technische universität dortmund

Computational Intelligence

Winter Term 2020/21

Prof. Dr. Günter Rudolph

Lehrstuhl für Algorithm Engineering (LS 11)

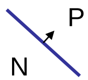
Fakultät für Informatik

TU Dortmund

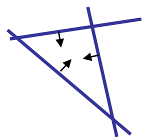
- Multi-Layer-Perceptron
  - Model
  - Backpropagation

What can be achieved by adding a layer?

- Single-layer perceptron (SLP)
  - ⇒ Hyperplane separates space in two subspaces

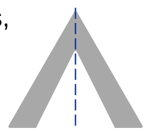


- Two-layer perceptron
  - ⇒ arbitrary convex sets can be separated



connected by AND gate in 2nd layer

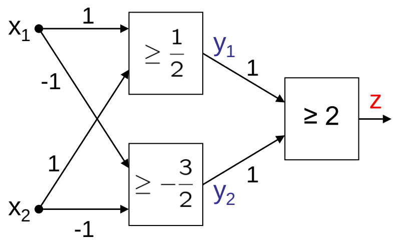
- Three-layer perceptron
  - ⇒ arbitrary sets can be partitioned into convex subsets,
  - convex subsets representable by 2nd layer,
  - resulting sets can be combined in 3rd layer



convex sets of 2nd layer connected by OR gate in 3rd layer

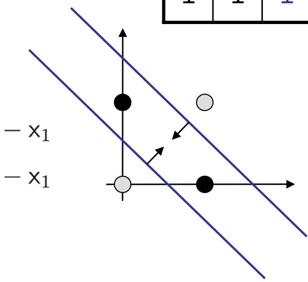
⇒ more than 3 layers not necessary (in principle)

XOR with 3 neurons in 2 steps



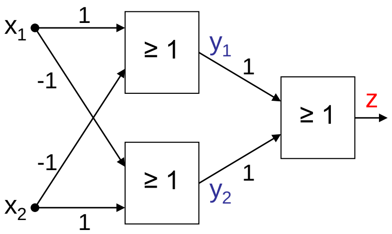
x_1	x_2	y_1	y_2	z
0	0	0	1	0
0	1	1	1	1
1	0	1	1	1
1	1	1	0	0

$$\left.\begin{array}{rcr} x_1 + x_2 & \geq & \frac{1}{2} \\ -x_1 - x_2 & \geq & -\frac{3}{2} \end{array}\right\} , \quad \left\{\begin{array}{rcl} x_2 & \geq & \frac{1}{2} - x_1 \\ x_2 & \leq & \frac{3}{2} - x_1 \end{array}\right.$$



convex set

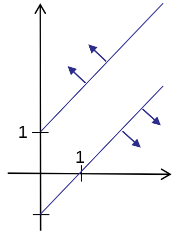
XOR with 3 neurons in 2 layers



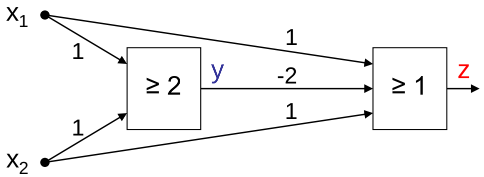
x_1	x_2	y_1	y_2	z
0	0	0	0	0
0	1	0	1	1
1	0	1	0	1
1	1	0	0	0

without AND gate in 2nd layer

$$\left.\begin{array}{l} x_1 - x_2 \geq 1 \\ x_2 - x_1 \geq 1 \end{array}\right\} \; , \quad \left\{\begin{array}{l} x_2 \leq x_1 - 1 \\ x_2 \geq x_1 + 1 \end{array}\right.$$



XOR can be realized with only 2 neurons!



x_1	x_2	y	-2y	x_1-2y+x_2	z
0	0	0	0	0	0
0	1	0	0	1	1
1	0	0	0	1	1
1	1	1	-2	0	0

BUT: this is not a layered network (no MLP) !

Evidently:

MLPs deployable for addressing significantly more difficult problems than SLPs!

But:

How can we adjust all these weights and thresholds?

Is there an efficient learning algorithm for MLPs?

History:

Unavailability of efficient learning algorithm for MLPs was a brake shoe ...

... until **Rumelhart, Hinton** and **Williams (1986): Backpropagation**

Actually proposed by **Werbos (1974)**

... but unknown to ANN researchers (was PhD thesis)

Quantification of classification error of MLP

- Total Sum Squared Error (TSSE)

$$f(w) = \sum_{x \in B} \| \underbrace{g(w;x)}_{\substack{\text{output of net} \\ \text{for weights w and input x}}} - \underbrace{g^*(x)}_{\substack{\text{target output of net} \\ \text{for input x}}} \|^2$$

- Total Mean Squared Error (TMSE)

$$f(w) = \frac{1}{|B| \cdot \ell} \sum_{x \in B} \| g(w;x) - g^*(x) \|^2 = \underbrace{\frac{1}{|B| \cdot \ell}}_{const.} \cdot \text{ TSSE}$$

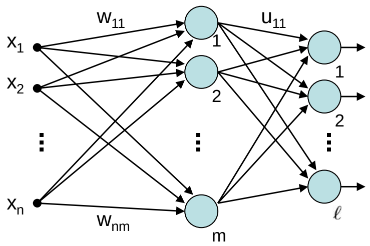
\# training patters   \# output neurons

⇒ leads to same solution as TSSE

Learning algorithms for Multi-Layer-Perceptron (here: 2 layers)

idea: minimize error!

$f(w_t, u_t)$ = TSSE $\rightarrow$ min!



Gradient method

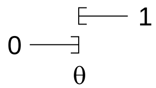
$$u_{t+1} = u_t - \gamma\, \nabla_u\, f(w_t, u_t)$$
$$w_{t+1} = w_t - \gamma\, \nabla_w\, f(w_t, u_t)$$

$$a(x) = \begin{cases} 1 & \text{if } x > \theta \\ 0 & \text{otherwise} \end{cases}$$

BUT:

f(w, u) cannot be differentiated!

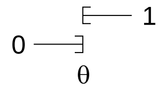
Why? → Discontinuous activation function a(.) in neuron!

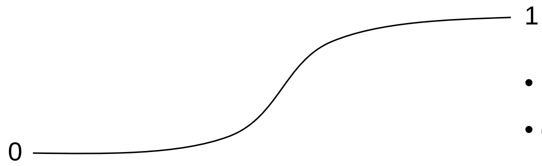


idea: find **smooth** activation function similar to original function !

Learning algorithms for Multi-Layer-Perceptron (here: 2 layers)

good idea: sigmoid activation function (instead of signum function)





- monotone increasing
- differentiable
- non-linear
- output ∈ [0,1] instead of ∈ { 0, 1 }
- threshold θ integrated in activation function

e.g.:

- $a(x) = \dfrac{1}{1+e^{-x}}$ $\quad a'(x) = a(x)(1-a(x))$
- $a(x) = \tanh(x)$ $\quad a'(x) = (1-a^2(x))$

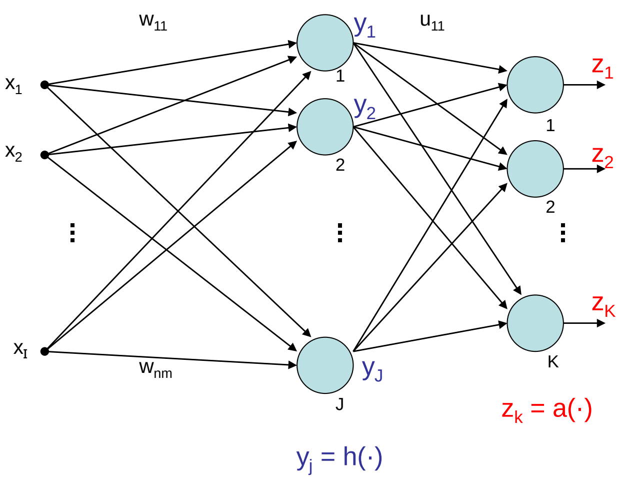
values of derivatives directly determinable from function values

Learning algorithms for Multi-Layer-Perceptron (here: 2 layers)

Gradient method

$f(w_t, u_t)$ = TSSE

$$u_{t+1} = u_t - \gamma\, \nabla_u\, f(w_t, u_t)$$
$$w_{t+1} = w_t - \gamma\, \nabla_w\, f(w_t, u_t)$$



x_i : inputs

y_j : values after first layer

z_k: values after second layer

$$y_j = h\left(\sum_{i=1}^{I} w_{ij} \cdot x_i\right) = h(w_j'\, x)$$

output of neuron j after 1st layer

$$z_k = a\left(\sum_{j=1}^{J} u_{jk} \cdot y_j\right) = a(u_k'\, y)$$

output of neuron k after 2nd layer

$$= a\left(\sum_{j=1}^{J} u_{jk} \cdot h\left(\sum_{i=1}^{I} w_{ij} \cdot x_i\right)\right)$$

error of input x:

$$f(w, u; x) = \sum_{k=1}^{K} (z_k(x) - z_k^*(x))^2 = \sum_{k=1}^{K} (z_k - z_k^*)^2$$

output of net

target output for input x

error for input x and target output z*:

$$f(w,u;x,z^*) \;=\; \underbrace{\sum_{k=1}^{K} \left[a\left(\sum_{j=1}^{J} u_{jk} \cdot \underbrace{h\left(\overbrace{\sum_{i=1}^{I} w_{ij} \cdot x_i}^{w_j' x} \right)}_{y_j} \right)}_{z_k} - z_k^*(x) \right]^2$$

total error for all training patterns (x, z*) ∈ B:

$$f(w,u) \;=\; \sum_{(x,z^*)\in B} f(w,u;x,z^*) \qquad \text{(TSSE)}$$

gradient of total error:

$$\nabla f(w,u) \;=\; \sum_{(x,z^*)\in B} \nabla f(w,u;x,z^*)$$

vector of partial derivatives w.r.t. weights u_{jk} and w_{ij}

thus:

$$\frac{\partial f(w,u)}{\partial u_{jk}} \;=\; \sum_{(x,z^*)\in B} \frac{\partial f(w,u;x,z^*)}{\partial u_{jk}}$$

and

$$\frac{\partial f(w,u)}{\partial w_{ij}} \;=\; \sum_{(x,z^*)\in B} \frac{\partial f(w,u;x,z^*)}{\partial w_{ij}}$$

assume: $a(x) = \dfrac{1}{1+e^{-x}} \;\Rightarrow\; \dfrac{d\,a(x)}{dx} = a'(x) = a(x)\cdot(1-a(x))$

and: $h(x) = a(x)$

chain rule of differential calculus:

$$[\,p(q(x))\,]' \;=\; \underbrace{p'(q(x))}_{\text{outer derivative}} \cdot \underbrace{q'(x)}_{\text{inner derivative}}$$

$$f(w,u;x,z^*) \;=\; \sum_{k=1}^{K} [\,a(u_k' y) - z_k^*\,]^2$$

partial derivative w.r.t. u_{jk}:

$$\begin{aligned}
\frac{\partial f(w,u;x,z^*)}{\partial u_{jk}} &= 2\,[\,a(u_k' y) - z_k^*\,] \cdot a'(u_k' y) \cdot y_j \\
&= 2\,[\,a(u_k' y) - z_k^*\,] \cdot a(u_k' y) \cdot (1 - a(u_k' y)) \cdot y_j \\
&= \underbrace{2\,[\,z_k - z_k^*\,] \cdot z_k \cdot (1 - z_k)}_{\text{“error signal“ } \delta_k} \cdot y_j
\end{aligned}$$

partial derivative w.r.t. w_{ij}:

$$\frac{\partial f(w,u;x,z^*)}{\partial w_{ij}} = 2\sum_{k=1}^{K} [\underbrace{a(u_k'y)}_{z_k} - z_k^*]\cdot \underbrace{a'(u_k'y)}_{z_k\,(1-z_k)}\cdot u_{jk}\cdot \underbrace{h'(w_j'x)}_{y_j\,(1-y_j)}\cdot x_i$$

$$= 2\cdot\sum_{k=1}^{K} [z_k - z_k^*]\cdot z_k\cdot(1-z_k)\cdot u_{jk}\cdot y_j\,(1-y_j)\cdot x_i$$

factors reordered

$$= \underbrace{x_i\cdot y_j\cdot(1-y_j)\cdot\sum_{k=1}^{K} \underbrace{2\cdot[z_k-z_k^*]\cdot z_k\cdot(1-z_k)}_{\text{error signal } \delta_k \text{ from previous layer}}\cdot u_{jk}}_{\text{error signal } \delta_j \text{ from “current“ layer}}$$

Generalization (> 2 layers)

Let neural network have L layers $S_1, S_2, \ldots S_L$.

Let neurons of all layers be numbered from 1 to N.

$j \in S_m \rightarrow$ neuron j is in m-th layer

All weights w_{ij} are gathered in weights matrix W.

Let o_j be output of neuron j.

error signal:

$$\delta_j = \begin{cases} o_j\cdot(1-o_j)\cdot(o_j - z_j^*) & \text{if } j\in S_L \text{ (output neuron)} \\ o_j\cdot(1-o_j)\cdot\displaystyle\sum_{k\in S_{m+1}} \delta_k\cdot w_{jk} & \text{if } j\in S_m \text{ and } m < L \end{cases}$$

correction:

$$w_{ij}^{(t+1)} = w_{ij}^{(t)} - \gamma\cdot o_i\cdot\delta_j$$

<u>in case of online learning</u>:
correction after **each** test pattern presented

error signal of neuron in inner layer determined by

- error signals of all neurons of subsequent layer and
- weights of associated connections.

$\Downarrow$

- First determine error signals of output neurons,
- use these error signals to calculate the error signals of the preceding layer,
- use these error signals to calculate the error signals of the preceding layer,
- and so forth until reaching the first inner layer.

$\Downarrow$

thus, error is propagated backwards from output layer to first inner
$\Rightarrow$ **backpropagation** (of error)

$\Rightarrow$ other optimization algorithms deployable!

in addition to **backpropagation** (gradient descent) also:

- **Backpropagation with Momentum**
  take into account also previous change of weights:
  $$\Delta w_{ij}^{(t)} = -\gamma_1\cdot o_i\cdot\delta_j - \gamma_2\cdot\Delta w_{ij}^{(t-1)}$$
- **QuickProp**
  assumption: error function can be approximated locally by quadratic function,
  update rule uses last two weights at step t – 1 and t – 2.
- **Resilient Propagation (RPROP)**
  exploits sign of partial derivatives:
  2 times negative or positive → increase step size!
  change of sign → reset last step and decrease step size!
  typical values: factor for decreasing 0,5 / factor for increasing 1,2
- **Evolutionary Algorithms**
  individual = weights matrix

Classification

given: set of training patterns (input / output) output = label
(e.g. class A, class B, ...)

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

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

$x \downarrow$ input (unknown)

$\hat{y} \downarrow$ output (guessed)

phase I:

train network

phase II:

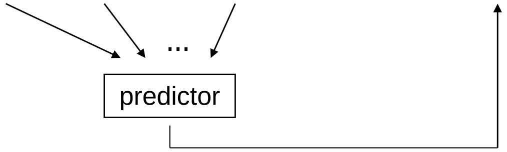
apply network to unkown inputs for classification

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

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



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: <u>Example for Creating Training Data</u>

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

$\underbrace{(10.5, 3.4, 5.6)}_{\text{known input}}$ 2.4 (known output) first input / output pair

further input / output pairs:

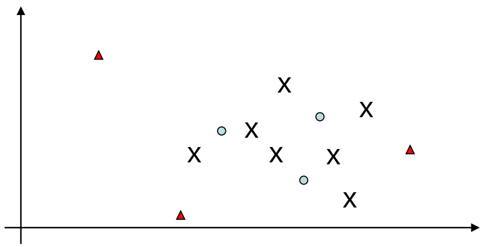
(3.4, 5.6, 2.4)	5.9
(5.6, 2.4, 5.9)	8.4
(2.4, 5.9, 8.4)	3.9
(5.9, 8.4, 3.9)	4.4
(8.4, 3.9, 4.4)	1.7

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