

Computational Intelligence

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Lehrstuhl für Algorithm Engineering (LS 11)

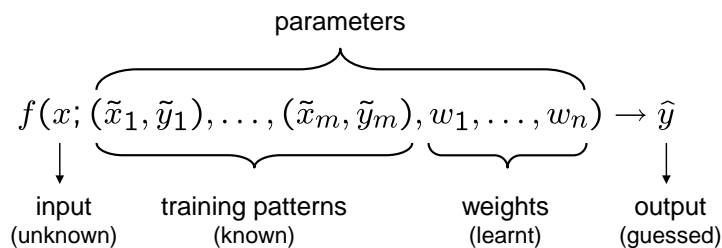
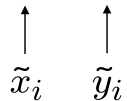
Fakultät für Informatik

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

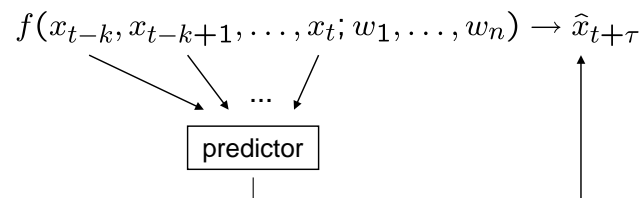


- phase I:**
train network
- phase II:**
apply network to unknown inputs for classification

Prediction of Time Series

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

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



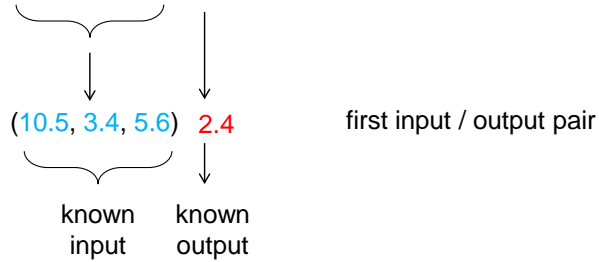
- phase I:**
train network
- phase II:**
apply network to historical inputs for predicting unknown outputs

training patterns:
 historical data where true output is known;
 error per pattern = $(\hat{x}_{t+\tau} - x_{t+\tau})^2$

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: $k=3$



further input / output pairs:

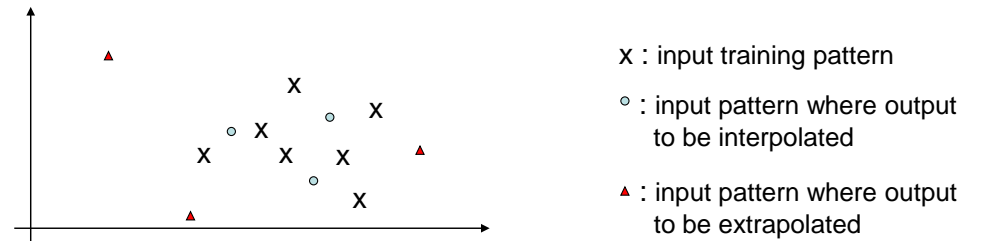
- (3.4, 5.6, 2.4) → 5.9
- (5.6, 2.4, 5.9) → 8.4
- (2.4, 5.9, 8.4) → 3.9
- (5.9, 8.4, 3.9) → 4.4
- (8.4, 3.9, 4.4) → 1.7

Function Approximation (the general case)

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

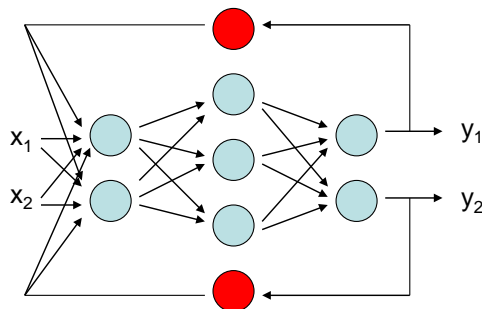
→ should give outputs close to true unknown function for arbitrary inputs

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



Jordan nets (1986)

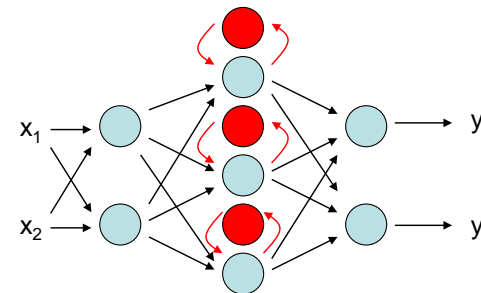
- **context neuron:** reads output from some neuron at step t and feeds value into net at step $t+1$



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 $\phi : \mathbb{R}^n \rightarrow \mathbb{R}$ is termed **radial basis function** iff $\exists \varphi : \mathbb{R} \rightarrow \mathbb{R} : \forall x \in \mathbb{R}^n : \phi(x; c) = \varphi(\|x - c\|)$. □

Definition:

RBF **local** iff $\varphi(r) \rightarrow 0$ as $r \rightarrow \infty$ □

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

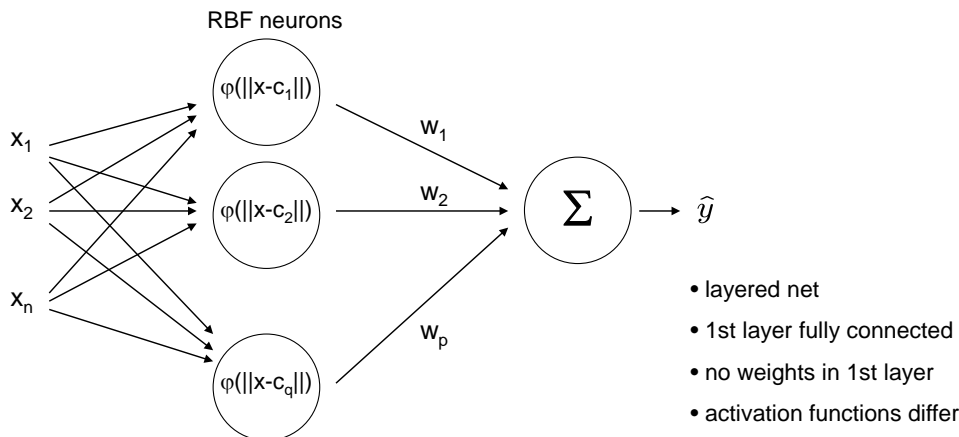
examples:

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

Definition:

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

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



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

find : weights w_1, \dots, w_q with minimal error

solution:

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

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

unknown known value known value

$$\Rightarrow \sum_{k=1}^q w_k \cdot p_{ik} = y_i \quad \Rightarrow N \text{ linear equations with } q \text{ unknowns}$$

in matrix form: $Pw = y$ 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

$Pw = y$ | $\cdot P'$ from left hand side (P' is transpose of P)

$P'Pw = P'y$ | $\cdot (P'P)^{-1}$ from left hand side

$(P'P)^{-1}P'Pw = (P'P)^{-1}P'y$ | simplify

unit matrix

P^+

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

Tikhonov Regularization (1963)

idea:

choose $(P'P + hI_q)^{-1}$ 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 $\Leftrightarrow \text{rank}(A) = n \Leftrightarrow A^{-1}$ 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)

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

question: how to justify this particular choice?

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

interpretation: minimize TSSE and prefer solutions with small values!

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

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

$2P'Pw - 2P'y + 2hw = 2(P'P + hI_q)w - 2P'y \stackrel{!}{=} 0$

$\Rightarrow w^* = (P'P + hI_q)^{-1}P'y$

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

Tikhonov Regularization (1963)

question: how to find appropriate $h > 0$ in $(P'P + hI_q)$?

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

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

\rightarrow several approaches in use

\rightarrow here: **grid search** and **crossvalidation**

(1) choose $n \in \mathbb{N}$ and $h_1, \dots, h_n \in (0, H] \subset \mathbb{R}^+$; set $p^* = 0$

(2) for $i = 1$ to n

(3) $p_i = \text{PERF}(h_i; T)$

(4) if $p_i > p^*$

(5) $p^* = p_i; k = i;$

(6) endif

(7) endfor

(8) return h_k

} grid search

Crossvalidation

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

$$T_1 \cup \dots \cup T_k = T$$

$$T_i \cap T_j = \emptyset \text{ for } i \neq j$$

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

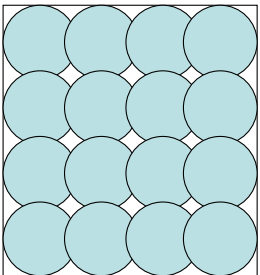
remark: if N large then inaccuracies for $P'P$ likely

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

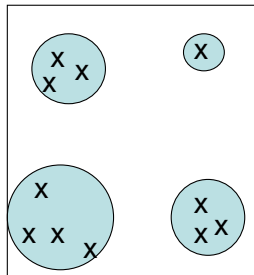
requires
differentiable
basis functions!

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)