

Computational Intelligence

Winter Term 2017/18

Prof. Dr. Günter Rudolph

Lehrstuhl für Algorithm Engineering (LS 11)

Fakultät für Informatik

TU Dortmund

- Single-Layer Perceptron
 - Accelerated Learning
 - Online- vs. Batch-Learning
- Multi-Layer-Perceptron
 - Model
 - Backpropagation

Acceleration of Perceptron Learning

Assumption: $x \in \{0, 1\}^n \Rightarrow \|x\| = \sum_{i=1}^n |x_i| \geq 1$ for all $x \neq (0, \dots, 0)$

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

$$\begin{aligned}
 w'_{t+1}x &= (w_t + (\delta + \varepsilon) x)' x \\
 &= \underbrace{w'_t x}_{-\delta} + (\delta + \varepsilon) x'x \\
 &= -\delta + \delta \|x\|^2 + \varepsilon \|x\|^2 \\
 &= \underbrace{\delta (\|x\|^2 - 1)}_{\geq 0} + \underbrace{\varepsilon \|x\|^2}_{> 0} > 0 \quad \checkmark
 \end{aligned}$$

Generalization:

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

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

$$\Rightarrow w'_{t+1} x = \underbrace{\delta (\|x\|^2 - 1)}_{< 0 \text{ possible!}} + \underbrace{\varepsilon \|x\|^2}_{> 0}$$

Idea: 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}

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

There exist numerous variants of Perceptron Learning Methods.

Theorem: (Duda & Hart 1973)

If rule for correcting weights is $w_{t+1} = w_t + \gamma_t x$ (if $w'_t x < 0$)

$$1. \quad \forall t \geq 0 : \gamma_t \geq 0$$

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

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

then $w_t \rightarrow w^*$ for $t \rightarrow \infty$ 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:

$$w_{t+1} = w_t + \gamma \sum_{\substack{w_t^i x < 0 \\ x \in B}} x \quad (\gamma > 0)$$

vague assessment in literature:

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

find weights by means of optimization

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

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

Optimum: $f(w) = 0$ iff $F(w)$ is empty

Possible approach: gradient method

$$w_{t+1} = w_t - \gamma \nabla f(w_t) \quad (\gamma > 0)$$

converges to a local minimum (dep. on w_0)

Gradient method

$$w_{t+1} = w_t - \gamma \nabla f(w_t)$$

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

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

Caution:

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

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

Gradient method

thus:

$$\begin{aligned}
 \text{gradient } \nabla f(w) &= \left(\frac{\partial f(w)}{\partial w_1}, \frac{\partial f(w)}{\partial w_2}, \dots, \frac{\partial f(w)}{\partial w_n} \right)' \\
 &= \left(-\sum_{x \in F(w)} x_1, -\sum_{x \in F(w)} x_2, \dots, -\sum_{x \in F(w)} x_n \right)' \\
 &= -\sum_{x \in F(w)} x
 \end{aligned}$$

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

gradient method \Leftrightarrow 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), $w_i \in \mathbb{R}$, $\theta \in \mathbb{R}$, $|B| = m$

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

$$x_{i1} w_1 + x_{i2} w_2 + \dots + x_{in} w_n \geq \theta \quad \rightarrow \text{trivial solution } w_i = \theta = 0 \text{ to be excluded!}$$

Therefore additionally: $\eta \in \mathbb{R}$

$$x_{i1} w_1 + x_{i2} w_2 + \dots + x_{in} w_n - \theta - \eta \geq 0$$

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

Matrix notation:

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

Linear Programming Problem:

$$f(z_1, z_2, \dots, z_n, z_{n+1}, z_{n+2}) = z_{n+2} \rightarrow \max!$$

$$\text{s.t. } Az \geq 0$$

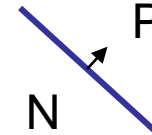
calculated by e.g. Kamarkar-
algorithm in **polynomial time**

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

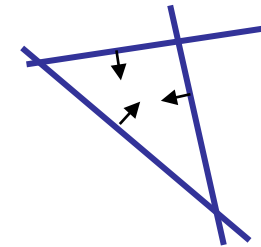
Otherwise separating hyperplane does not exist!

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

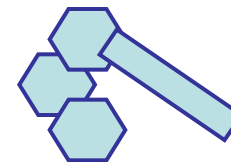


connected by
AND gate in
2nd layer

- Three-layer perceptron
 ⇒ arbitrary sets can be separated (depends on number of neurons)-

several convex sets representable by 2nd layer,

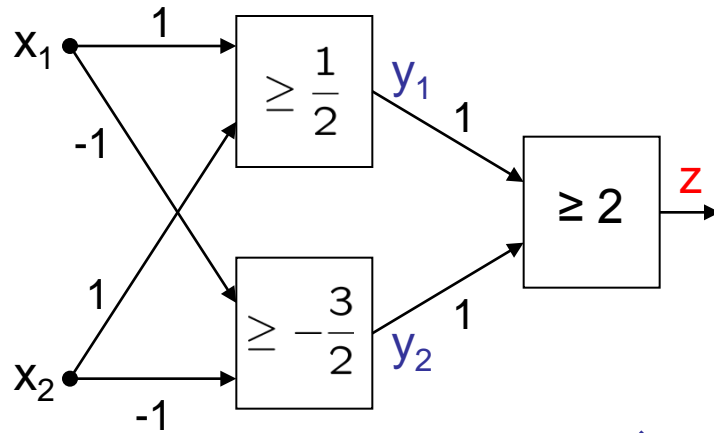
these sets can be combined in 3rd layer



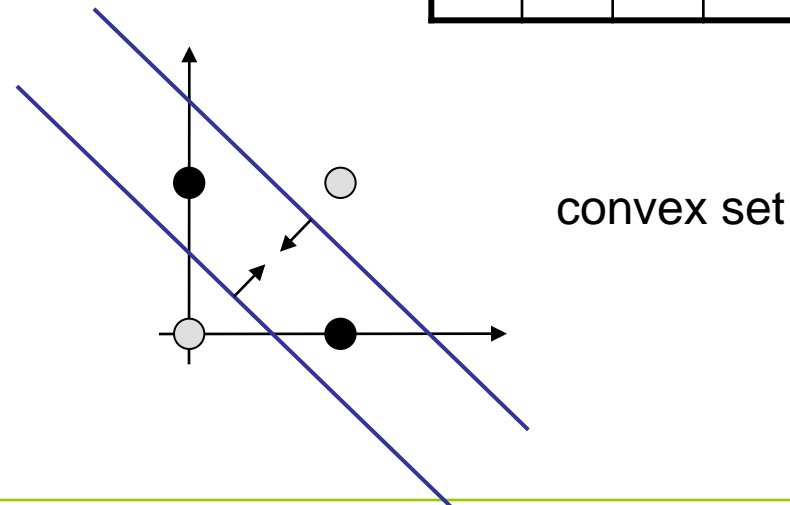
convex sets
of 2nd layer
connected by
OR gate in
3rd layer

⇒ more than 3 layers not necessary!

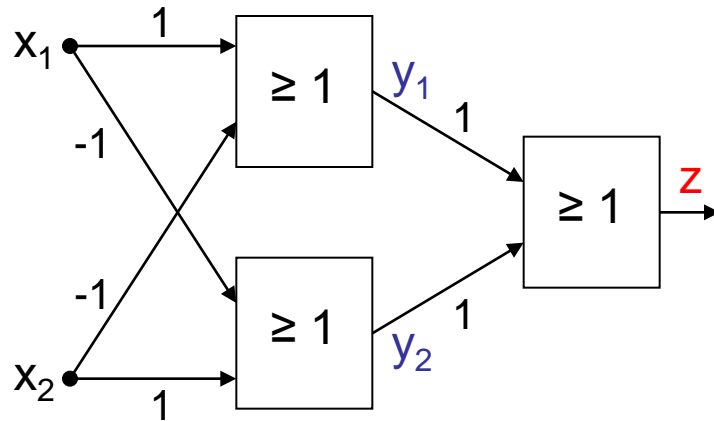
XOR with 3 neurons in 2 steps



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



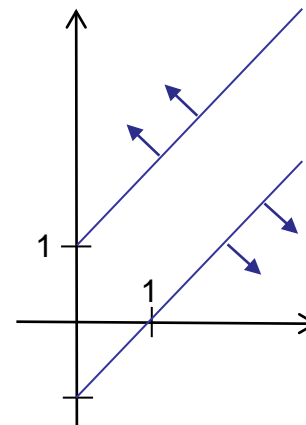
XOR with 3 neurons in 2 layers



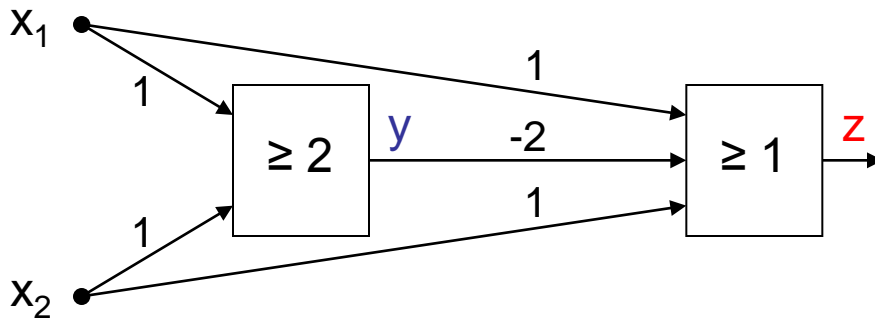
x_1	x_2	y_1	y_2	z
0	0	0	0	0
0	1	0	1	1
1	0	1	0	1
1	1	0	0	0

without AND gate in 2nd layer

$$\left. \begin{array}{l} x_1 - x_2 \geq 1 \\ x_2 - x_1 \geq 1 \end{array} \right\} \Leftrightarrow \begin{cases} x_2 \leq x_1 - 1 \\ x_2 \geq x_1 + 1 \end{cases}$$



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)

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

output of net for weights w and input x target output of net for input x

- Total Mean Squared Error (TMSE)

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

training patterns

output neurons

leads to same solution as TSSE

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

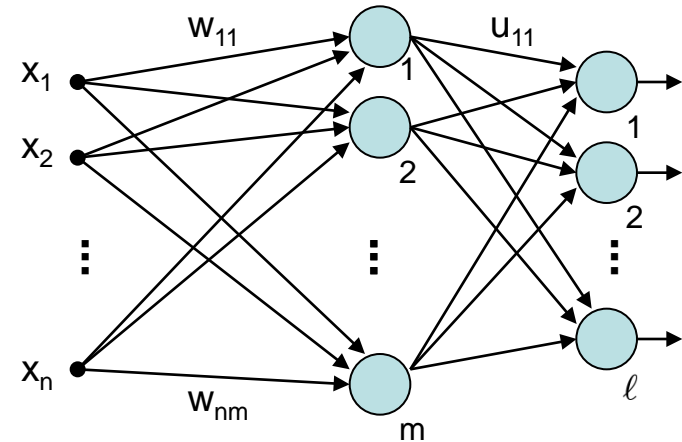
idea: minimize error!

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

Gradient method

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

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

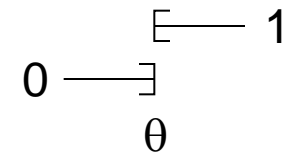


BUT:

$f(w, u)$ cannot be differentiated!

Why? \rightarrow Discontinuous activation function $a(\cdot)$ in neuron!

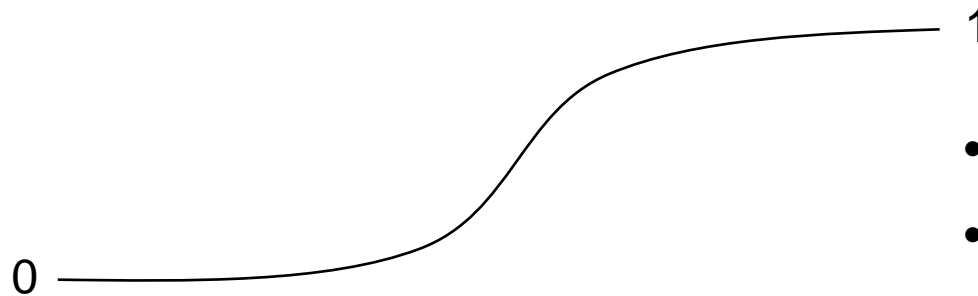
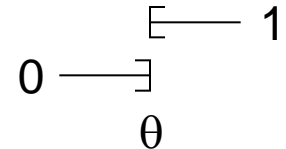
$$a(x) = \begin{cases} 1 & \text{if } x > \theta \\ 0 & \text{otherwise} \end{cases}$$



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 $\in [0,1]$ instead of $\in \{ 0, 1 \}$
- threshold θ integrated in activation function

e.g.:

- $a(x) = \frac{1}{1 + e^{-x}}$ $a'(x) = a(x)(1 - a(x))$
 - $a(x) = \tanh(x)$ $a'(x) = (1 - a^2(x))$
- } values of derivatives directly determinable from function values

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

Gradient method

$$f(w_t, u_t) = \text{TSSE}$$

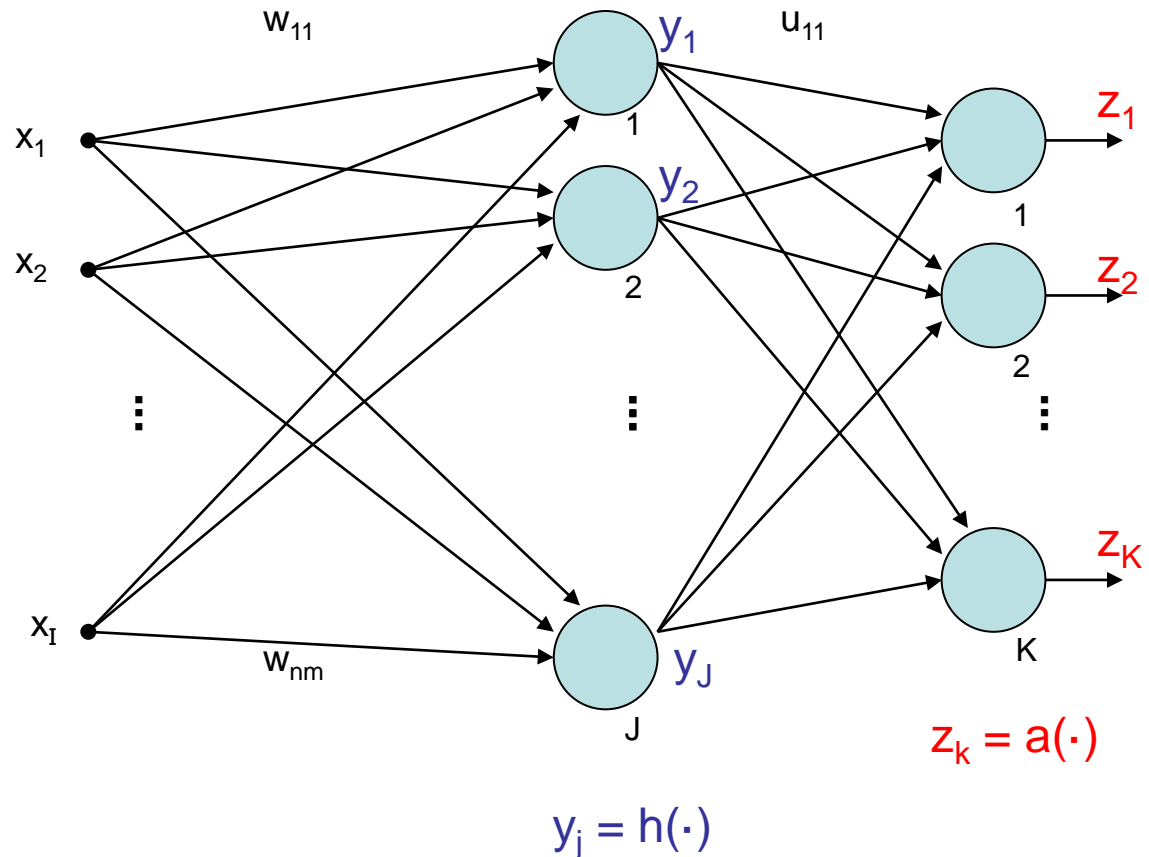
$$u_{t+1} = u_t - \gamma \nabla_u f(w_t, u_t)$$

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

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^* :

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

$w'_j x$
 y_j
 z_k

total error for all training patterns $(x, z^*) \in B$:

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

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: $a(x) = \frac{1}{1 + e^{-x}} \Rightarrow \frac{d a(x)}{d x} = a'(x) = a(x) \cdot (1 - a(x))$

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} :

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

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

$$\begin{aligned} \frac{\partial f(w, u; x, z^*)}{\partial w_{ij}} &= 2 \sum_{k=1}^K \underbrace{[a(u'_k y) - z_k^*]}_{z_k} \cdot \underbrace{a'(u'_k y)}_{z_k(1-z_k)} \cdot u_{jk} \cdot \underbrace{h'(w'_j x)}_{y_j(1-y_j)} \cdot x_i \\ &= 2 \cdot \sum_{k=1}^K [z_k - z_k^*] \cdot z_k \cdot (1 - z_k) \cdot u_{jk} \cdot y_j (1 - y_j) \cdot x_i \\ &\stackrel{\text{factors reordered}}{=} x_i \cdot y_j \cdot (1 - y_j) \cdot \underbrace{\sum_{k=1}^K 2 \cdot [z_k - z_k^*] \cdot z_k \cdot (1 - z_k) \cdot u_{jk}}_{\text{error signal } \delta_k \text{ from previous layer}} \\ &\quad \underbrace{\hspace{15em}}_{\text{error signal } \delta_j \text{ from "current" layer}} \end{aligned}$$

Generalization (> 2 layers)

Let neural network have L layers S_1, S_2, \dots, 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:

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

correction:

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

in case of online learning:

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.



- 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.



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

⇒ 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

} later more
about this!