarrow P'P$ p.s.d.

Proof : $\forall x \in \mathbb{R}^n : x'(P'P)x = (x'P') \cdot (Px) = (Px)'(Px) = \|Px\|_2^2 \geq 0$ q.e.d.

Tikhonov Regularization (1963)

$\Rightarrow (P'P + h\,I_q)$ is p.d. $\Rightarrow (P'P + h\,I_q)^{-1}$ exists

question: how to justify this particular choice?

$$\|Pw - y\|^2 + h \cdot \|w\|^2 \quad \to \min_w!$$

interpretation: minimize TSSE and prefer solutions with small values!

$$\frac{d}{dw}[\,(Pw - y)'(Pw - y) + h \cdot w'w\,] =$$

$$\frac{d}{dw}[\,(w'P'Pw - w'P'y - y'Pw + y'y + h \cdot w'w\,] =$$

$$2\,P'Pw - 2\,P'y + 2h\,w = 2\,(P'P + h\,I_q)\,w - 2\,P'y \stackrel{!}{=} 0$$

$$\Rightarrow \boxed{w^* = (P'P + h\,I_q)^{-1}P'y}$$

$\frac{d}{dw}[\,2\,(P'P + h\,I_q)\,w - 2\,P'y\,] = 2\,(P'P + h\,I_q)$ is p.d. $\quad \Rightarrow$ minimum

Tikhonov Regularization (1963)

<u>question:</u> how to find appropriate $h > 0$ in $(P'P + h\, I_q)$?

let $\text{PERF}(h; T)$ with $\text{PERF} : \mathbb{R}^+ \to \mathbb{R}^+$ measure the performance of RBF net for positive h and given training set T

find h^* such that $\text{PERF}(h^*; T) = \max\{\text{PERF}(h; T) : h \in \mathbb{R}^+\}$

→ several approaches in use
→ <u>here:</u> **grid search** and **crossvalidation**

(1) choose $n \in \mathbb{N}$ and $h_1, \ldots, h_n \in (0, H] \subset \mathbb{R}^+$; set $p^* = 0$
(2) for $i = 1$ to n
(3) $\quad p_i = \text{PERF}(h_i; T)$
(4) $\quad$ if $p_i > p^*$
(5) $\quad\quad p^* = p_i; k = i;$
(6) $\quad$ endif
(7) endfor
(8) return h_k

grid search

Crossvalidation

choose $k \in \mathbb{N}$ with $k < |T|$
let $T_1, \ldots, T_k$ be partition of training set T

$T_1 \cup \ldots \cup T_k = T$
$T_i \cap T_j = \emptyset$ for $i \neq j$

$\textsc{perf}(h; T) =$

(1) set $err = 0$
(2) `for` $i = 1$ `to` k
(3) build matrix P and vector y from $T \setminus T_i$
(4) get weights $w = (P'P + h\,I)^{-1} P'y$
(5) build matrix P and vector y from T_i
(6) get error $e = (Pw - y)'(Pw - y)$
(7) $err = err + e$
(8) `endfor`
(9) `return` $1/err$

complexity (naive)

$w = (P'P)^{-1} P' y$

$$\underbrace{P'P: N^2 q \qquad \text{inversion: } q^3 \qquad P'y: qN \qquad \text{multiplication: } q^2}_{O(N^2 q) \text{ elementary operations}}$$

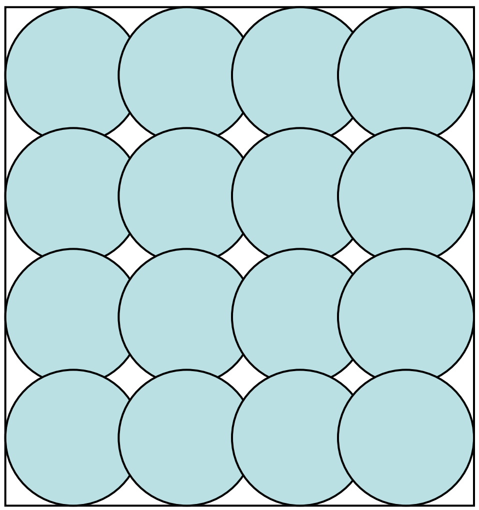
remark: if N large then inaccuracies for P'P likely

$\Rightarrow$ first analytic solution, then $\underbrace{\text{gradient descent}}_{\text{requires differentiable basis functions!}}$ starting from this solution

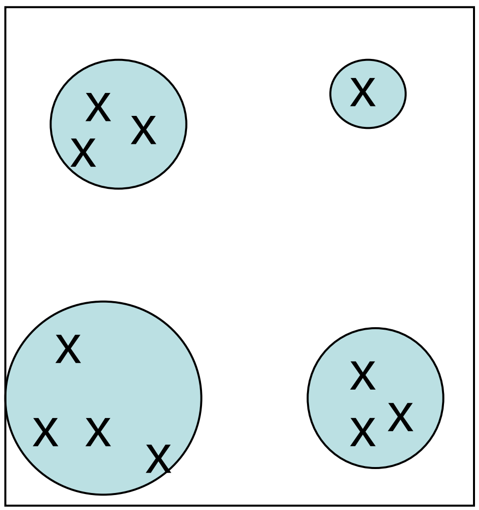
so far: tacitly assumed that RBF neurons are given

$\Rightarrow$ center c_k and radii σ considered given and known

how to choose c_k and σ ?



uniform covering



if training patterns inhomogenously distributed then first cluster analysis

choose center of basis function from each cluster, use cluster size for setting σ

advantages:

- additional training patterns → only local adjustment of weights
- optimal weights determinable in polynomial time
- regions not supported by RBF net can be identified by zero outputs

  (if output close to zero, verify that output of each basis function is close to zero)

disadvantages:

- number of neurons increases exponentially with input dimension
- unable to extrapolate (since there are no centers and RBFs are local)