technische universität dortmund

Computational Intelligence

Winter Term 2018/19

Prof. Dr. Günter Rudolph

Lehrstuhl für Algorithm Engineering (LS 11)

Fakultät für Informatik

TU Dortmund

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

Classification

given: set of training patterns (input / output)

$\tilde{x}_i$ (input), $\tilde{y}_i$ (output)

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

parameters:

$$f(x; (\tilde{x}_1, \tilde{y}_1), \ldots, (\tilde{x}_m, \tilde{y}_m), w_1, \ldots, w_n) \to \hat{y}$$

- x: input (unknown)
- $(\tilde{x}_1, \tilde{y}_1), \ldots, (\tilde{x}_m, \tilde{y}_m)$: training patterns (known)
- $w_1, \ldots, w_n$: weights (learnt)
- $\hat{y}$: output (guessed)

phase I:

train network

phase II:

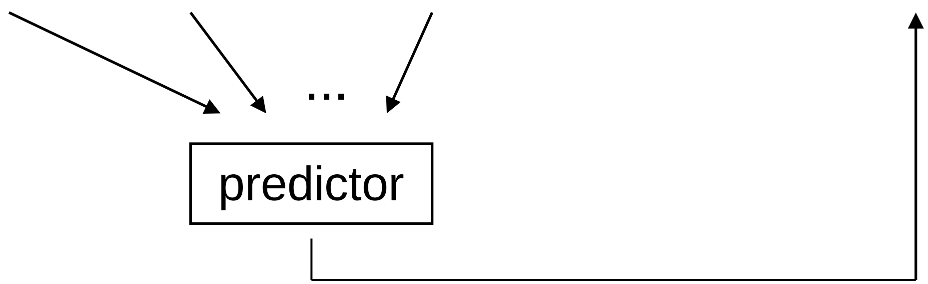
apply network to unkown inputs for classification

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

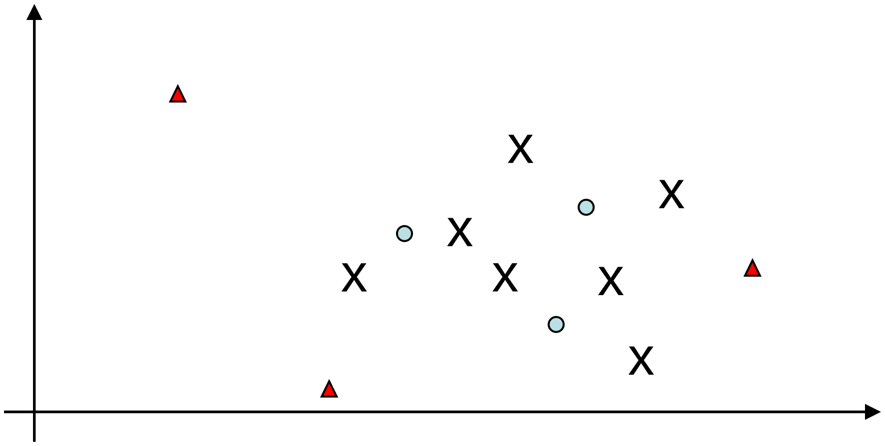
Function Approximation (the general case)

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**



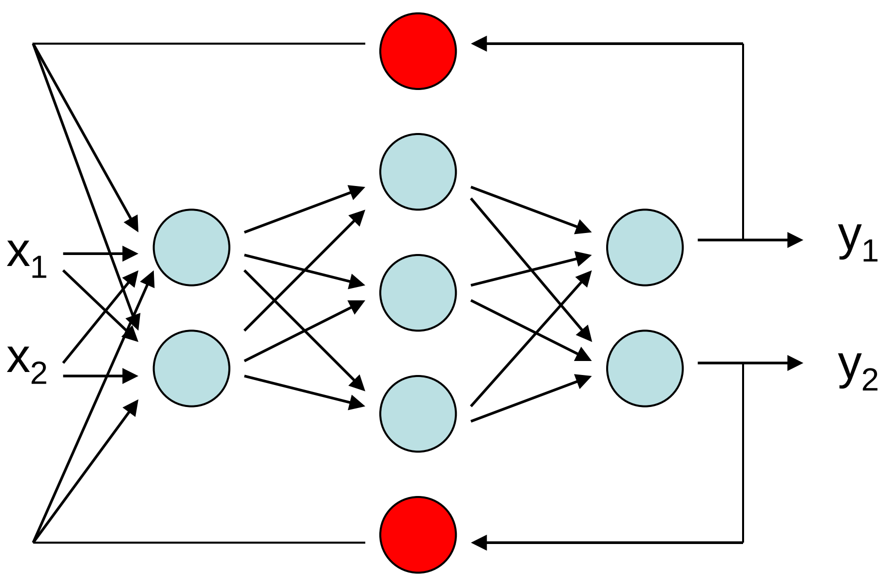
x : input training pattern

○ : 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



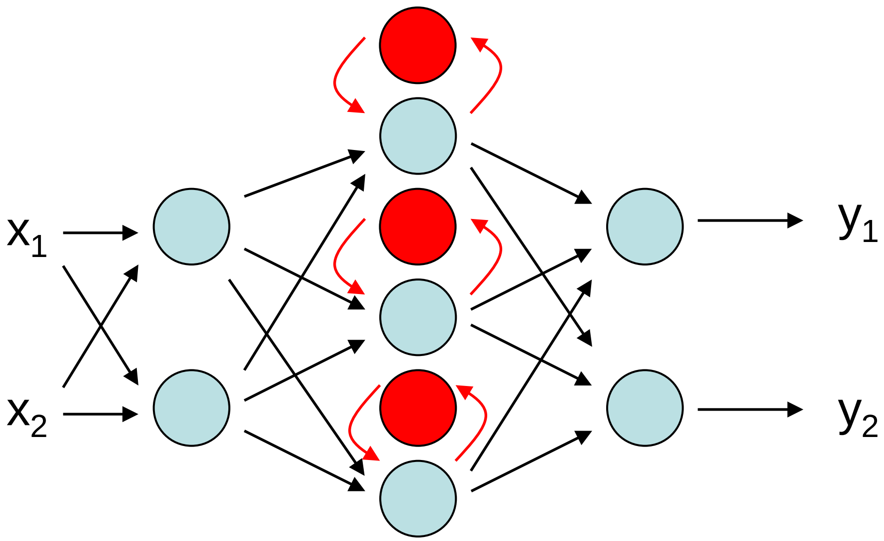
Jordan net =

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

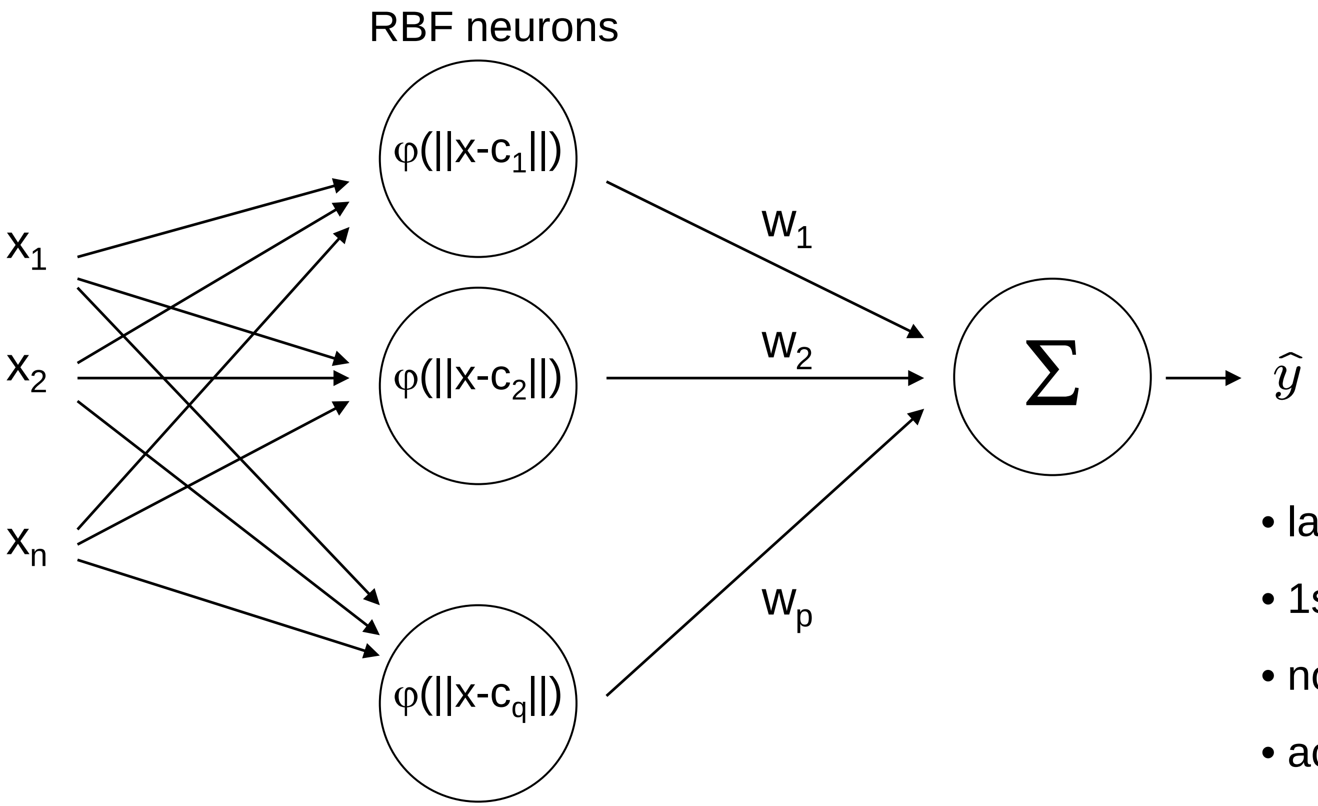
examples:

$\varphi(r) = \exp\left(-\frac{r^2}{\sigma^2}\right)$	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, ..., 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 $P: N \times q$, $y: N \times 1$, $w: q \times 1$,

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

<u>question:</u> how to justify this particular choice?

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

interpretation: minimize TSSE and prefer solutions with small values!

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

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

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

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

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

Tikhonov Regularization (1963)

question: 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
→ here: **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 $i \neq j$

$\text{PERF}(h; T) =$

(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)

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

$P'P$: $N^2 q$ inversion: q^3 $P'y$: qN multiplication: q^2

$O(N^2 q)$ elementary operations

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

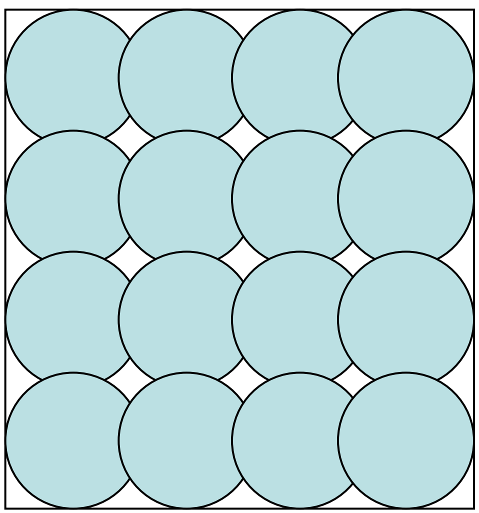
⇒ first analytic solution, then gradient descent starting from this solution

gradient descent: requires differentiable basis functions!

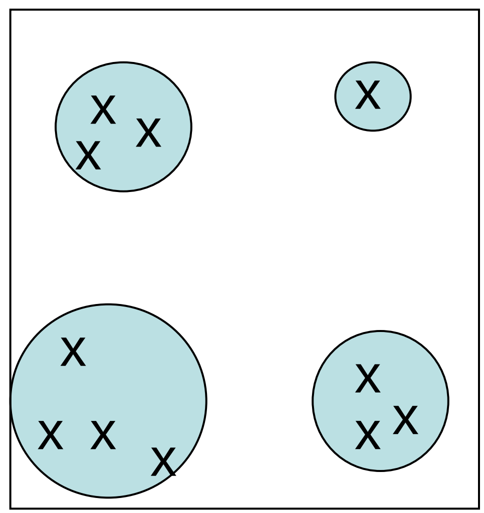
so far: tacitly assumed that RBF neurons are given

⇒ 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)

Example: XOR via RBF

training data: (0,0), (1,1) with value –1
(0,1), (1,0) with value +1

$$\varphi(r) = \exp\left(-\frac{1}{\sigma^2}\, r^2\right)$$

choose Gaussian kernel; set $\sigma = 1$; set centers c_i to training points

$$\hat{f}(x) = w_1\, \varphi(\|x - c_1\|) + w_2\, \varphi(\|x - c_2\|) + w_3\, \varphi(\|x - c_3\|) + w_4\, \varphi(\|x - c_4\|)$$

$$\begin{array}{lcccccccccc}
\hat{f}(0,0) & = & w_1 & + & e^{-1}\cdot w_2 & + & e^{-1}\cdot w_3 & + & e^{-2}\cdot w_4 & \overset{!}{=} & -1 \\
\hat{f}(0,1) & = & e^{-1}\cdot w_1 & + & w_2 & + & e^{-2}\cdot w_3 & + & e^{-1}\cdot w_4 & \overset{!}{=} & 1 \\
\hat{f}(1,0) & = & e^{-1}\cdot w_1 & + & e^{-2}\cdot w_2 & + & w_3 & + & e^{-1}\cdot w_4 & \overset{!}{=} & 1 \\
\hat{f}(1,1) & = & e^{-2}\cdot w_1 & + & e^{-1}\cdot w_2 & + & e^{-1}\cdot w_3 & + & w_4 & \overset{!}{=} & -1
\end{array}$$

$$P = \begin{pmatrix} 1 & e^{-1} & e & e^{-2} \\ e^{-1} & 1 & e^{-2} & e^{-1} \\ e^{-1} & e^{-2} & 1 & e^{-1} \\ e^{-2} & e^{-1} & e^{-1} & 1 \end{pmatrix} \quad y = \begin{pmatrix} -1 \\ 1 \\ 1 \\ -1 \end{pmatrix} \quad w^* = P^{-1}\, y = \frac{e^2}{(e-1)^2} \begin{pmatrix} -1 \\ 1 \\ 1 \\ -1 \end{pmatrix}$$

Example: XOR via RBF

$$\hat{f}(x) = \frac{e^2}{(e-1)^2} \cdot \left[-e^{-x_1^2 - x_2^2} + e^{-x_1^2 - (x_2-1)^2} + e^{-(x_1-1)^2 - x_2^2} - e^{-(x_1-1)^2 - (x_2-1)^2} \right]$$