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Neural Networks

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Neural Networks:

Self-Organization

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Neural Networks:

Contents:

- Associative Memories
- **Self-Organization**
- Kohonen Maps, Hybrid Models, and Genetic Algorithms

Contents:

- Associative Memories
- **Self-Organization**
 - **Unsupervised Competitive Learning**
 - The Main Principles
 - The Competitive Learning Algorithm
 - Stability of the Results
 - PCA Analysis and the Oja's Learning Algorithm
 - Convergence of the Oja's Algorithm
- Kohonen Maps, Hybrid Models, and Genetic Algorithms
 - Kohonen Maps: Motivation and the Training Algorithm
 - Stability of the Solution
 - Supervised Variants of Kohonen Maps
 - Hybrid Models: Counterpropagation Networks, RBF-networks, the ART Model, Cascade Correlation
 - Genetic Algorithms and the Schemata Theorem

Self-Organization

- Unsupervised training:
 - Self-organization and clustering
- Motivation:
 - The network decides by itself what response fits best for the presented input pattern and adjusts its weights accordingly
- Problem:
 - Determine the number and location of clusters present in the feature space

Self-Organization (2)

Competitive learning:

- Compete for the „right to represent the patterns“
- *Winner - Takes - All* rule (WTA)
- *Inhibition* of opponents
- Network *plasticity*
- Learning with conscience

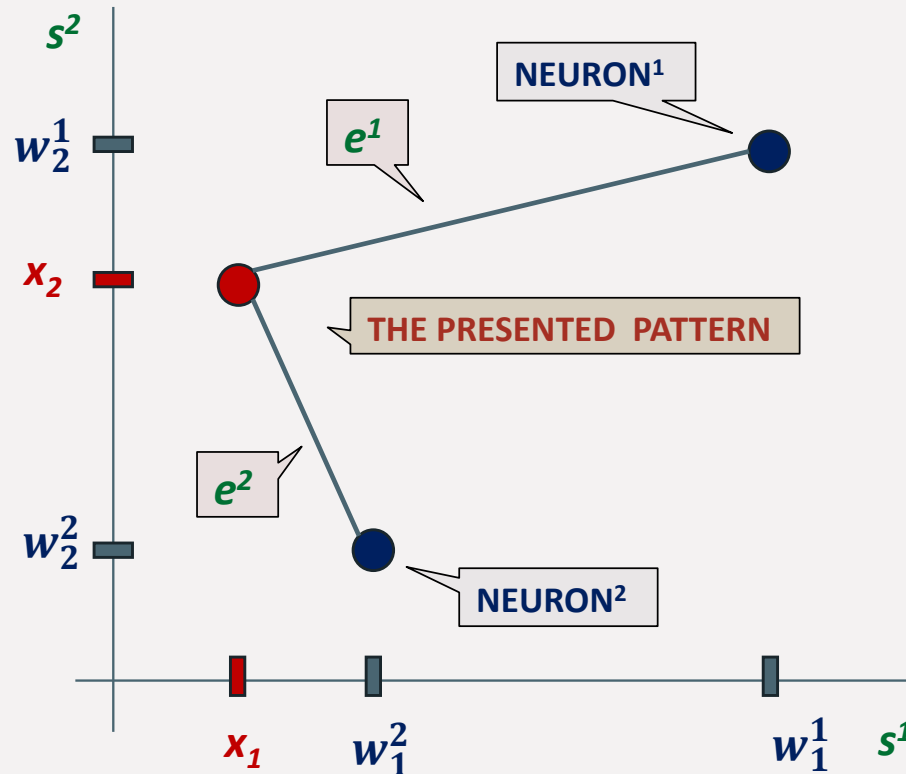
Reinforcement learning:

- Emphasizes the best reproduction of inputs

Unsupervised Competitive Learning

- n -dimensional input patterns are processed by such a number of neurons, that corresponds to the (assumed) number of clusters
- the neurons compute the (Euclidean) *distance* between the presented pattern and their weight vector

Unsupervised Competitive Learning (2)



- ◆ Competition „is won“ by the neuron situated the closest to the presented pattern
- ◆ The winning neuron becomes the most active one and will *inhibit* the activity of other neurons

Unsupervised Competitive Learning (3)

- Inhibition by means of „lateral connections“
⇒ *lateral inhibition*
- Global information about the state of all the neurons in the network is necessary to decide whether a neuron will be active or not
- The activity of a neuron signals the membership of the presented input to the cluster of vectors represented by this neuron

Unsupervised Competitive Learning (4)

- The winning neuron adjusts its weights towards the presented pattern:

$$\Delta \vec{w} = \alpha \cdot (\vec{x} - \vec{w})$$

network plasticity (decays slowly during training)



Our objective:

- Position the neurons into the cluster centers
- Keep the already formed network structure

Unsupervised Competitive Learning (5)

- Strategies speeding-up the training:
 - An appropriate weight initialization, e.g., according to randomly selected patterns
- Problems:
 - Dead (never used) neurons
 - A grid in the Kohonen layer
 - Topological neighborhood of neurons
 - Controlled competition and the mechanism of conscience

Unsupervised Competitive Learning (6)

- During training, the weights of the neurons should be set in such a way that they correspond to the „centers of gravity of the respective clusters“
- The energy function of a set of n -dimensional ($n \geq 2$) normalized input patterns $X = \{\vec{x}_1, \dots, \vec{x}_m\}$ is given for 1 neuron with the weight vector \vec{w} by means of:

$$E_X(\vec{w}) = \sum_{i=1}^m \|\vec{x}_i - \vec{w}\|^2 ; \quad \vec{w} \in R^n$$

Unsupervised Competitive Learning (7)

⇒ in the optimum case, the weight vector is located in the center of the input pattern cluster:

$$\begin{aligned} E_X(\vec{w}) &= \sum_{i=1}^m \|\vec{x}_i - \vec{w}\|^2 = \sum_{i=1}^m \sum_{j=1}^n (x_{ij} - w_j)^2 = \\ &= \sum_{i=1}^m \sum_{j=1}^n (x_{ij}^2 - 2x_{ij}w_j + w_j^2) = \\ &= m \left(\sum_{j=1}^n w_j^2 - \frac{2}{m} \sum_{j=1}^n w_j \left(\sum_{i=1}^m x_{ij} \right) \right) + \sum_{i=1}^m \sum_{j=1}^n x_{ij}^2 = \end{aligned}$$

$$m \left(\sum_{j=1}^n w_j^2 - \frac{2}{m} \sum_{j=1}^n w_j \left(\sum_{i=1}^m x_{ij} \right) \right) + \sum_{i=1}^m \sum_{j=1}^n x_{ij}^2$$

Unsupervised Competitive Learning (8)

$$\begin{aligned}
 E_X(\vec{w}) &= m \sum_{j=1}^n \left(w_j^2 - \frac{2}{m} w_j \left(\sum_{i=1}^m x_{ij} \right) + \frac{1}{m^2} \left(\sum_{i=1}^m x_{ij} \right) \left(\sum_{i=1}^m x_{ij} \right) \right) - \\
 &\quad - \underbrace{\frac{1}{m} \sum_{j=1}^n \left[\left(\sum_{i=1}^m x_{ij} \right) \left(\sum_{i=1}^m x_{ij} \right) \right] + \sum_{i=1}^m \sum_{j=1}^n x_{ij}^2}_{= K} = \\
 &= m \left(\sum_{j=1}^n \left(w_j - \frac{1}{m} \sum_{i=1}^m x_{ij} \right)^2 \right) + K = \\
 &= m \|\vec{w} - \vec{x}^*\|^2 + K
 \end{aligned}$$

Unsupervised Competitive Learning (9)

- the vector \vec{x}^* is the centroid of the cluster $\{\vec{x}_1, \vec{x}_2, \dots, \vec{x}_m\}$ and K is a constant
- the energy function has a global minimum at \vec{x}^*

Unsupervised Competitive Learning (10)

Clustering methods for empirical multidimensional data:

- Two basic approaches:
 - k nearest neighbors – for labeled data
 - k -means algorithm – for unlabeled data
- k nearest neighbors (supervised training)
 - The training patterns are stored and classified into one of l different classes
 - A new input vector is classified into the class that contains the majority of its k nearest neighbors (from the stored set)

Unsupervised Competitive Learning (11)

- k -means clustering algorithm:
 - unsupervised learning
 - Input vectors are grouped into k different clusters
(at the beginning, each cluster contains exactly 1 vector)
 - A new vector \vec{x} is assigned to the cluster i , the centroid of which lies the closest to this pattern

Unsupervised Competitive Learning (12)

- k -means clustering algorithm (continue)

- The centroid \vec{c}_i is then adjusted by means of:

$$\vec{c}_i(\text{new}) = \vec{c}_i(\text{old}) + \frac{1}{n_i} (\vec{x} - \vec{c}_i(\text{old}))$$

n_i ... the number of vectors already assigned to cluster i

- This procedure is iteratively repeated for the entire data set (its structure is then captured by the „weight vectors“ \vec{c}_i ; $i = 1, \dots, k$).

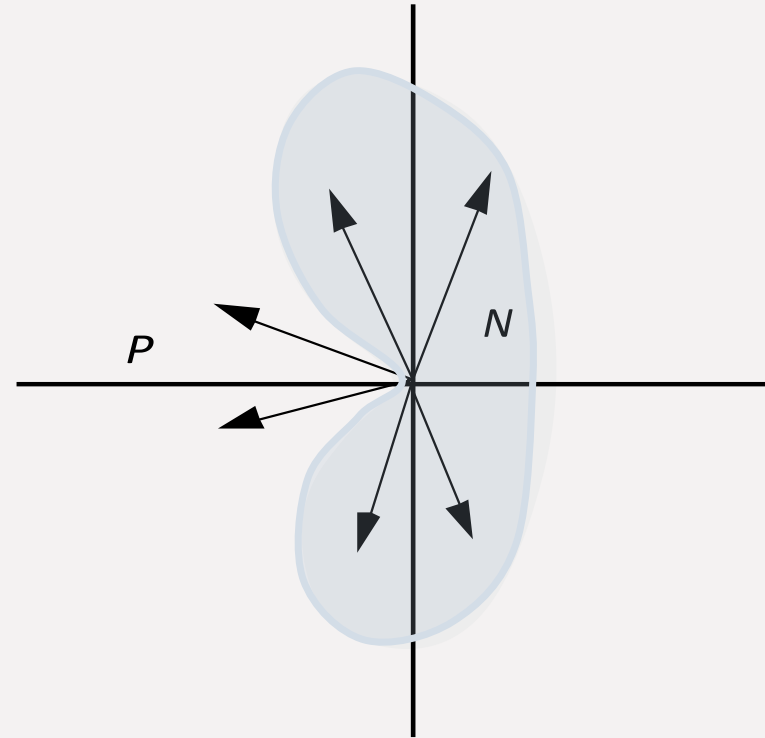
→ Vector quantization

The Clustering Problem

- Two sets of vectors: P and N
- Difficult to „separate“ the clusters by means of a simple perceptron such that:

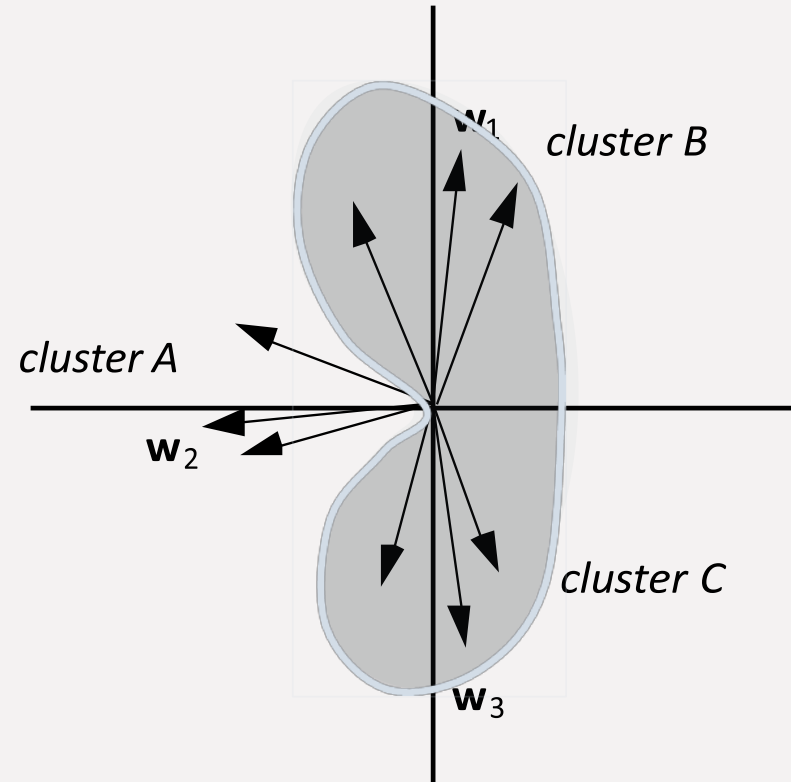
$$\vec{w} \cdot \vec{p} \geq 0 \quad \forall \vec{p} \in P$$

$$\wedge \quad \vec{w} \cdot \vec{n} < 0 \quad \forall \vec{n} \in N$$



The Clustering Problem (2)

- Example: Three weight vectors for three clusters
- 3 different vectors \vec{w}_1, \vec{w}_2 and \vec{w}_3 can be used as „representants“ of the respective clusters A, B and C



The Clustering Problem (3)

- Each one of these vectors is „relatively close“ to any vector from the respective cluster
- Each weight vector corresponds to a single neuron which is active only if the input vector is close enough to its own weight vector

==> How could we determine the number and distribution of the clusters?

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Competitive Learning: The Algorithm

- Let $X = \{\vec{x}_1, \vec{x}_2, \dots, \vec{x}_l\}$ be a set of normalized input vectors in the n -dimensional space which we want to classify into k different clusters
- The neural network consists of k neurons, each of which has n inputs and zero threshold

Initialization:

- The normalized weight vectors $\vec{w}_1, \dots, \vec{w}_k$ are generated randomly

Competitive Learning: The Algorithm (2)

Test:

- Select randomly a vector $\vec{x}_j \in X$
- Compute $\vec{w}_i \cdot \vec{x}_j$ for $i = 1, \dots, k$
- Select \vec{w}_m such that $\vec{w}_m \cdot \vec{x}_j \geq \vec{w}_i \cdot \vec{x}_j \quad (\forall i = 1, \dots, k)$
- Continue with Update

Update:

- Substitute $\vec{w}_m(\text{new})$ with $\vec{w}_m(\text{old}) + \vec{x}_j$ and normalize
- Continue with Test

Competitive Learning: The Algorithm (3)

- The algorithm can be stopped after a pre-determined number of steps
- The weight vectors of the k neurons are „attracted“ towards the centers of the respective clusters in the input space
- The algorithm is based on the principle known as „winner-takes-all“

Competitive Learning: The Algorithm (4)

- Normalized vectors prevent the weight vectors from becoming so large that they would win the competition too often
 - Other neurons would then never be updated and would remain useless → „dead neurons“
- Since both the input and weight vectors are normalized, the scalar product $\vec{w}_i \cdot \vec{x}_j$ of a weight and input vector is equal to the cosine of the angle between these two vectors

Competitive Learning: The Algorithm (5)

- The selection rule guarantees that the weight vector \vec{w}_m of the cluster that is updated is the one that lies closest to the tested input vector
- The update rule rotates the weight vector \vec{w}_m towards \vec{x}_j

Different learning rules:

- Update with a learning constant
 $\Delta \vec{w}_m = \eta \vec{x}_j$; $\eta \in (0,1)$ decays slowly in time
→ network plasticity

Competitive Learning: The Algorithm (6)

Different learning rules (continue):

- **Difference update:** $\Delta \vec{w}_m = \eta (\vec{x}_j - \vec{w}_m)$
 - „correction“ proportional to the difference of both vectors
- **Batch update** → a more stable learning process
 - Weight „corrections“ are computed for each respective pattern and then cumulated
 - After a number of iterations, the weight corrections are added to the weights at once

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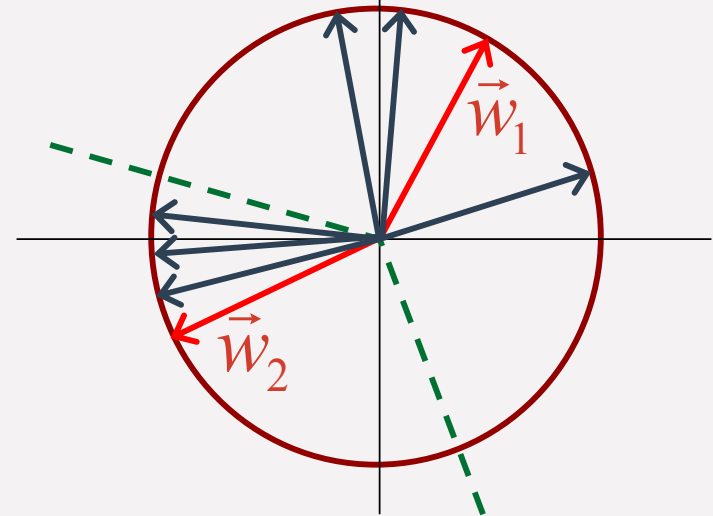
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Competitive Learning: The Algorithm (7)

Stability of the solutions

- Necessity of a suitable measure for a „good clustering“
 - a simple approach: find the distance between clusters
- Two clusters of vectors and two „representative weight vectors“:
 - Both „representative vectors“ lie close to the vectors from their respective cluster

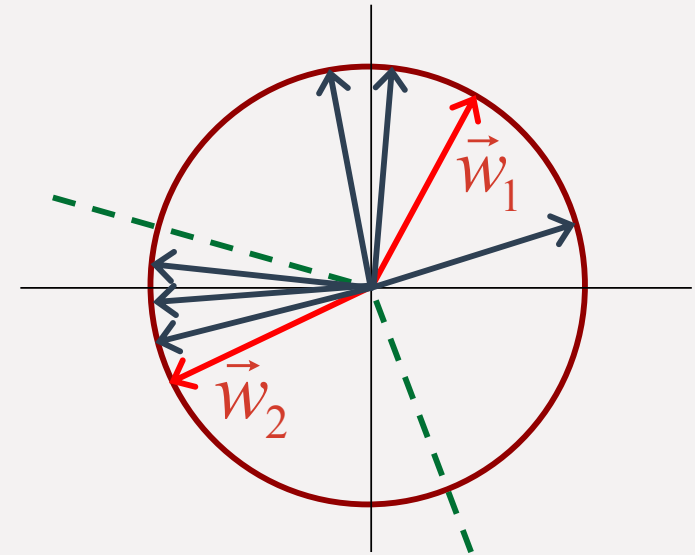


Competitive Learning: The Algorithm (8)

Stability of the solutions (continue):

- \vec{w}_1 lies inside a „cone“ defined by the vectors from its cluster
- \vec{w}_2 lies outside of the „cone“ of \vec{w}_1
- The vector \vec{w}_1 will not jump outside of its „cone“ in future iterations
- The vector \vec{w}_2 will jump inside the cone defined by its cluster at some point and will remain there

→ such a solution will be stable



Competitive Learning: The Algorithm (9)

The solution in a stable equilibrium:

- Intuitive idea:
 - A stable equilibrium requires clearly delimited clusters
- If the clusters overlap or are very extended, it can be the case that no stable solution can be found
==> unstable equilibrium

Stability of the Solutions: The Analysis

Definition:

Let P denote the set $\{\vec{p}_1, \dots, \vec{p}_m\}$ of n -dimensional ($n \geq 2$) vectors located in the same half-space (\sim a formal restriction of the cluster size).

The cone K defined by P is the set of all vectors \vec{x} of the form $\vec{x} = \alpha_1 \vec{p}_1 + \dots + \alpha_m \vec{p}_m$, where $\alpha_1, \dots, \alpha_m$ are positive real numbers.

- The cone of a cluster contains all vectors „within“ the cluster
- The diameter of a cone defined by normalized vectors is proportional to the maximum possible angle between two vectors in the cluster

Stability of the Solutions: The Analysis (2)

Definition:

The (angular) diameter ϕ of a cone K defined by normalized vectors $\{\vec{p}_1, \dots, \vec{p}_m\}$ corresponds to:

$$\phi = \sup \left\{ \arccos(\vec{a} \cdot \vec{b}) \mid \forall \vec{a}, \vec{b} \in K; \|\vec{a}\| = \|\vec{b}\| = 1 \right\}$$

where $0 \leq \arccos(\vec{a} \cdot \vec{b}) \leq \pi$

- A sufficient condition for stable equilibrium is that the angular diameter of the cluster's cone must be smaller than the distance between clusters.

Stability of the Solutions: The Analysis (3)

Definition:

Let $P = \{\vec{p}_1, \dots, \vec{p}_m\}$ and $N = \{\vec{n}_1, \dots, \vec{n}_k\}$ be two non-empty sets of normalized vectors in an n -dimensional space ($n \geq 2$) that define the cones K_P and K_N

- If the intersection of the two cones is empty, the (angular) distance between K_N and K_P is given by:

$$\psi_{P,N} = \inf\{ \arccos(\vec{p} \cdot \vec{n}) ; \vec{p} \in K_P, \vec{n} \in K_N \text{ and } \|\vec{p}\| = \|\vec{n}\| = 1 \}$$

where $0 \leq \arccos(\vec{p} \cdot \vec{n}) \leq \pi$

- If the two cones K_P and K_N intersect, $\psi_{P,N} = 0$

Stability of the Solutions: The Analysis (4)

- If angular distance between clusters is greater than angular diameter of the clusters, a stable solution exists
 - The weight vectors will lie inside their respective cluster cones
 - Once inside their respective cluster cones, the weight vectors will not leave them

Clustering quality control:

- A smaller number of „more compact“ clusters is usually preferred
- A cost function penalizing a too big number of clusters

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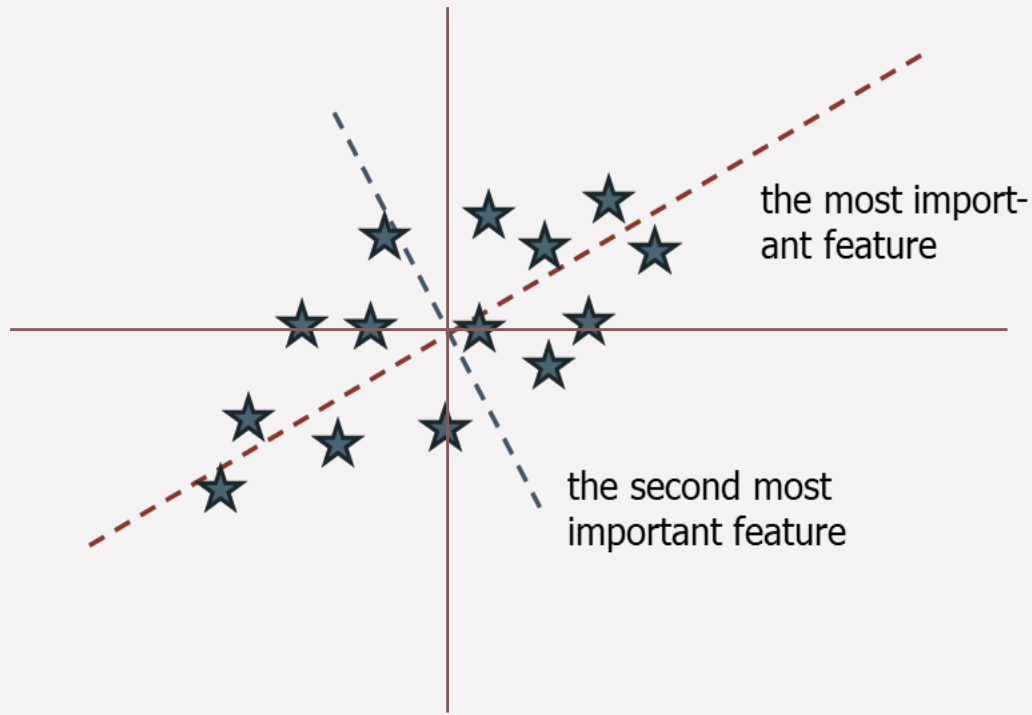
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PCA – Principal Component Analysis

- ~ reduces the dimensionality of the input data
 - use fewer features without losing essential information
 - selection of the most important features
- ~ a set of m n -dimensional vectors is given: $\{\vec{x}_1, \vec{x}_2, \dots, \vec{x}_m\}$
- ~ the first principal component of this set of vectors is a vector \vec{w} which maximizes the expression

$$\frac{1}{m} \sum_{i=1}^m (\vec{w} \cdot \vec{x}_i)^2$$

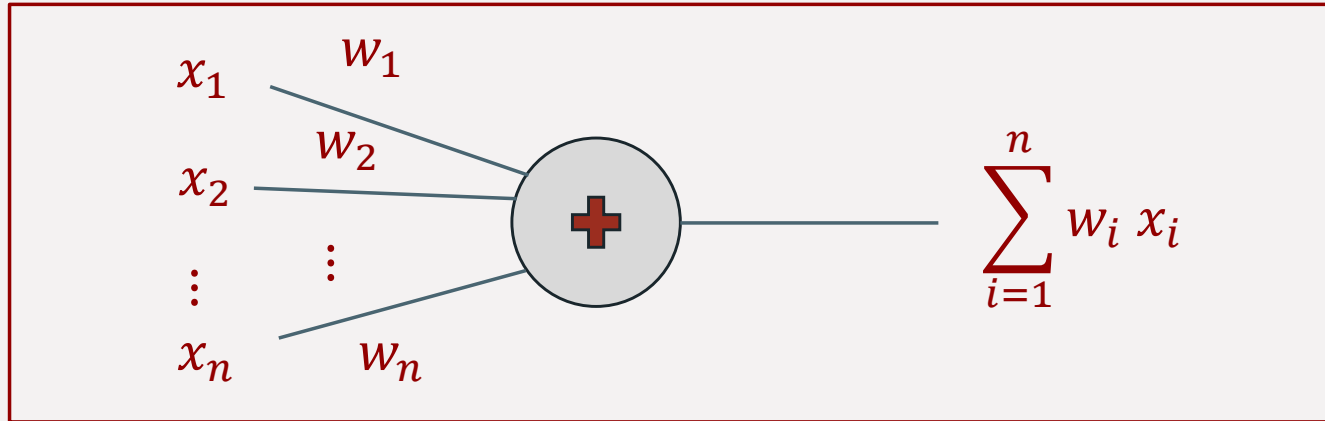
PCA – Principal Component Analysis (2)



■ Distribution of the input data:

- The first principal component: direction of maximum variance in the data
- The second principal component: orthogonal to 1. PC and maximum variance
(~ subtract from \vec{x} its orthogonal projection on 1. PC)

PCA – Principal Component Analysis (3)



The applied model:

- Linear associator – outputs the weighted input as a result
- **Unsupervised reinforcement learning** – Oja's algorithm

Computation of the Principal Components with Artificial Neural Networks

Oja's learning algorithm (E. Oja, 1982)
(for the computation of the first principal component)

Assumption:

- The centroid of the input data is located at the origin

Start:

- Let X be a set of n -dimensional vectors
- The vector \vec{w} is initialized randomly ($\vec{w} \neq 0$)
- A learning constant γ with $0 < \gamma \leq 1$ is selected

Computation of the Principal Components with Artificial Neural Networks (2)

Oja's learning algorithm (continue):

Update:

- From the set X a vector \vec{x} is selected randomly
- The dot product $\Phi = \vec{x} \cdot \vec{w}$ is computed
- The new weight vector is set to: $\vec{w} + \gamma \Phi(\vec{x} - \Phi \vec{w})$
- Make γ smaller and go to „Update“

Stopping condition for update

- e.g., a predetermined number of iterations

Computation of the Principal Components with Artificial Neural Networks (3)

- The learning constant γ
 - The learning constant must be chosen small enough to guarantee adequate weight updates (limit big oscillations)
- „Automatic normalization“ of the weight vector
 - global information about all patterns is not necessary
 - local information about the updated weight, input, and scalar product of the associator is sufficient
- The first principal component is equivalent to the direction of the longest eigenvector of the correlation matrix of the considered input vectors

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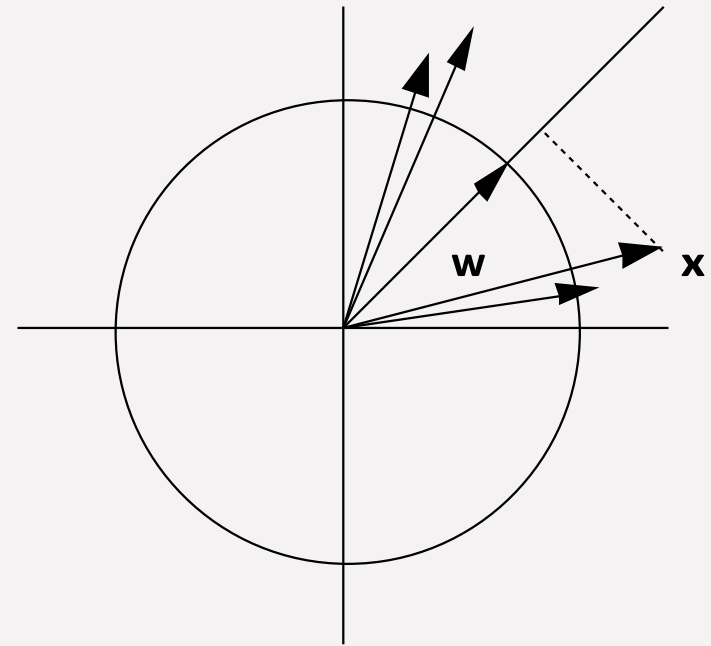
Convergence of The Oja's Algorithm

When a unique solution to the task exists,
Oja's algorithm will converge:

Idea of the proof:

Update of \vec{w} towards \vec{x}

- if Oja's algorithm is started for a weight vector inside a cone, it will oscillate in it, but will not leave it
- for $\|\vec{w}\| = 1$ the dot product $\Phi = \vec{x} \cdot \vec{w}$ corresponds to the length of the projection of \vec{x} on \vec{w}



Convergence of The Oja's Algorithm (2)

Idea of the proof (continue):

-) the vector $\vec{x} - \Phi \vec{w}$ is orthogonal to \vec{w}
-) an iteration of Oja's algorithm attracts \vec{w} to the vectors from cluster X
-) if the length of \vec{w} remains equal to 1 (or close to 1), \vec{w} will be brought into the middle of the cluster
-) further, it is necessary to show that the vector \vec{w} is automatically normalized by the Oja's learning algorithm:

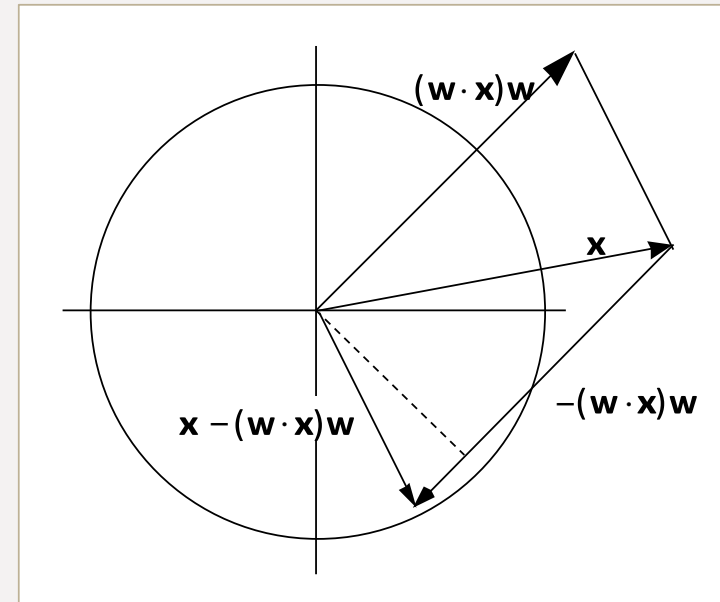
- Idea:
- a) the length of the vector \vec{w} is bigger than 1
 - b) the length of the vector \vec{w} is smaller than 1

Convergence of The Oja's Algorithm (3)

a) the length of the vector \vec{w} is bigger than 1

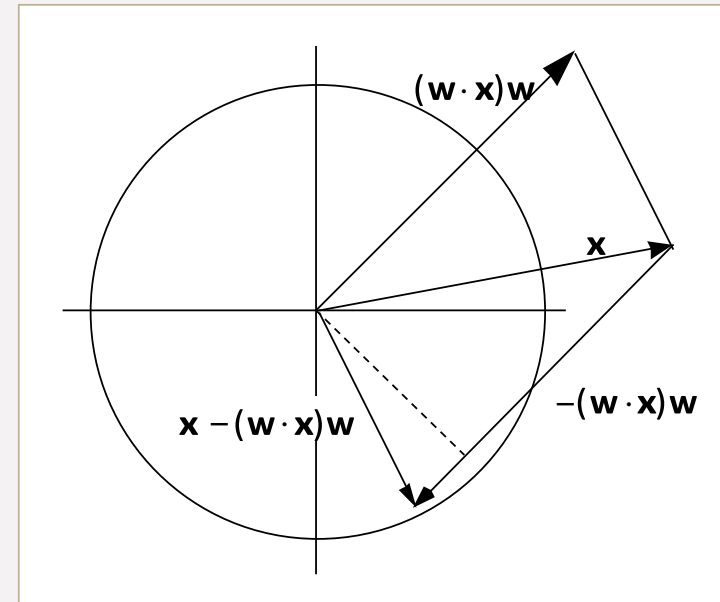
- The length of the vector $(\vec{x} \cdot \vec{w}) \vec{w}$ is bigger than the length of the orthogonal projection of \vec{x} on \vec{w}
- Further, assume that $\vec{x} \cdot \vec{w} > 0$, i.e., the vectors \vec{x} and \vec{w} are not too far away one from the other
- The vector $\vec{x} - (\vec{x} \cdot \vec{w}) \vec{w}$ has a negative projection on \vec{w} , as:

$$(\vec{x} - (\vec{x} \cdot \vec{w}) \vec{w}) \cdot \vec{w} = \vec{x} \cdot \vec{w} - \|\vec{w}\|^2 \vec{x} \cdot \vec{w} < 0$$



Convergence of The Oja's Algorithm (4)

- The result of many iterations:
 - (the vector $\vec{x} - (\vec{x} \cdot \vec{w})\vec{w}$ has one component normal to \vec{w} and another one with the opposite direction of \vec{w})
 - \vec{w} will be brought into the middle of the cluster of vectors (and the normal component cancels in average)
 - \vec{w} will become smaller with the growing number of iterations of this type (!avoid making \vec{w} too small or reversing its direction in an iteration!)



Convergence of The Oja's Algorithm (5)

- A suitable choice of the learning parameter γ and normalization of the training vectors:
 - if the vector \vec{x} has a positive dot product Φ with \vec{w} , then this should hold also for the new weight vector; it should thus hold:

$$\vec{x} \cdot (\vec{w} + \gamma\Phi(\vec{x} - \Phi\vec{w})) > 0$$

$$\Phi + \gamma\Phi\|\vec{x}\|^2 - \gamma\Phi\Phi^2 > 0$$

$$\underbrace{\Phi}_{> 0} \underbrace{(1 + \gamma(\|\vec{x}\|^2 - \Phi^2))}_{> 0} > 0 \Rightarrow \gamma(\|x^2\| - \Phi^2) > -1$$

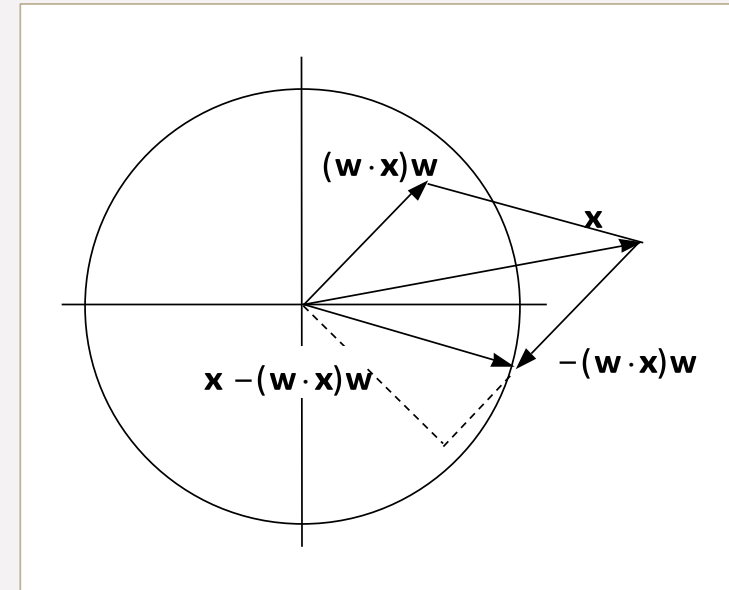
- For positive small enough γ , is always satisfied

Convergence of The Oja's Algorithm (6)

b) the length of the vector \vec{w} is smaller than 1

(similarly to a))

- The vector $\vec{x} - (\vec{x} \cdot \vec{w})\vec{w}$ has a positive projection on \vec{w}
 - growing of \vec{w}
- **Combining a) and b)** $\Rightarrow \vec{w}$ will be brought into the middle of the cluster and the length of \vec{w} will oscillate around 1 (for a small enough γ)
- Problems: „sparse“ clusters

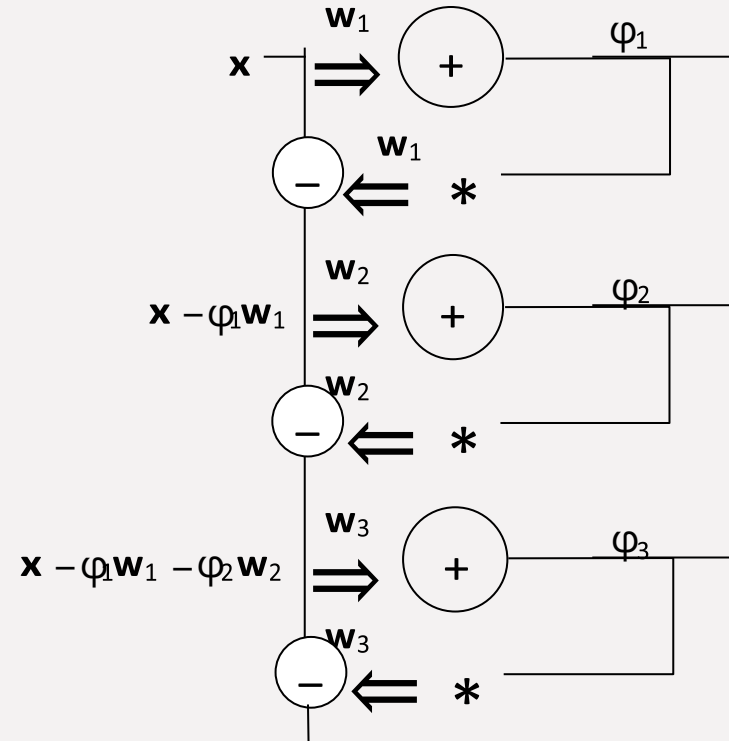


Oja's Learning Algorithm: Problems and Generalization

Problems:

- „sparse“ clusters
- big differences in the length of the input vectors

Computation of more
principal components:



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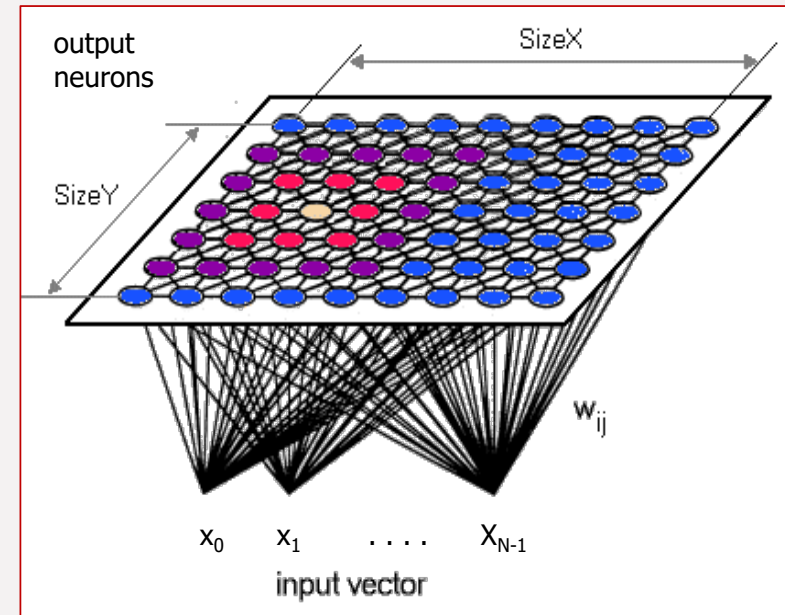
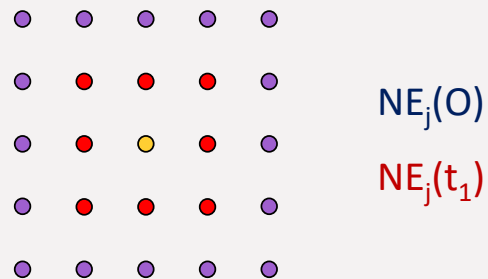
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Kohonen Self-Organizing Feature Maps

- Teuvo Kohonen – phonetic typewriter
 - Unsupervised training
 - Recall
 - Applications: economics, text and image processing, etc.
 - topological neighborhood



Kohonen Model: The Training Algorithm

Motivation:

- The grid of (topologically ordered) neurons allows us to identify the immediate neighbors of a given neuron
 - during training, the weights of the respective neurons and their neighbors will be updated

The objective: neighboring neurons should respond to closely related signals

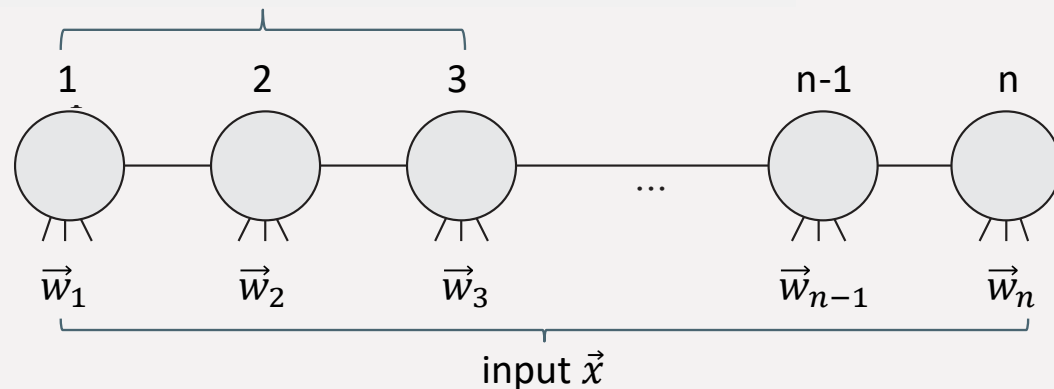
Kohonen Model: The Training Algorithm (2)

The problem (1-dimensional):

- divide the n -dimensional space by means of a one-dimensional chain of „Kohonen neurons“
- The neurons are arranged in a sequence and numbered from 1 to n

A one-dimensional
lattice of neurons

the neighborhood of neuron 2 (with radius 1)



Kohonen Model: The Training algorithm (3)

Problem (1-dimensional – continued):

- One-dimensional grid of neurons:
 - Each neuron receives an n -dimensional input \vec{x} and based on an n -dimensional weight vector $\vec{w} = (w_1, \dots, w_n)$, it computes its excitation

The objective: „specialization“ of each neuron to a different region of the input space (this „specialization“ is characterized by maximum excitation of the respective neurons for patterns from the given region)

Kohonen Model: The Training algorithm (4)

Problem (1-dimensional – continued):

- „Kohonen“ neurons compute the Euclidean distance between the input \vec{x} and the corresponding weight vector \vec{w}
 - „the closest“ neuron will be characterized by maximum excitation

Kohonen Model: The Training Algorithm (5)

Neighborhood definition:

- In a one-dimensional Kohonen map, the neighborhood of neuron k with radius 1 contains neuron $k-1$ and $k+1$
- Neurons on both ends of a one-dimensional Kohonen map have an asymmetric neighborhood
- In a 1 – dimensional Kohonen map, the neighborhood of neuron k with radius r contains all the neurons located up to r positions from k to the left or to the right
- Similarly for multidimensional Kohonen maps and the chosen grid metrics (rectangular, hexagonal, ...)

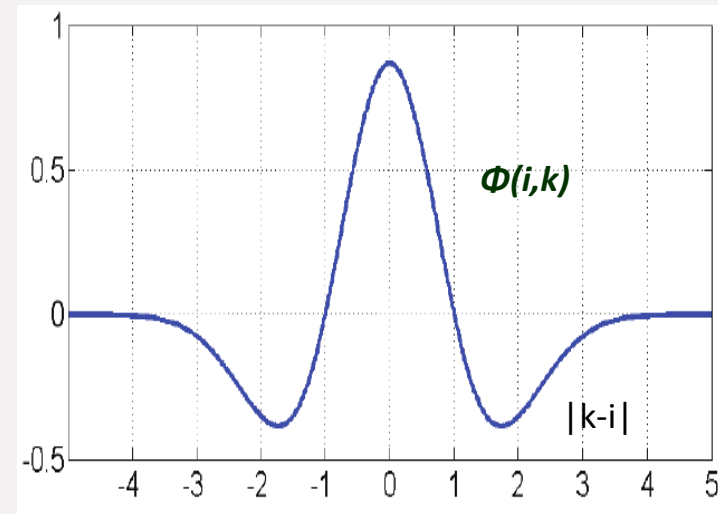
Kohonen Model: The Training Algorithm (6)

Lateral interaction function $\Phi(i,k)$:

~ „the strength of the lateral interconnection“ between neuron i and k during training

Example:

- $\Phi(i,k)=1 \ \forall i$ from the neighborhood of k with radius r and $\Phi(i,k)=0$ for all remaining i
- „Mexican hat“ function
- ... and others ...



Kohonen Self-Organizing Feature Maps: The Training Algorithm

Step 1: Initialize the weights between N input and M output neurons to small random values. Initialize also the neighborhood and the lateral interaction function Φ .

Step 2: Present a new training pattern to the network.

Step 3: Compute the distance d_j between the input pattern and the weight vectors of all output neurons j as:

$$d_j = \sum_{i=0}^{N-1} \left(x_i(t) - w_{ij}(t) \right)^2$$

where $x_i(t)$ denotes the input of neuron i at time t and $w_{ij}(t)$ corresponds to the synaptic weight between the input neuron i and the output neuron j at time t . This distance can contain weight coefficients.

Kohonen Self-Organizing Feature Maps: The Training Algorithm (2)

Step 4: Select (e.g., by means of lateral inhibition) the output neuron c with the minimum distance d_j from the presented input pattern and denote it to be „the winner“.

Step 5: Adjust the weights of the winning neuron c and all the neurons from its neighborhood N_c . The new weights are:

$$w_{ij}(t+1) = w_{ij}(t) + \alpha(t) \Phi(c,j) (x_i(t) - w_{ij}(t))$$

for $j \in N_c$; $0 \leq i \leq N-1$

$\alpha(t)$ is the vigilance coefficient ($0 < \alpha(t) < 1$) decreasing with time.

Kohonen Self-Organizing Feature Maps: The Training Algorithm (3)

For the choice of $\alpha(t)$ it should hold:

$$\sum_{t=1}^{\infty} \alpha(t) = \infty \quad \wedge \quad \sum_{t=1}^{\infty} \alpha^2(t) < \infty$$

e.g., for $\alpha(t) = \frac{1}{t}$: $\sum_{t=1}^{\infty} 1/t = \infty$
 $\sum_{t=1}^{\infty} 1/t^2 = \frac{\pi^2}{6}$

During training, the winning neuron adjusts its weight vector towards current input patterns. The same holds also for neurons from the neighborhood of the winner.

The value of the function $\Phi(c,j)$ decreases with growing distance of the neurons from the center of the neighborhood N_c .

Step 6: Repeat by Going to **Step 2**.

Neural Networks:

Contents:

- Self-Organization
- Kohonen Maps, Hybrid Models, and Genetic Algorithms

Contents:

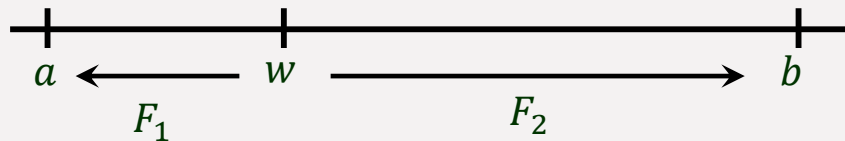
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Analysis of Convergence: Stability of The Solution and an Ordered State

Stability when supposed that the network has already arrived at an ordered state:

1) One-dimensional case:

- a) interval $[a, b]$, 1 neuron with the weight w , no neighborhood considered:



→ convergence of w towards the center of $[a, b]$

Analysis of Convergence:

Stability of The Solution and an Ordered State (2)

- The update rule: $w_n = w_{n-1} + \alpha(x - w_{n-1})$
 $w_n, w_{n-1} \dots$ weight values at time n and $n - 1$
 x a random number from the interval $[a, b]$
- If $0 < \alpha \leq 1$, the series w_1, w_2, \dots cannot leave $[a, b]$
- Bounded is also the expected value $\langle w \rangle$ of the weight w
- The expected value of the derivative of w with respect to t is zero:
 $\left\langle \frac{dw}{dt} \right\rangle = 0$, otherwise $\langle w \rangle$ would be $\langle w \rangle < a$ or $\langle w \rangle > b$
- As $\left\langle \frac{dw}{dt} \right\rangle = \alpha(\langle x \rangle - \langle w \rangle) = \alpha\left(\frac{a+b}{2} - \langle w \rangle\right)$, it follows: $\langle w \rangle = (a + b)/2$

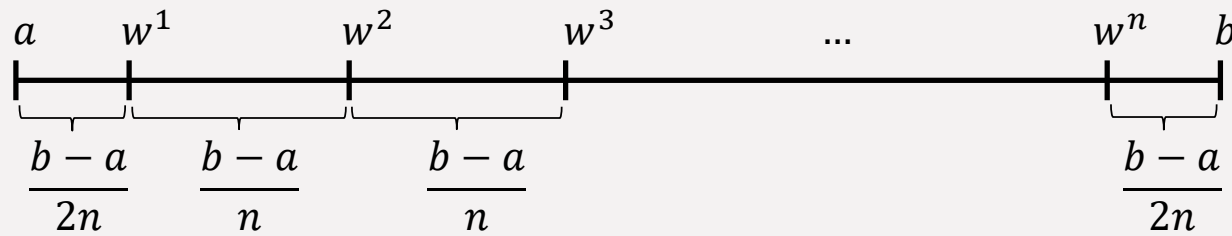
Analysis of Convergence: Stability of The Solution and an Ordered State (3)

b) interval $[a, b]$, n neurons with the weights w^1, w^2, \dots, w^n

- no neighborhood considered,
- the weights are assumed to be monotonically ordered:

$$a < x^1 < x^2 < \dots < x^n < b$$

→ the weights converge to: $\langle w^i \rangle = a + (2i - 1) \frac{b-a}{2n}$



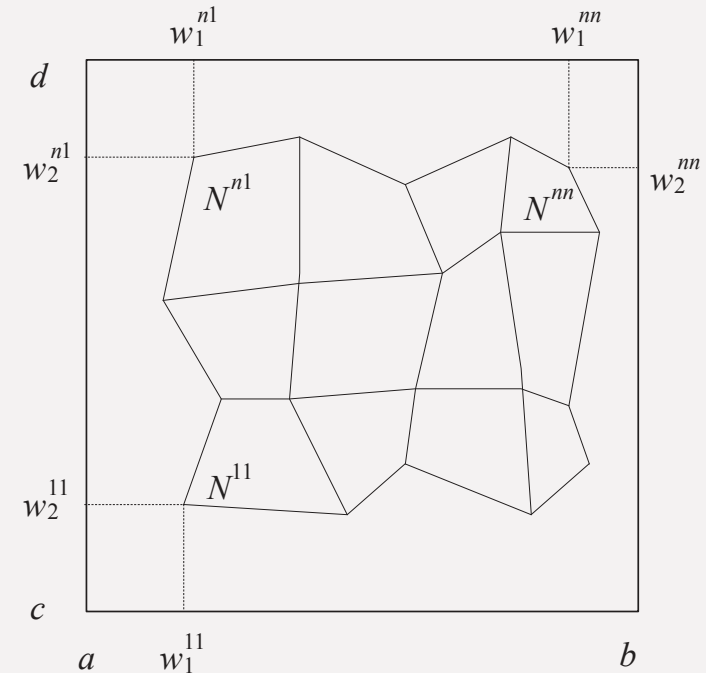
Analysis of Convergence: Stability of The Solution and an Ordered State (4)

2) Two-dimensional case:

- interval $[a, b] \times [c, d]$, $n \times n$ neurons
- no neighborhood considered, monotonically ordered weights:

$$\begin{aligned} w_1^{ij} &< w_1^{ik} && \text{for } j < k \\ w_2^{ij} &< w_2^{kj} && \text{for } j < k \end{aligned}$$

→ The problem will be reduced
to two 1-dimensional problems



N^{ij} is the neuron at row i and column j with the weights w_1^{ij} and w_2^{ij}

Analysis of Convergence: Stability of The Solution and an Ordered State (5)

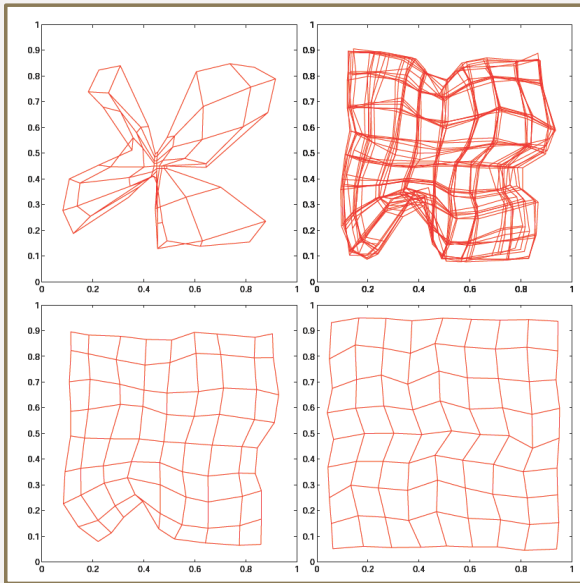
2) Two-dimensional case (continued):

- Let $w_j^1 = \frac{1}{n} \sum_{i=1}^n w_1^{ij}$ denote the average weight value of the neurons from the j -th column
 - Since $w_1^{ij} < w_1^{ik}$ for $j < k$, these average values w_1^j will be monotonically arranged: $a < w_1^1 < w_1^2 < \dots < b$
 - In the first column, the average weight value will oscillate around the expected value $\langle w_1^1 \rangle$
 - Similarly for the average weight values in each row
- convergence to a stable state (for small enough learning rates)

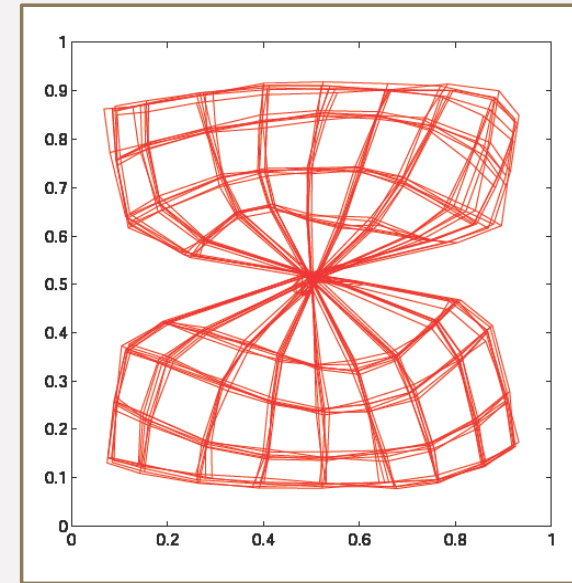
Analysis of Convergence: Stability of The Solution and an Ordered State (6)

PROBLEMS:

- „unfolding“ a planar mesh and conditions, under which it will happen



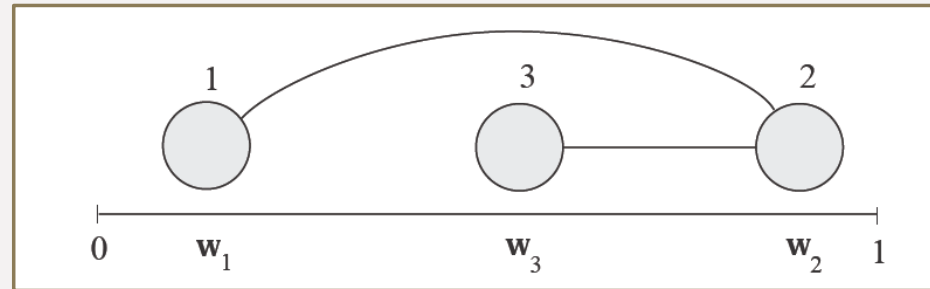
But sometimes



Analysis of Convergence: Stability of The Solution and an Ordered State (7)

PROBLEMS:

- „meta-stable states“ and improper choice of lateral interaction (a too fast decrease)



- convergence of 1-dimensional Kohonen networks to an ordered state if the input is selected from a uniform distribution and the following update rule is used

$$w_k^{new} = w_k^{old} + \gamma(x - w_k^{old})$$

where k denotes the winning neuron and its two neighbors (Cottrell & Fort, 1986)

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Variants of The Training Algorithm for Kohonen Maps

Supervised training:

(LVQ ~ Learning Vector Quantization)

LVQ1:

- Motivation:

-) \vec{x} should belong to the same class as the closest \vec{w}_i
- let $c = \arg \min_i \{\|\vec{x} - \vec{w}_i\|\}$ denotes the \vec{w}_i that is the closest one to \vec{x} ($c \sim$ the winning neuron)

Variants of The Training Algorithm for Kohonen Maps (2)

LVQ1 (continued):

→ adjustment rules ($0 < \alpha(t) < 1$):

- $\vec{w}_c(t+1) = \vec{w}_c(t) + \alpha(t)[\vec{x}(t) - \vec{w}_c(t)]$

if \vec{x} and \vec{w}_c are classified identically

- $\vec{w}_c(t+1) = \vec{w}_c(t) - \alpha(t)[\vec{x}(t) - \vec{w}_c(t)]$

if \vec{x} and \vec{w}_c are classified differently

- $\vec{w}_i(t+1) = \vec{w}_i(t)$ if $i \neq c$

Variants of The Training Algorithm for Kohonen Maps (3)

LVQ2.1:

- Motivation: mutual update of 2 nearest neighbors of \vec{x}
 - One must belong to the correct class, the other to the incorrect
 - Furthermore, \vec{x} must be from the area close to the separating hyperplane between \vec{w}_i and \vec{w}_j (~ from „the window“)
 - If d_i (resp. d_j) denotes the Euclidean distance between \vec{x} and \vec{w}_i (resp. between \vec{x} and \vec{w}_j), „the window“ can be defined by means of:

$$\min\left(\frac{d_i}{d_j}, \frac{d_j}{d_i}\right) > s, \text{ where } s = \frac{1 - \omega}{1 + \omega}$$

(recommended values for ω (~ the width of the window): 0.2 – 0.3)

Variants of The Training Algorithm for Kohonen Maps (4)

LVQ2.1 (continued):

→ adjustment rules ($0 < \alpha(t) < 1$):

- $\vec{w}_i(t + 1) = \vec{w}_i(t) - \alpha(t)[\vec{x}(t) - \vec{w}_i(t)]$
- $\vec{w}_j(t + 1) = \vec{w}_j(t) + \alpha(t)[\vec{x}(t) - \vec{w}_j(t)]$
 - \vec{w}_i and \vec{w}_j are the closest to \vec{x}
 - at the same time, \vec{x} and \vec{w}_j belong to the same class
 - and \vec{x} and \vec{w}_i belong to different classes
 - \vec{x} comes from the „window“

Variants of The Training Algorithm for Kohonen Maps (5)

LVQ3 (motivation):

- approximation of the class distributions and stabilization of the solution
→ adjustment rules ($0 < \alpha(t) < 1$):
 - $\vec{w}_i(t+1) = \vec{w}_i(t) - \alpha(t)[\vec{x}(t) - \vec{w}_i(t)]$
 - $\vec{w}_j(t+1) = \vec{w}_j(t) + \alpha(t)[\vec{x}(t) - \vec{w}_j(t)]$
 - \vec{w}_i and \vec{w}_j are the closest to \vec{x} ; \vec{x} and \vec{w}_j belong to the same class; while \vec{x} and \vec{w}_i belong to different classes and \vec{x} comes from the „window“
 - $\vec{w}_k(t+1) = \vec{w}_k(t) + \varepsilon\alpha(t)[\vec{x}(t) - \vec{w}_k(t)]$
 - for $k \in \{i, j\}$ if \vec{x} , \vec{w}_i and \vec{w}_j belong to the same class
 - The choice of parameters for the „window“: $0.1 \leq \varepsilon \leq 0.5$ and $0.2 \leq \omega \leq 0.3$

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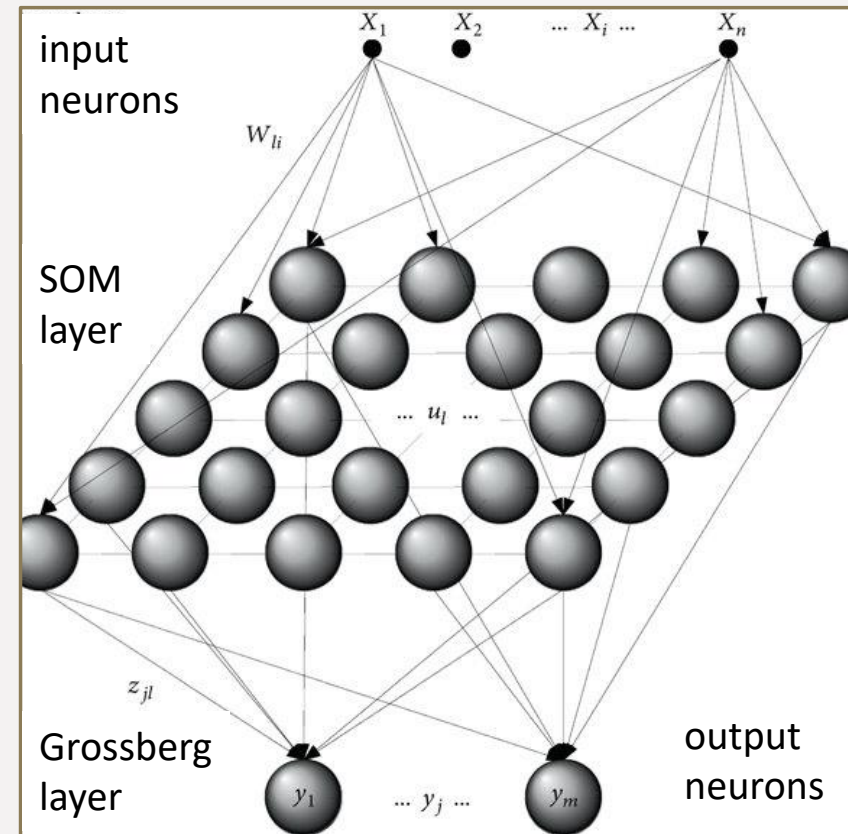
Variants of The Training Algorithm for Kohonen Maps (7)

Further variants:

- Multi-layered Kohonen maps
 - Abstraction tree
- Counterpropagation networks
 - Supervised training – two phases
 - Kohonen (clustering) layer
 - Grossberg layer (weight adjustment only for the winning neurons from the Kohonen layer)

Counterpropagation Networks

- Training: supervised
- Recall
- Application:
 - Heteroassociative memory



The Training Algorithm for Counterpropagation Networks (1)

Step 1: Initialize synaptic weights to small random values.

Step 2: Present a new training pattern to the network as:

$$(input, desired\ output) = (\vec{x}(t), \vec{d}(t)).$$

Step 3: In the Kohonen layer, find the winning neuron c , the synaptic weights of which best correspond to the presented pattern $\vec{x}(t)$. For this neuron, it thus follows that the distance e_c between the selected weight vector $\vec{v}_c(t)$ and the presented pattern $\vec{x}(t)$ is minimal. E.g., the Euclidean metrics can be used; then:

$$e_c = \min_k e_k = \min_k \sqrt{\sum_i (x_i(t) - v_{ik}(t))^2}$$

The Training Algorithm for Counterpropagation Networks (2)

Step 4: Update the weights v_{ik} between the input neuron i and the neurons from Kohonen layer that belong to the neighborhood N_c of neuron c to better correspond to the presented pattern $\vec{x}(t)$:

$$v_{ik}(t + 1) = v_{ik}(t) + \alpha(t)(x_i(t) - v_{ik}(t))$$

$\alpha(t)$, where $0 < \alpha(t) < 1$, is the training parameter for the weights between the input and Kohonen layer that decreases with time. t represents the current training step, $t + 1$ the following one.

The Training Algorithm for Counterpropagation Networks (3)

Step 5: Update the weights w_{cj} between the „winning“ neuron c from the Kohonen layer and the neurons of the Grossberg layer such that the output vector \vec{y} better corresponds to the desired output $\vec{d}(t)$:

$$w_{cj}(t + 1) = (1 - \beta)w_{cj}(t) + \gamma z_c d_j(t)$$

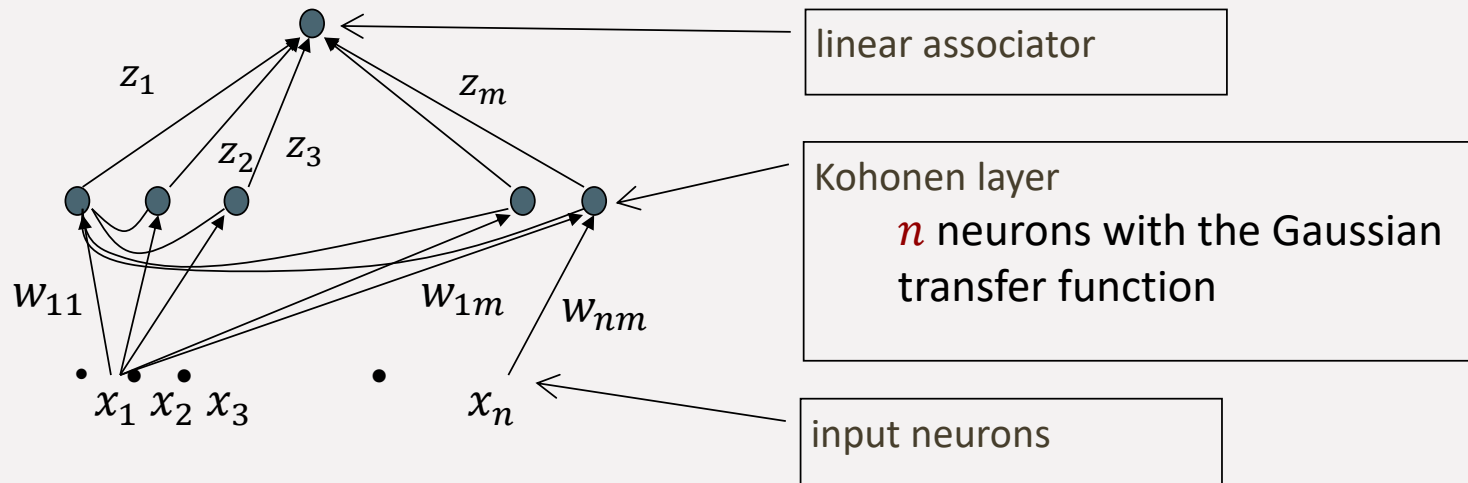
$w_{cj}(t)$ is the weight of the synaptic connection between the c -th neuron of the Kohonen layer and the j -th neuron of the Grossberg layer in time t , $w_{cj}(t + 1)$ denotes the value of this synaptic connection in time $t + 1$.

β is a positive constant influencing the dependence of the new value of the synaptic weight on its value in the preceding training step. A positive constant γ represents the learning rate for the weights between the Kohonen and Grossberg layer, z_c denotes the activity of the „winning“ neuron from the Kohonen layer.

Step 6: Go to Step 2.

RBF-networks (Radial Basis Functions)

- Hybrid architecture (Moody & Darken)
- Supervised training



RBF-networks (Radial Basis Functions)

- Every neuron j computes its output $g_j(t)$ according to:

$$g_j(\vec{x}) = \frac{\exp\left(-\frac{(\vec{x} - \vec{w}_j)^2}{2\sigma_j^2}\right)}{\sum_k \exp\left(-\frac{(\vec{x} - \vec{w}_k)^2}{2\sigma_k^2}\right)}$$

\vec{x} ... input vector

$\vec{w}_1, \dots, \vec{w}_n$... weight vectors of hidden neurons

$\sigma_1, \dots, \sigma_n$... constants (set, e.g., according to the distance between the respective weight vector and its closest neighbor)

RBF-networks (Radial Basis Functions)

- the output of each hidden neuron is normalized
 - mutual inter-connection of all the neurons
- the weights z_1, \dots, z_m can be found, e.g., by means of the back-propagation training algorithm:

$$E = \frac{1}{2} \sum_p \left(\sum_{j=1}^m g_j(\vec{x}_p) z_j - d_p \right)^2$$

The error function on the whole training set

Adaptation for a single training pattern (x, d)

$$\Delta z_i \cong -\frac{\partial E}{\partial z_i} = \gamma g_i(\vec{x}) \left(d - \sum_{j=1}^m g_j(\vec{x}) z_j \right)$$

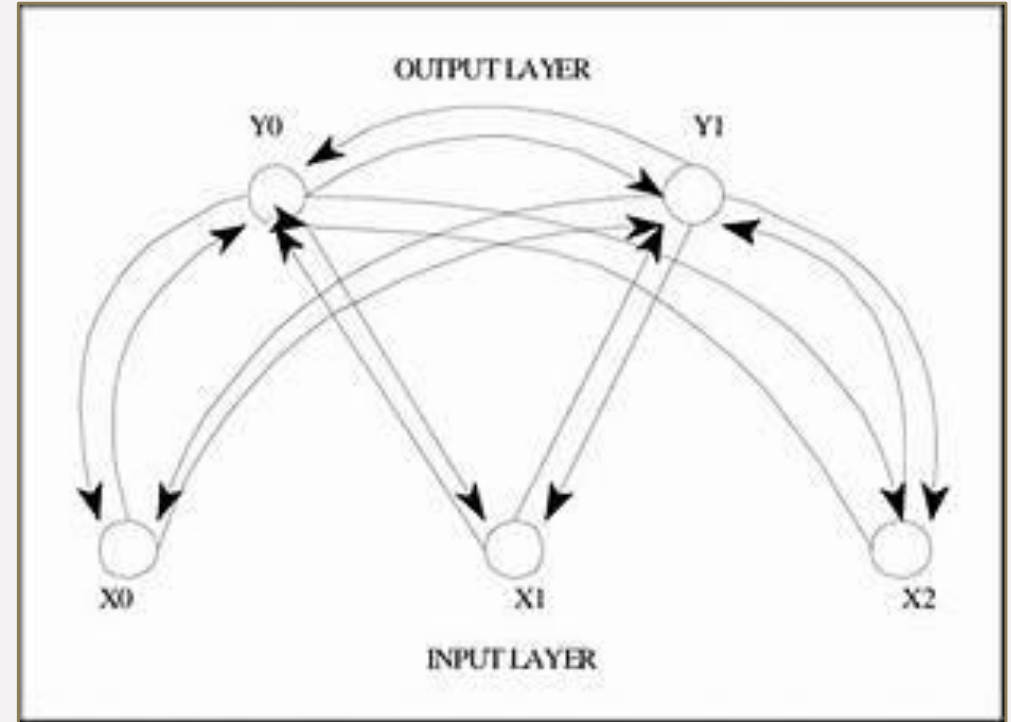
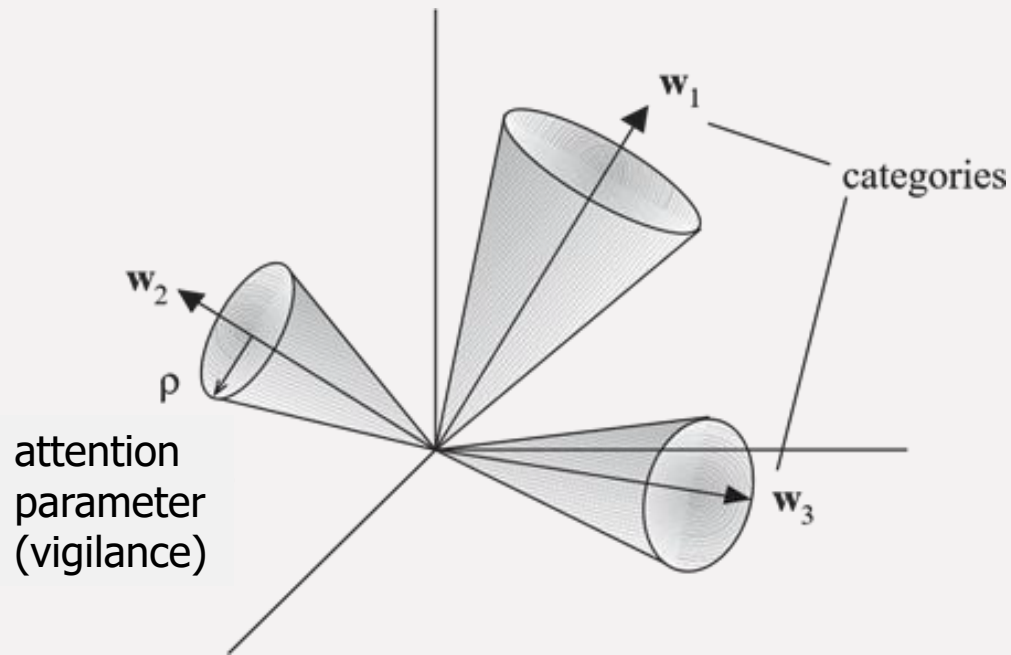
d ... the desired output

p ... the number of training patterns

γ ... training parameter

ART – Adaptive Resonance Theory

(Carpenter & Grossberg)



ART – Adaptive Resonance Theory (2)

(Carpenter & Grossberg)

ART 1:

- Binary inputs, unsupervised training
- Lateral inhibition is used to find the output neuron with maximum response
- Feedback weights (from the output neurons to the input neurons) are used to compare the actual similarity of the processed input pattern with the recalled pattern (stored in the weights)

ART – Adaptive Resonance Theory (3)

(Carpenter & Grossberg)

ART 1 (continued):

- Vigilance test – attention parameter ρ
- A mechanism to „switch off“ the output neuron with maximum response
 - stability × plasticity of the network
- × the network has big problems even for „moderately noise-corrupted patterns“
 - a growing number of stored patterns

ART 1 – The Training Algorithm

Step 1: Initialization

$$t_{ij}(0) = 1 \quad 0 \leq i \leq N - 1$$

$$b_{ij}(0) = 1/(1 + N) \quad 0 \leq j \leq M - 1$$

$$\rho \quad 0 \leq \rho \leq 1$$

$b_{ij}(t)$ ~ the weight between the input neuron i and the output neuron j in time t

$t_{ij}(t)$ ~ the weight between the output neuron j and the input neuron i in time t (determine the pattern specified by the output neuron j)

ρ ~ vigilance parameter (determines, how close should be the presented input to the stored pattern to belong to the same category)

ART 1 – The Training Algorithm (2)

Step 2: Present a new input pattern

Step 3: Compute the activation of output neurons

$$\mu_j = \sum_{i=0}^{N-1} b_{ij}(t) x_i; \quad 0 \leq j \leq M - 1$$

$\mu_j \sim$ output of the output neuron j

$x_i \sim i$ -th component of the input vector ($\in \{0,1\}$)

Step 4: Find the stored pattern, that best represents the presented pattern (e.g., by means of lateral inhibition):

$$\mu_{j^*} = \max_j \{\mu_j\}$$

ART 1 – The Training Algorithm (3)

Step 5: Vigilance test (using feedback weights)

$$\|\vec{x}\| = \sum_{i=0}^{N-1} x_i \text{ and } \|T \cdot \vec{x}\| = \sum_{i=0}^{N-1} t_{ij^*} x_i \quad (x_i \in \{0,1\})$$

if $\frac{\|T \cdot \vec{x}\|}{\|\vec{x}\|} > \rho$, go to Step 7

else go to Step 6

Step 6: Inhibit the best matching neuron

the output of neuron j^* selected in Step 4 is temporarily set to zero
(and not considered in the following maximization in Step 4).

Afterwards go to Step 4.

ART 1 – The Training Algorithm (4)

Step 7: Adjustment of the best matching neuron

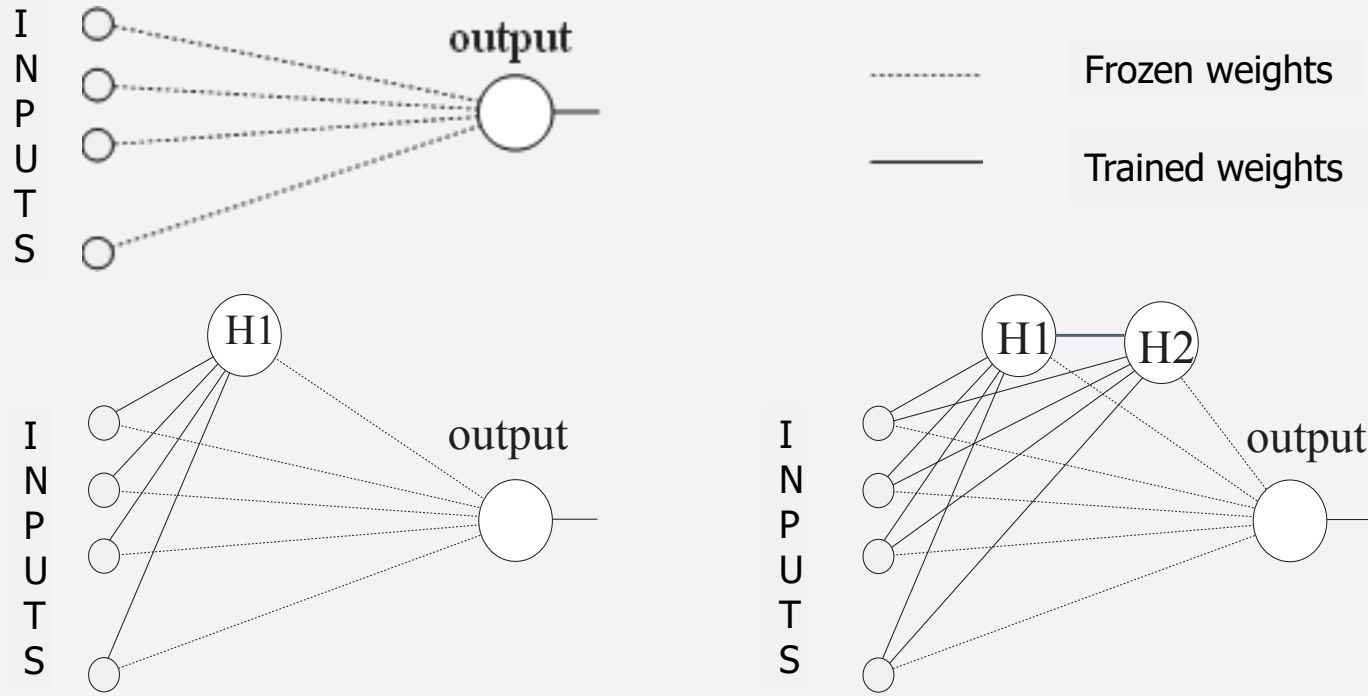
$$t_{ij^*}(t + 1) = t_{ij^*}(t) \cdot x_i$$

$$b_{ij^*}(t + 1) = \frac{t_{ij^*}(t) \cdot x_i}{0.5 + \sum_{i=0}^{N-1} t_{ij^*}(t) \cdot x_i}$$

Step 8: Go to Step 2 and repeat

(Before that, „switch on“ all the neurons „switched off“ in Step 6)

Cascade Correlation (2) (Fahlman & Lebiere, 1990)



Cascade Correlation (3) (Fahlman & Lebiere, 1990)

Training of the network (proceeds in 2 phases):

- a) During the first phase, the already existing network is trained by means of Quickprop
- If the current error value is small enough, the algorithm stops
 - If the average quadratic error remains bigger than its desired level, a new neuron is added to the network

Cascade Correlation (4) (Fahlman & Lebiere, 1990)

Training of the network (continued):

- b) The new added neuron is trained to maximize correlation between its output and the error at network output
- **the output of the trained added neuron strongly correlates with the „residual“ error**
- The input weights of the added neuron will be frozen
 - Only the weights from the added neuron to the output will be „retrained“

Cascade Correlation (5) (Fahlman & Lebiere, 1990)

Training of the network (continued):

While training hidden neurons, our objective is to maximize S :

$$S = \left| \sum_{i=1}^p (V_i - \bar{V}) (E_i - \bar{E}) \right|$$

p the number of training patterns

V_i output of the added neuron for the i -th pattern

\bar{V} average output of the added neuron

E_i error for the i -th pattern

\bar{E} average error

Cascade Correlation (Fahlman & Lebiere, 1990)

~ a robust growing architecture

- The system starts training with a direct interconnection between the inputs and outputs
- Subsequently, hidden neurons are added
- The inputs of each new neuron are interconnected with all original inputs and previously created neurons

$$S = \left| \sum_{i=1}^p (V_i - \bar{V}) (E_i - \bar{E}) \right|$$

Cascade Correlation (6) (Fahlman & Lebiere, 1990)

Training of the network (continued):

$$\frac{\partial S}{\partial w_k} = \sum_{i=1}^p \sigma(E_i - \bar{E}) f'_i I_{i,k}$$

σ the sign of correlation between the added neuron and the output

f'_i the derivative of the transfer function for pattern i

$I_{i,k}$ k -th input of the added neuron for pattern i

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Genetic Algorithms (GA)

- Lawrence Fogel
 - studied **recombination and mutating** of populations
 - *L. Fogel et al.: Artificial Intelligence Through Simulated Evolution, John Wiley and Sons, New York, 1966*
- John Holland
 - proposed the **concept of schemata** and studied their diffusion dynamics
 - *J. Holland: Adaptation in Natural and Artificial Systems: An Introductory Analysis with Applications to Biology, Control and Artificial Systems, The University of Michigan Press, Ann Arbor, MI, 1975*
- David Goldberg
 - summarized **evolutionary methods** for the solution of optimization problems
 - *D. Goldberg: Genetic Algorithms in Search, Optimization, and Machine Learning, Addison-Wesley, Reading, MA, 1989*

Genetic Algorithms (GA)

- Artificial chromosome (genotype)
 - ~ a string of symbols that code the properties of the individual (phenotype), e.g., a binary value of a variable or their sequence
 - many coding types – binary, Grey, real values, ...
 - various alphabets – binary, ternary, ...

with the Grey code, only one bit changes state from one position to another, i.e., if more than one bit changes, the data must be incorrect

	Binary code	Grey code
0	000	000
1	001	001
2	010	011
3	011	010
4	100	110

Genetic Algorithms (GA)

■ Population

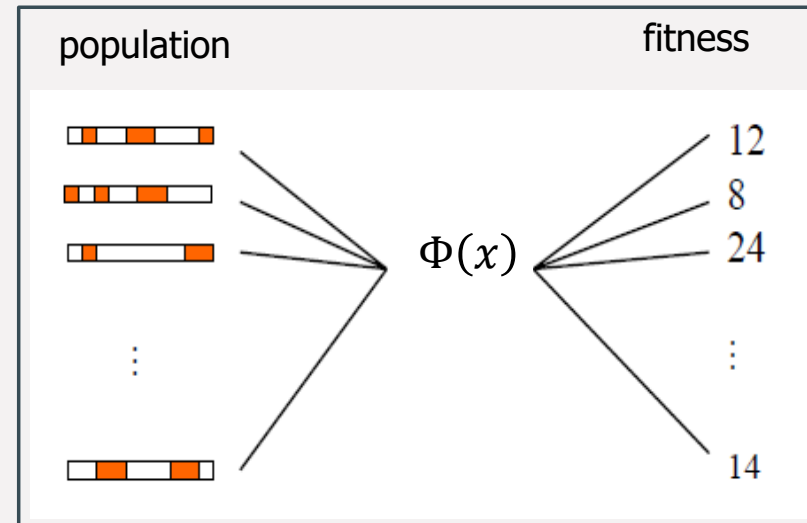
~ a set of artificial chromosomes that cyclically undergo selective reproduction with random changes

- more efficient individuals are favored

■ Fitness function (performance criterion)

~ a mapping $\Phi: \text{genotype} \rightarrow \mathbb{R}$

- better individuals get higher values



Genetic Algorithms (GA)

A general genetic algorithm (Goldberg, 1989)

- create a population of N randomly generated chromosomes x_1, x_2, \dots, x_N
- repeat
 - decode all the chromosomes and evaluate their fitness, $f_i = \Phi(x_i)$
 - form a new population by means of selective reproduction
 - recombine the chromosomes – crossover
 - mutate the chromosomes
- until the wanted individual has been found or the fitness of the so-far best individual does not improve

GA: Simple Selection

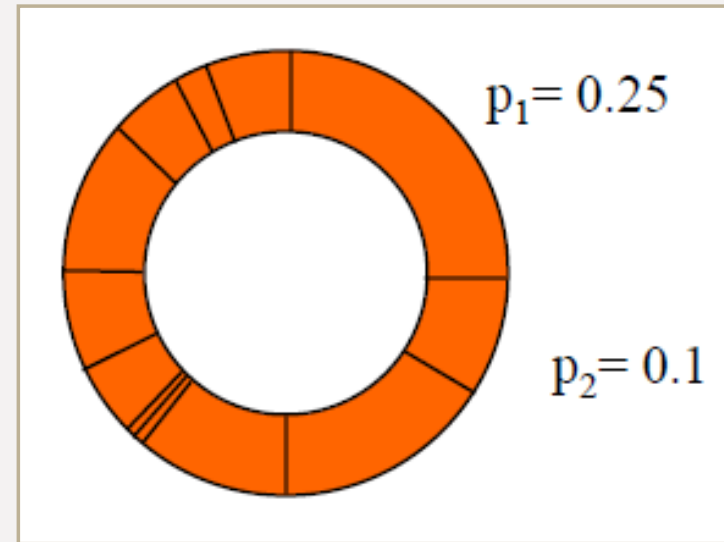
- a new population is created by copying the chromosomes from the previous population
 - the better is the copied individual, the more copies should be contained in the new population

- Roulette wheel selection:

- the chance of an individual's being selected is proportional to its fitness:

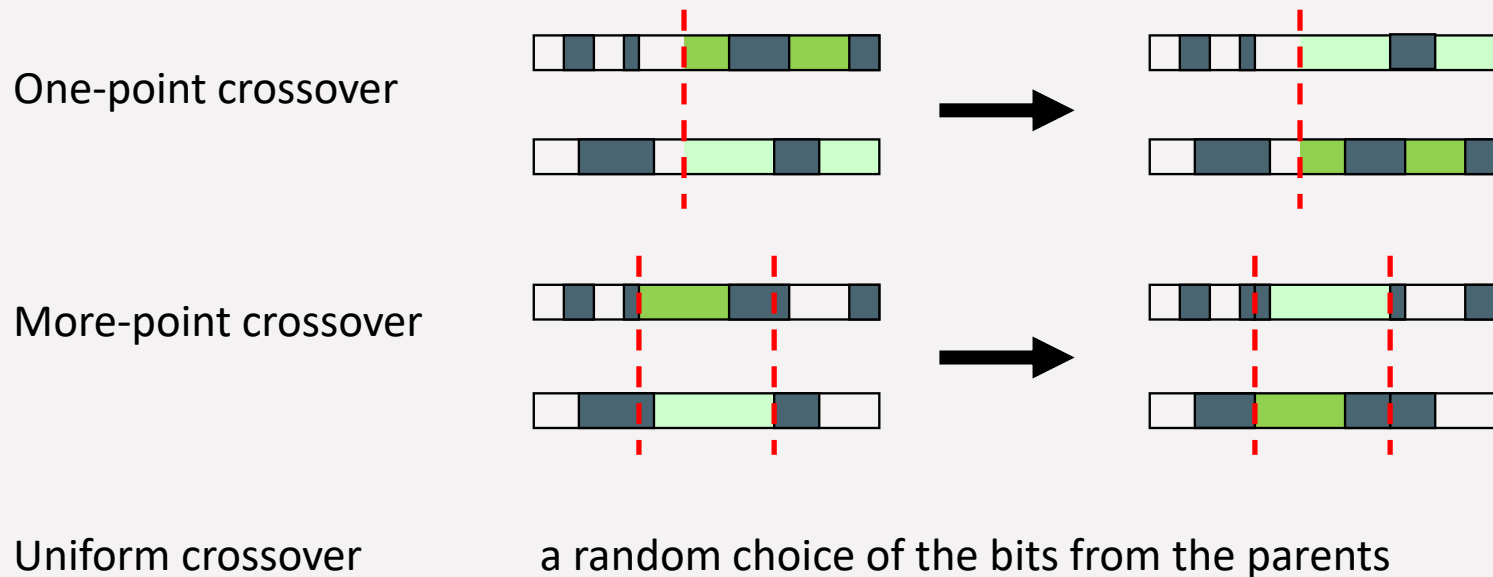
$$p_i = \frac{f_i}{\sum_{j=1}^N f_j}$$

- for a population of N individuals, the roulette wheel will be spun N -times



GA: Crossover

- individuals are randomly paired
- each pair of individuals will be „crossed over“ with a given probability



Mutation and distributed GA

- Mutation: ~ alter each element of the chromosome with a given probability
 - (binary-valued) bits will be negated
 - in the case of other ranges, a randomly chosen value can be used directly or in addition to the original value
 - probability of mutation is, in general, very low, e.g., 0.001
 - Exception: local minima (analogy to niche populations, e.g., hemophilia in European royalty, ectrodactyly in isolated tribes)



Mutation and distributed GA (2)

■ Distributed genetic algorithms:

- the individuals of a population are arranged, e.g., into a 2D- space
- selection and crossover proceed only locally, yet individual sub-populations overlap
~ analogy to settler populations

=> propagation of „advantageous“ properties over entire populations



GA: Non-determinism

- The whole GA is non-deterministic and uses random variables
- Typically, we are interested in the average and maximum fitness
- GA stops after the desired fitness value has been achieved, a preset number of generations has been completed or if the fitness did not change during several past generations
- Afterwards, GA can be run again with other parameters
- The result represents the best individual selected from final generations over all the GA-runs

Neural Networks:

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- Self-Organization
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GA: Schemata

- a schema is a mask describing a certain group of strings / chromosomes
 - $1**1 = \{1001, 1011, 1101, 1111\}$; * stands for any allowed value
- binary strings of length l allow for at most 3^l different schemata
- a population of N individuals represented by strings of length l yields between 2^l and $N2^l$ schemata
- a schema may define a property that guarantees high fitness
- it potentially allows to investigate more strings than actually contained within the population
- GA processes at most N^3 schemata in each step, even if it contains only N strings (an implicit parallelism in GA – Holland, 1975)

GA: Schemata (continued)

- some schemata yield a higher average fitness
- long schemata can be easily destroyed: **1*****1** vs. *****01****
- *short schemata yielding a high average fitness grow exponentially during GA*
- schemata are considered to be the basic building blocks of evolution; crossover represents its main operator as it allows to investigate the combinations of schemata. In this respect, however, appropriate coding is required with short building blocks
- Note: sometimes, crossover worsens the results – in such a case, its probability shall be set to very small values or zero

GA: Schemata Theorem

- The order of the schema H , $o(H)$, is the number of fixed positions in the schema H (i.e., with values **0** or **1** for a binary alphabet), e.g.:
 - $o(011*1**) = 4$
 - $o(1*****) = 1$
- The length of the schema H , $\delta(H)$, corresponds to the distance between the first and the last fixed position of H :
 - $\delta(011*1**) = 4$
 - $\delta(1*****) = 0$
- *The Schemata Theorem analyzes the influence of reproduction, crossover and mutation on the number of strings corresponding to a given schema*

GA – Convergence Analysis: the Influence of Reproduction

The influence of reproduction on the expected number of individuals with a given schema in the population:

- At time t , the population contains m strings of the schema H ($m = m(H, t)$)
- During reproduction, a string A_i is selected to the following population (according to its fitness $f_i = \Phi(A_i)$) with the probability: $p_i = \frac{f_i}{\sum_{j=1}^N f_j}$
- In the following population of the size n , the expected number of strings complying with the schema H ($m = m(H, t + 1)$) can be estimated as:

$$m(H, t + 1) = m(H, t) \cdot N \cdot \frac{f(H)}{\sum_{j=1}^N f_j}$$

where $f(H)$ is the average fitness of strings complying with the schema H

GA – Convergence Analysis: the Influence of Reproduction (2)

The influence of reproduction on the expected number of individuals with a given schema in the population (cont.):

- For the average fitness $f(H)$ of strings complying with the schema H at time t and for the average fitness of the entire population of n strings:

$$\bar{f} = \frac{\sum_{j=1}^N f_j}{N}$$

we obtain: $m(H, t + 1) = m(H, t) \cdot \frac{f(H)}{\bar{f}}$

- During fitness-based reproduction, the number of strings complying with a given schema grows / drops according to the average fitness

GA – Convergence Analysis: the Influence of Crossover

The influence of crossover on the expected number of individuals with a given schema in the population:

- for each schema, we can assess the probability p_s of surviving crossover as:

$$p_s = 1 - \frac{\delta(H)}{l-1}$$

- if crossover is performed randomly with probability p_c , the probability of surviving crossover corresponds to: $p_s = 1 - p_c \frac{\delta(H)}{l-1}$

→ During reproduction combined with crossover, the number of strings complying with a given schema grows / drops in the population according to the length of the schema and its average fitness:

$$m(H, t + 1) \geq m(H, t) \cdot \frac{f(H)}{\bar{f}} \cdot \left[1 - p_c \frac{\delta(H)}{l-1} \right]$$

GA – Convergence Analysis: the Influence of Mutation

The influence of mutation on the expected number of individuals with a given schema in the population:

- a random change occurs at each position with probability p_m
⇒ each position survives mutation with probability $1 - p_m$
- all the respective mutations are mutually independent
- for a schema, each of the $o(H)$ fixed positions has to survive
⇒ the probability of surviving mutation is for schema H : $(1 - p_m)^{o(H)}$
- approximation for very small values of p_m ($\ll 1$):
$$(1 - p_m)^{o(h)} \sim 1 - o(H)p_m$$

GA – Convergence Analysis: the Influence of Mutation (2)

The influence of mutation on the expected number of individuals with a given schema in the population (cont.):

- The expected number of strings complying with schema H in the population after reproduction, crossover, and mutation:

$$m(H, t + 1) \geq m(H, t) \cdot \frac{f(H)}{\bar{f}} \cdot \left[1 - p_c \frac{\delta(H)}{l - 1} - o(H) \cdot p_m \right]$$

→ During reproduction combined with crossover and mutation, the highest chance to survive possess short schemata with few fixed positions and above-average fitness

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