

Computational Intelligence

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Computational Intelligence

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- Radial Basis Function Nets (RBF Nets)

- Model
- Training

- Hopfield Networks

- Model
- Optimization

Definition:

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

Definition:

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

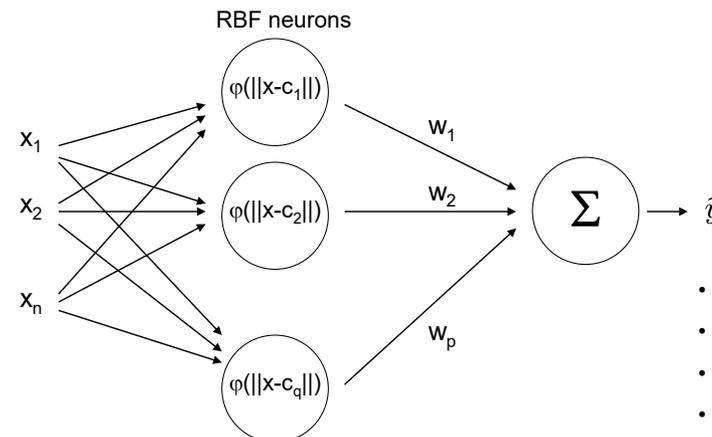
typically, $\|x\|$ denotes Euclidean norm of vector x

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



- 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, \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: $P w = y$ 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

$$\begin{array}{ll}
 P w = y & | \cdot P' \text{ from left hand side (} P' \text{ is transpose of } P) \\
 P' P w = P' y & | \cdot (P' P)^{-1} \text{ from left hand side} \\
 \underbrace{(P' P)^{-1}}_{\text{unit matrix}} P' P w = \underbrace{(P' P)^{-1}}_{P^+} P' y & | \text{ simplify}
 \end{array}$$

- 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 $\forall x \in \mathbb{R}^n : x' A x \geq 0$
 Def : matrix A positive definite (p.d.) iff $\forall x \in \mathbb{R}^n \setminus \{0\} : x' A x > 0$
 Thm : matrix A : $n \times n$ regular $\Leftrightarrow \text{rank}(A) = n \Leftrightarrow A^{-1}$ exists $\Leftrightarrow A$ 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 : $\forall x \in \mathbb{R}^n \setminus \{0\} : x'(a \cdot A + b \cdot B)x = \underbrace{a \cdot x' A x}_{> 0} + \underbrace{b \cdot x' B x}_{\geq 0} > 0$ q.e.d.

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

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

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

interpretation: minimize TSSE and prefer solutions with small values!

avoid overfitting

$$\begin{aligned}
 \frac{d}{dw} [(P w - y)'(P w - y) + h \cdot w' w] &= \\
 \frac{d}{dw} [(w' P' P w - w' P' y - y' P w + y' y + h \cdot w' w)] &= \\
 2 P' P w - 2 P' y + 2 h w &= 2 (P' P + h I_q) w - 2 P' y \stackrel{!}{=} 0 \\
 \Rightarrow w^* &= (P' P + h I_q)^{-1} P' y
 \end{aligned}$$

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

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

→ several approaches in use
→ 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

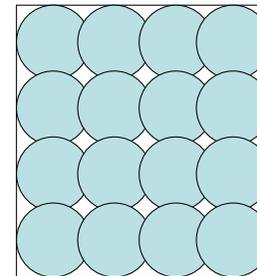
⇒ first analytic solution, then gradient descent starting from this solution

requires differentiable basis functions!

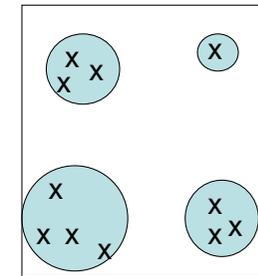
so far: tacitly assumed that RBF neurons are given

⇒ center c_k and radii σ considered given and known

how to choose c_k and σ ?



uniform covering



if training patterns inhomogeneously 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

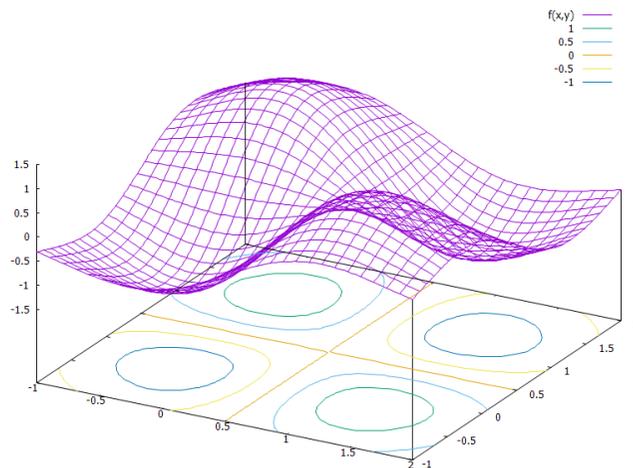
$$\hat{f}(x) = w_1 \varphi(\|x - c_1\|) + w_2 \varphi(\|x - c_2\|) + w_3 \varphi(\|x - c_3\|) + w_4 \varphi(\|x - c_4\|)$$

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

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

Example: XOR via RBF

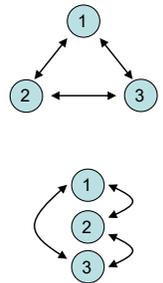
$$\hat{f}(x) = \frac{e^2}{(e-1)^2} \cdot \left[-e^{-x_1^2 - x_2^2} + e^{-x_1^2 - (x_2-1)^2} + e^{-(x_1-1)^2 - x_2^2} - e^{-(x_1-1)^2 - (x_2-1)^2} \right]$$



proposed 1982

characterization:

- neurons preserve state until selected at random for update
- bipolar states: $x \in \{-1, +1\}^n$
- n neurons fully connected
- symmetric weight matrix
- no self-loops (→ zero main diagonal entries)
- thresholds θ , neuron i fires if excitations larger than θ_i



transition: select index k at random, new state is $\tilde{x} = \text{sgn}(xW - \theta)$

$$\text{where } \tilde{x} = (x_1, \dots, x_{k-1}, \tilde{x}_k, x_{k+1}, \dots, x_n)$$

energy of state x is $E(x) = -\frac{1}{2} xWx' + \theta x'$

Fixed Points

Definition

x is **fixed point** of a Hopfield network iff $x = \text{sgn}(x' W - \theta)$. \square

Example:

Set $W = x x'$ and choose θ with $|\theta_i| < n$, where $x \in \{-1, +1\}^n$.

$$\rightarrow \text{sgn}(x' W - \theta) = \text{sgn}(x' (x x')) = \text{sgn}(x' x x' - \theta) = \text{sgn}(\|x\|^2 x' - \theta)$$

Note that $\|x\|^2 = n$ for all $x \in \{-1, +1\}^n$.

$$\rightarrow x_i = +1: \text{sgn}(n \cdot (+1) - \theta_i) = +1 \text{ iff } +n - \theta_i \geq 0 \Leftrightarrow \theta_i \leq +n$$

$$\rightarrow x_i = -1: \text{sgn}(n \cdot (-1) - \theta_i) = -1 \text{ iff } -n - \theta_i < 0 \Leftrightarrow \theta_i > -n$$

Theorem:

If $W = x x'$ and $|\theta_i| < n$ then x is fixed point of a Hopfield network. \square

Concept of Energy Function

given: HN with $W = x x'$ $\Rightarrow x$ is stable state of HN

starting point $x^{(0)}$ $\Rightarrow x^{(1)} = \text{sgn}(x^{(0)'} W - \theta)$

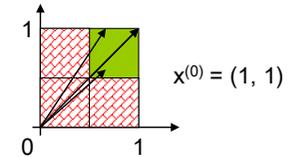
\Rightarrow excitation $e = W x^{(1)} - \theta$

\Rightarrow if $\text{sign}(e) = x^{(0)}$ then $x^{(0)}$ stable state

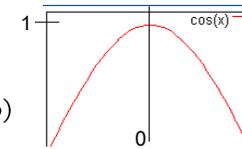
small angle between e' and $x^{(0)}$



true if e' close to $x^{(0)}$



recall: $\frac{ab'}{\|a\| \cdot \|b\|} = \cos \angle(a, b)$



small angle $\alpha \Rightarrow$ large $\cos(\alpha)$

Concept of Energy Function

required:

small angle between $e = W x^{(0)} - \theta$ and $x^{(0)}$

\Rightarrow larger cosine of angle indicates greater similarity of vectors

$$\Rightarrow \forall e' \text{ of equal size: try to maximize } x^{(0)'} e' = \underbrace{\|x^{(0)}\|}_{\text{fixed}} \cdot \underbrace{\|e'\|}_{\text{fixed}} \cdot \underbrace{\cos \angle(x^{(0)}, e')}_{\rightarrow \text{max!}}$$

\Rightarrow maximize $x^{(0)'} e = x^{(0)'} (W x^{(0)} - \theta) = x^{(0)'} W x^{(0)} - \theta' x^{(0)}$

\Rightarrow identical to minimize $-x^{(0)'} W x^{(0)} + \theta' x^{(0)}$

Definition

Energy function of HN at iteration t is $E(x^{(t)}) = -\frac{1}{2} x^{(t)'} W x^{(t)} + \theta' x^{(t)}$ \square

Theorem:

Hopfield network converges to local minimum of energy function after a finite number of updates. \square

Proof: assume that x_k has been updated $\tilde{x}_k = -x_k$ and $\tilde{x}_i = x_i$ for $i \neq k$

$$\begin{aligned} E(x) - E(\tilde{x}) &= -\frac{1}{2} x' W x + \theta' x + \frac{1}{2} \tilde{x}' W \tilde{x} - \theta' \tilde{x} \\ &= -\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n w_{ij} x_i x_j + \sum_{i=1}^n \theta_i x_i + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n w_{ij} \tilde{x}_i \tilde{x}_j - \sum_{i=1}^n \theta_i \tilde{x}_i \\ &= -\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n w_{ij} (x_i x_j - \tilde{x}_i \tilde{x}_j) + \sum_{i=1}^n \theta_i \underbrace{(x_i - \tilde{x}_i)}_{=0 \text{ if } i \neq k} \\ &= -\frac{1}{2} \sum_{\substack{i=1 \\ i \neq k}}^n \sum_{j=1}^n w_{ij} (x_i x_j - \tilde{x}_i \tilde{x}_j) - \frac{1}{2} \sum_{j=1}^n w_{kj} \underbrace{(x_k x_j - \tilde{x}_k \tilde{x}_j)}_{\substack{0 \text{ if } j = k \\ x_j \text{ if } j \neq k}} + \theta_k (x_k - \tilde{x}_k) \end{aligned}$$

$$\begin{aligned}
&= -\frac{1}{2} \sum_{\substack{i=1 \\ i \neq k}}^n \sum_{j=1}^n w_{ij} x_i \underbrace{(x_j - \tilde{x}_j)}_{=0 \text{ if } j \neq k} - \frac{1}{2} \sum_{\substack{j=1 \\ j \neq k}}^n w_{kj} x_j (x_k - \tilde{x}_k) + \theta_k (x_k - \tilde{x}_k) \\
&= -\frac{1}{2} \sum_{\substack{i=1 \\ i \neq k}}^n w_{ik} x_i (x_k - \tilde{x}_k) - \frac{1}{2} \sum_{\substack{j=1 \\ j \neq k}}^n w_{kj} x_j (x_k - \tilde{x}_k) + \theta_k (x_k - \tilde{x}_k) \\
&\quad \text{(rename } j \text{ to } i, \text{ recall } W = W', w_{kk} = 0) \\
&= -\sum_{i=1}^n w_{ik} x_i (x_k - \tilde{x}_k) + \theta_k (x_k - \tilde{x}_k) \\
&= -(x_k - \tilde{x}_k) \underbrace{\left[\sum_{i=1}^n w_{ik} x_i - \theta_k \right]}_{\text{excitation } e_k} > 0 \quad \text{since:} \\
&\quad > 0 \text{ if } x_k < 0 \text{ and vice versa}
\end{aligned}$$

x_k	$x_k - \tilde{x}_k$	$e_k - \theta_k$	ΔE
+1	> 0	< 0	> 0
-1	< 0	> 0	> 0

⇒ every update (change of state) decreases energy function
 ⇒ since number of different bipolar vectors is finite
 update stops after finite #updates

remark: dynamics of HN get stable in local minimum of energy function!

q.e.d.

⇒ Hopfield network can be used to optimize combinatorial optimization problems!

Application to Combinatorial Optimization

Idea:

- transform combinatorial optimization problem as objective function with $x \in \{-1, +1\}^n$
- rearrange objective function to look like a Hopfield energy function
- extract weights W and thresholds θ from this energy function
- initialize a Hopfield net with these parameters W and θ
- run the Hopfield net until reaching stable state (= local minimizer of energy function)
- stable state is local minimizer of combinatorial optimization problem

Example I: Linear Functions

$$f(x) = \sum_{i=1}^n c_i x_i \rightarrow \min! \quad (x_i \in \{-1, +1\})$$

Evidently: $E(x) = f(x)$ with $W = 0$ and $\theta = c$

⇓

choose $x^{(0)} \in \{-1, +1\}^n$
 set iteration counter $t = 0$
 repeat
 choose index k at random

$$x_k^{(t+1)} = \text{sgn}(x^{(t)} \cdot W_{\cdot, k} - \theta_k) = \text{sgn}(x^{(t)} \cdot 0 - c_k) = -\text{sgn}(c_k) = \begin{cases} -1 & \text{if } c_k > 0 \\ +1 & \text{if } c_k < 0 \end{cases}$$
 increment t
 until reaching fixed point

⇒ fixed point reached after $\Theta(n \log n)$ iterations on average

[proof: → black board]

Example II: MAXCUT

given: graph with n nodes and symmetric weights $\omega_{ij} = \omega_{ji}$, $\omega_{ii} = 0$, on edges

task: find a partition $V = (V_0, V_1)$ of the nodes such that the weighted sum of edges with one endpoint in V_0 and one endpoint in V_1 becomes maximal

encoding: $\forall i=1, \dots, n$: $y_i = 0$, node i in set V_0 ; $y_i = 1$, node i in set V_1

objective function: $f(y) = \sum_{i=1}^{n-1} \sum_{j=i+1}^n \omega_{ij} [y_i(1-y_j) + y_j(1-y_i)] \rightarrow \max!$

preparations for applying Hopfield network

step 1: conversion to minimization problem

step 2: transformation of variables

step 3: transformation to "Hopfield normal form"

step 4: extract coefficients as weights and thresholds of Hopfield net

Example II: MAXCUT (continued)

step 1: conversion to minimization problem

\Rightarrow multiply function with $-1 \Rightarrow E(y) = -f(y) \rightarrow \min!$

step 2: transformation of variables

$\Rightarrow y_i = (x_i + 1) / 2$

$$\Rightarrow f(x) = \sum_{i=1}^{n-1} \sum_{j=i+1}^n \omega_{ij} \left[\frac{x_i + 1}{2} \left(1 - \frac{x_j + 1}{2} \right) + \frac{x_j + 1}{2} \left(1 - \frac{x_i + 1}{2} \right) \right]$$

$$= \frac{1}{2} \sum_{i=1}^{n-1} \sum_{j=i+1}^n \omega_{ij} [1 - x_i x_j]$$

$$= \frac{1}{2} \sum_{i=1}^{n-1} \sum_{j=i+1}^n \omega_{ij} - \frac{1}{2} \sum_{i=1}^{n-1} \sum_{j=i+1}^n \omega_{ij} x_i x_j$$

constant value (does not affect location of optimal solution)

Example II: MAXCUT (continued)

step 3: transformation to "Hopfield normal form"

$$E(x) = \frac{1}{2} \sum_{i=1}^{n-1} \sum_{j=i+1}^n \omega_{ij} x_i x_j = -\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \underbrace{\left(-\frac{1}{2} \omega_{ij} \right)}_{w_{ij}} x_i x_j$$

$$= -\frac{1}{2} x' W x + \theta' x$$

$$\downarrow$$

$$0'$$

step 4: extract coefficients as weights and thresholds of Hopfield net

$$w_{ij} = -\frac{\omega_{ij}}{2} \text{ for } i \neq j, \quad w_{ii} = 0, \quad \theta_i = 0$$

remark: ω_{ij} : weights in graph — w_{ij} : weights in Hopfield net