

Computational Intelligence

Winter Term 2020/21

Prof. Dr. Günter Rudolph

Lehrstuhl für Algorithm Engineering (LS 11)

Fakultät für Informatik

TU Dortmund

- Introduction to Artificial Neural Networks
 - McCulloch Pitts Neuron (MCP)
 - Minsky / Papert Perceptron (MPP)

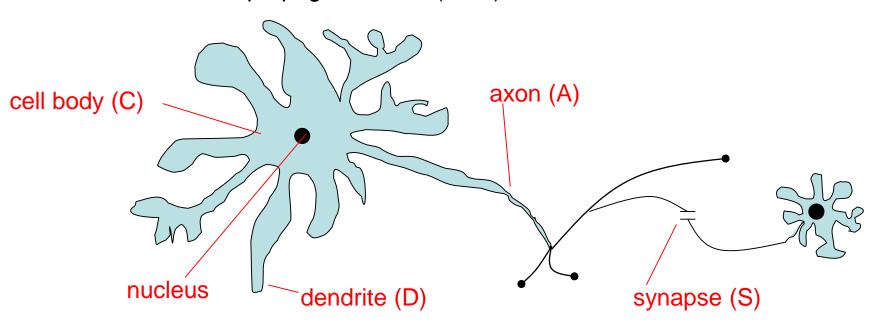
Biological Prototype

- Neuron
 - Information gathering (D)
 - Information processing (C)
 - Information propagation (A / S)

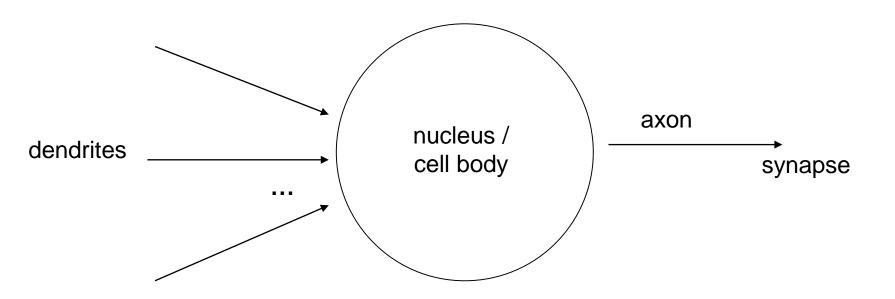
human being: 10¹² neurons

electricity in mV range

speed: 120 m/s



Abstraction

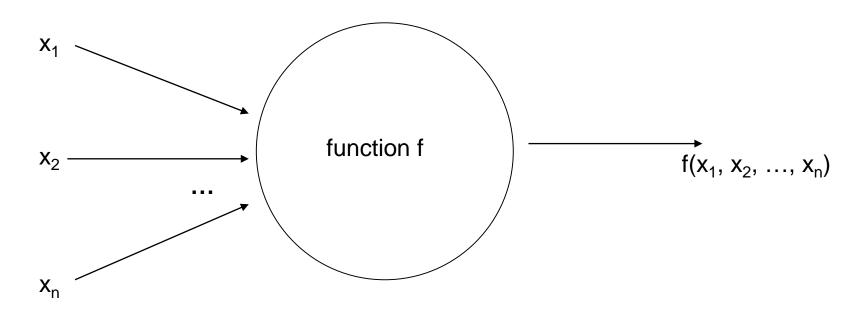


signal input

signal processing

signal output

Model



McCulloch-Pitts-Neuron 1943:

$$x_i \in \{0, 1\} =: B$$

 $f: B^n \to B$

1943: Warren McCulloch / Walter Pitts

- description of neurological networks
 - → modell: McCulloch-Pitts-Neuron (MCP)
- basic idea:
 - neuron is either active or inactive
 - skills result from *connecting* neurons
- considered static networks
 (i.e. connections had been constructed and not learnt)

McCulloch-Pitts-Neuron

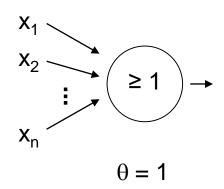
n binary input signals $x_1, ..., x_n$

threshold $\theta > 0$

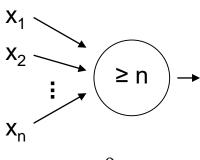
$$f(x_1, \dots, x_n) = \begin{cases} 1 & \text{if } \sum_{i=1}^n x_i \ge \theta \\ 0 & \text{else} \end{cases}$$

boolean OR

⇒ can be realized:



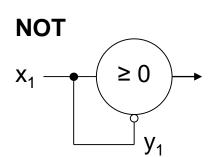
boolean AND



McCulloch-Pitts-Neuron

n binary input signals $x_1, ..., x_n$ threshold $\theta > 0$

in addition: m binary inhibitory signals y₁, ..., y_m

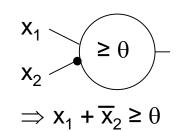


$$\tilde{f}(x_1,\ldots,x_n;y_1,\ldots,y_m) = f(x_1,\ldots,x_n) \cdot \prod_{j=1}^m (1-y_j)$$

- if at least one $y_i = 1$, then output = 0
- otherwise:
 - sum of inputs ≥ threshold, then output = 1 else output = 0

Assumption:

inputs also available in inverted form, i.e. ∃ inverted inputs.

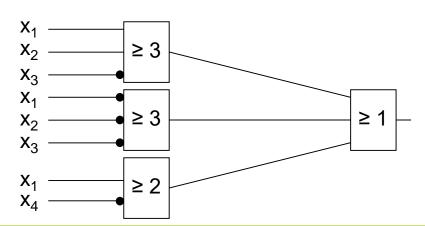


Theorem:

Every logical function F: $B^n \to B$ can be simulated with a two-layered McCulloch/Pitts net.

Example:

$$F(x) = x_1 x_2 \bar{x}_3 \vee \bar{x}_1 \bar{x}_2 \bar{x}_3 \vee x_1 \bar{x}_4$$



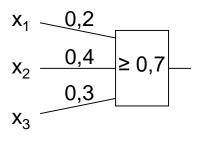
Proof: (by construction)

Every boolean function F can be transformed in disjunctive normal form

- ⇒ 2 layers (AND OR)
- 1. Every clause gets a decoding neuron with $\theta = n$ \Rightarrow output = 1 only if clause satisfied (AND gate)
- 2. All outputs of decoding neurons are inputs of a neuron with $\theta = 1$ (OR gate)

q.e.d.

Generalization: inputs with weights



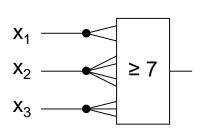
fires 1 if

$$0.2 x_1 + 0.4 x_2 + 0.3 x_3 \ge 0.7$$

$$2 x_1 + 4 x_2 + 3 x_3 \ge 7$$

$$\downarrow \downarrow$$

duplicate inputs!



Theorem:

Weighted and unweighted MCP-nets are equivalent for weights $\in \mathbb{Q}^+$.

Proof:

Let $\sum_{i=1}^{n} \frac{a_i}{b_i} x_i \geq \frac{a_0}{b_0}$ with $a_i, b_i \in \mathbb{N}$

Multiplication with $\prod_{i=0}^{n} b_i$ yields inequality with coefficients in N

Duplicate input x_i , such that we get $a_i b_1 b_2 \cdots b_{i-1} b_{i+1} \cdots b_n$ inputs.

Threshold $\theta = a_0 b_1 \cdots b_n$

Set all weights to 1.

q.e.d.

Conclusion for MCP nets:

- + feed-forward: able to compute any Boolean function
- + recursive: able to simulate DFA (deterministic finite automaton)
- very similar to conventional logical circuits
- difficult to construct
- no good learning algorithm available

Perceptron (Rosenblatt 1958)

- → complex model → reduced by Minsky & Papert to what is "necessary"
- \rightarrow Minsky-Papert perceptron (MPP), 1969 \rightarrow essential difference: $x \in [0,1] \subset \mathbb{R}$

What can a single MPP do?

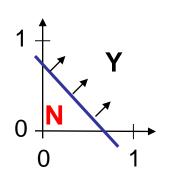
$$w_1 x_1 + w_2 x_2 \ge \theta$$

isolation of x₂ yields:

Example:

$$0,9x_1+0,8x_2 \ge 0,6$$

$$\Leftrightarrow x_2 \ge \frac{3}{4} - \frac{9}{8}x_1$$



separating line

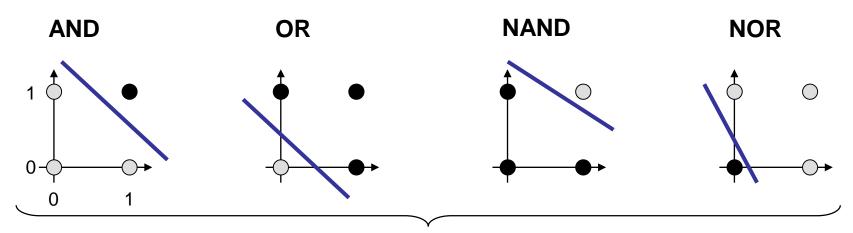
 $\underline{\text{separates}} \ \mathbb{R}^2$

in 2 classes

Introduction to Artificial Neural Networks

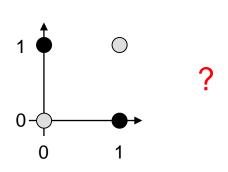
Lecture 09

$$\bigcirc = 0$$
 $\bullet = 1$

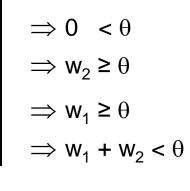


→ MPP at least as powerful as MCP neuron!





| X ₁ | X_2 | xor |
|-----------------------|-------|-----|
| 0 | 0 | 0 |
| 0 | 1 | 1 |
| 1 | 0 | 1 |
| 1 | 1 | 0 |



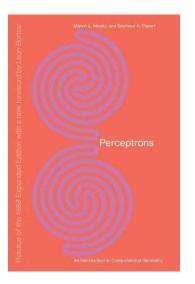
$$\begin{array}{c} w_1, w_2 \ge \theta > 0 \\ \Rightarrow w_1 + w_2 \ge 2\theta \\ \hline \\ \text{contradiction!} \end{array}$$

$$W_1 X_1 + W_2 X_2 \ge \theta$$

1969: Marvin Minsky / Seymor Papert

- book Perceptrons → analysis math. properties of perceptrons
- disillusioning result:perceptions fail to solve a number of trivial problems!
 - XOR Problem
 - Parity Problem
 - Connectivity Problem
- "conclusion": all artificial neurons have this kind of weakness!
 - ⇒ research in this field is a scientific dead end!

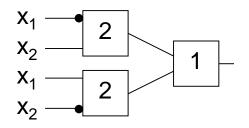






how to leave the "dead end":

<u>Multilayer</u> Perceptrons:

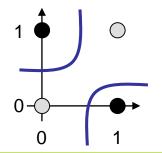


⇒ realizes XOR

Nonlinear separating functions:

XOR

$$g(x_1, x_2) = 2x_1 + 2x_2 - 4x_1x_2 - 1$$
 with $\theta = 0$



$$g(0,0) = -1$$

 $g(0,1) = +1$

$$g(0,1) = +1$$

$$g(1,0) = +1$$

$$g(1,1) = -1$$

How to obtain weights w_i and threshold θ ?

as yet: by construction

example: NAND-gate

| X ₁ | X ₂ | NAND |
|-----------------------|----------------|------|
| 0 | 0 | 1 |
| 0 | 1 | 1 |
| 1 | 0 | 1 |
| 1 | 1 | 0 |

$$\Rightarrow 0 \ge \theta$$

$$\Rightarrow w_2 \ge \theta$$

$$\Rightarrow w_1 \ge \theta$$

$$\Rightarrow w_1 + w_2 < \theta$$

requires solution of a system of linear inequalities (∈ P)

(e.g.:
$$W_1 = W_2 = -2$$
, $\theta = -3$)

now: by "learning" / training

Perceptron Learning

Assumption: test examples with correct I/O behavior available

Principle:

- (1) choose initial weights in arbitrary manner
- (2) feed in test pattern
- (3) if output of perceptron wrong, then change weights
- (4) goto (2) until correct output for all test paterns

graphically:

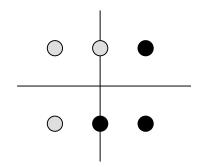


→ translation and rotation of separating lines

Introduction to Artificial Neural Networks

Lecture 09

Example



$$P = \left\{ \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \begin{pmatrix} 0 \\ -1 \end{pmatrix} \right\} \quad \bullet$$

$$N = \left\{ \begin{pmatrix} -1 \\ -1 \end{pmatrix}, \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\} \quad \bigcirc$$

threshold as a weight: $w = (\theta, w_1, w_2)^{\circ}$



$$P = \left\{ \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \right\}$$

$$N = \left\{ \begin{pmatrix} 1 \\ -1 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \right\}$$

$$\begin{array}{c|c}
1 & -\theta \\
x_1 & w_1 \\
x_2 & w_2
\end{array} \ge 0$$

$$w_1x_1 + w_2x_2 \ge \theta \iff w_1x_1 + w_2x_2 - \theta \cdot 1 \ge 0$$

$$w_0 \quad x_0$$

 \Rightarrow separating hyperplane:

$$H(w) = \{ x : h(x;w) = 0 \}$$

where

$$h(x;w) = w'x = w_0x_0 + w_1x_1 + ... + w_nx_n$$

 \Rightarrow origin $0 \in H(w)$ since h(0;w) = 0

Introduction to Artificial Neural Networks

Lecture 09

Perceptron Learning

P: set of positive examples N: set of negative examples

→ output 1 \rightarrow output 0

threshold θ integrated in weights

- 1. choose w_0 at random, t = 0
- 2. choose arbitrary $x \in P \cup N$
- 3. if $x \in P$ and w_t 'x > 0 then goto 2 if $x \in N$ and $w_t, x \le 0$ then goto 2
- 4. if $x \in P$ and w_t ' $x \le 0$ then $W_{t+1} = W_t + X$; t++; goto 2
- 5. if $x \in N$ and w_t 'x > 0 then $W_{t+1} = W_t - X$; t++; goto 2

6. stop? If I/O correct for all examples!

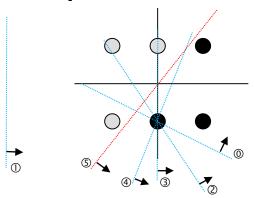
I/O correct!

let w'x \leq 0, should be > 0! (w+x)'x = w'x + x'x > w'x

let w'x > 0, should be $\leq 0!$ (w-x)'x = w'x - x'x < w'x

remark: if separating H(w*) exists, then algorithm converges, is finite (but in worst case: exponential runtime)

Example



suppose initial vector of weights is

$$W^{(0)} = (1, \frac{1}{2}, 1)$$

```
> w = SPL(m,c(1,0.5,1))
[1] 1.0 0.5 1.0
[1] 2.0 0.5 0.0
[1] 1.0 1.5 1.0
[1] 0.0 2.5 0.0
[1] -1.0 2.5 -1.0
[1] 0.0 2.5 -2.0
```

```
SPL <- function(m,w) {</pre>
  print(w)
  repeat {
    OK <- TRUE
    for (i in 1:nrow(m)) {
      x <- m[i,]
       s \leftarrow x[1]*w[1]+x[2]*w[2]+x[3]*w[3]
       if (s <= 0) {
         OK <- FALSE
         W \leftarrow W + X
         print(w) # show every change
    if (OK) break;
  return(w)
}
```

```
m <- matrix( # only positive examples
  c(c(1,1,1),c(1,1,-1),c(1,0,-1),
      c(-1,1,1),c(-1,1,-1),c(-1,0,-1)),
  nrow=6,byrow=TRUE)</pre>
```

Acceleration of Perceptron Learning

Assumption:
$$x \in \{0, 1\}^n \Rightarrow ||x|| = \sum_{i=1}^n |x_i| \ge 1 \text{ for all } x \ne (0, ..., 0)$$

Let B = P
$$\cup$$
 { -x : x \in N }

(only positive examples)

If classification incorrect, then w'x < 0. ◆

Consequently, size of error is just $\delta = -w'x > 0$.

$$\Rightarrow$$
 $w_{t+1} = w_t + (\delta + \varepsilon) x$ for $\varepsilon > 0$ (small) corrects error in a single step, since

$$w'_{t+1}x = (w_t + (\delta + \varepsilon) x)' x$$

$$= w'_t x + (\delta + \varepsilon) x' x$$

$$= -\delta + \delta ||x||^2 + \varepsilon ||x||^2$$

$$= \delta (||x||^2 - 1) + \varepsilon ||x||^2 > 0$$

$$\geq 0 > 0$$

Generalization:

Assumption:
$$x \in \mathbb{R}^n \implies ||x|| > 0$$
 for all $x \neq (0, ..., 0)$

as before:
$$w_{t+1} = w_t + (\delta + \epsilon) x$$
 for $\epsilon > 0$ (small) and $\delta = -w_t' x > 0$

$$\Rightarrow W'_{t+1}x = \delta(||x||^2 - 1) + \varepsilon ||x||^2$$

$$< 0 \text{ possible!} > 0$$

Claim: Scaling of data does not alter classification task (if threshold 0)!

Let
$$\ell = \min \{ || x || : x \in B \} > 0$$

Set
$$\hat{X} = \frac{X}{\ell}$$
 \Rightarrow set of scaled examples \hat{B}

$$\Rightarrow || \hat{\mathbf{x}} || \ge 1 \quad \Rightarrow \quad || \hat{\mathbf{x}} ||^2 - 1 \ge 0 \quad \Rightarrow \quad \mathbf{w'}_{t+1} \hat{\mathbf{x}} > 0 \quad \mathbf{\square}$$

Theorem:

Let $X = P \cup N$ with $P \cap N = \emptyset$ be training patterns (P: positive; N: negative examples). Suppose training patterns are embedded in \mathbb{R}^{n+1} with threshold 0 and origin $0 \notin X$.

If separating hyperplane H(w) exists, then scaling of data does not alter classification task!

Proof:

Suppose $\exists x \in P \cup N$ with ||x|| < 1 and let $\ell = \min\{ ||x|| : x \in P \cup N \} > 0$.

Set
$$\hat{x} = \frac{1}{\ell} x$$
 so that $\hat{P} = \{ \frac{x}{\ell} : x \in P \}$ and $\hat{N} = \{ \frac{x}{\ell} : x \in N \}$.

Suppose $\exists w \text{ with } \forall \hat{x} \in \hat{P} : w'\hat{x} > 0 \text{ and } \forall \hat{x} \in \hat{N} : w'\hat{x} \leq 0.$

Then holds:

$$\mathbf{w}'\hat{\mathbf{x}} > 0 \iff \mathbf{w}'\frac{\mathbf{x}}{\ell} > 0 \iff \mathbf{w}'\mathbf{x} > 0$$

$$w'\hat{x} \le 0 \Leftrightarrow w'\frac{x}{\ell} \le 0 \Leftrightarrow w'x \le 0$$

q.e.d.

There exist numerous variants of Perceptron Learning Methods.

Theorem: (Duda & Hart 1973)

If rule for correcting weights is $w_{t+1} = w_t + \gamma_t x$ (i.e., if $w_t' x < 0$) and

1.
$$\forall t \ge 0 : \gamma_t \ge 0$$

$$2. \sum_{t=0}^{\infty} \gamma_t = \infty$$

3.
$$\lim_{m \to \infty} \frac{\sum_{t=0}^{m} \gamma_t^2}{\left(\sum_{t=0}^{m} \gamma_t\right)^2} = 0$$

then $w_t \to w^*$ for $t \to \infty$ with $\forall x: x'w^* > 0$.

e.g.:
$$\gamma_t = \gamma > 0$$
 or $\gamma_t = \gamma / (t+1)$ for $\gamma > 0$

as yet: Online Learning

→ Update of weights after each training pattern (if necessary)

now: Batch Learning

- → Update of weights only after test of all training patterns
- → Update rule:

$$W_{t+1} = W_t + \gamma \sum_{\substack{w'_t x < 0 \\ x \in B}} x \qquad (\gamma > 0)$$

vague assessment in literature:

- advantage : "usually faster"
- disadvantage : "needs more memory" ← just a single vector!

find weights by means of optimization

Let $F(w) = \{ x \in B : w \le 0 \}$ be the set of patterns incorrectly classified by weight w.

$$f(w) = -\sum_{x \in F(w)} w'x \rightarrow min!$$

$$f(w) = 0$$

f(w) = 0 iff F(w) is empty

Possible approach: gradient method

$$W_{t+1} = W_t - \gamma \nabla f(W_t)$$
 $(\gamma > 0)$

converges to a <u>local</u> minimum (dep. on w_0)

Gradient method

$$\mathbf{W}_{t+1} = \mathbf{W}_t - \gamma \ \nabla \mathbf{f}(\mathbf{W}_t)$$

Gradient points in direction of steepest ascent of function $f(\cdot)$

Gradient
$$\nabla f(w) = \left(\frac{\partial f(w)}{\partial w_1}, \frac{\partial f(w)}{\partial w_2}, \dots, \frac{\partial f(w)}{\partial w_n}\right)$$

$$\frac{\partial f(w)}{\partial w_i} = -\frac{\partial}{\partial w_i} \sum_{x \in F(w)} w'x = -\frac{\partial}{\partial w_i} \sum_{x \in F(w)} \sum_{j=1}^n w_j \cdot x_j$$

$$= -\sum_{x \in F(w)} \underbrace{\frac{\partial}{\partial w_i} \left(\sum_{j=1}^n w_j \cdot x_j \right)}_{x_i} = -\sum_{x \in F(w)} x_i$$

Caution:

Indices i of w_i
here denote
components of
vector w; they are
not the iteration
counters!

Gradient method

thus:

gradient
$$\nabla f(w) = \left(\frac{\partial f(w)}{\partial w_1}, \frac{\partial f(w)}{\partial w_2}, \dots, \frac{\partial f(w)}{\partial w_n}\right)'$$

$$= \left(\sum_{x \in F(w)} x_1, -\sum_{x \in F(w)} x_2, \dots, -\sum_{x \in F(w)} x_n\right)'$$

$$= -\sum_{x \in F(w)} x$$

$$\Rightarrow w_{t+1} = w_t + \gamma \sum_{x \in F(w_t)} x$$

gradient method ⇔ batch learning

How difficult is it

- (a) to find a separating hyperplane, provided it exists?
- (b) to decide, that there is no separating hyperplane?

Let
$$B = P \cup \{ -x : x \in N \}$$
 (only positive examples), $w_i \in R$, $\theta \in R$, $|B| = m$

For every example $x_i \in B$ should hold:

$$x_{i1} w_1 + x_{i2} w_2 + ... + x_{in} w_n \ge \theta$$
 \rightarrow trivial solution $w_i = \theta = 0$ to be excluded!

Therefore additionally: $\eta \in R$

$$x_{i1} W_1 + x_{i2} W_2 + ... + x_{in} W_n - \theta - \eta \ge 0$$

Idea: η maximize \rightarrow if $\eta^* > 0$, then solution found

Matrix notation:

$$A = \begin{pmatrix} x'_1 & -1 & -1 \\ x'_2 & -1 & -1 \\ \vdots & \vdots & \vdots \\ x'_m & -1 & -1 \end{pmatrix} \qquad z = \begin{pmatrix} w \\ \theta \\ \eta \end{pmatrix}$$

Linear Programming Problem:

$$f(z_1, z_2, ..., z_n, z_{n+1}, z_{n+2}) = z_{n+2} \rightarrow max!$$
 calculated by e.g. Kamarkar-algorithm in **polynomial time**

If $z_{n+2} = \eta > 0$, then weights and threshold are given by z.

Otherwise separating hyperplane does not exist!