Artificial Neural Networks
Unsupervised learning: SOM

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Outline

- Competitive learning.
- Self-organization, Vector Quantization, Cluster Analysis.
- SOM architecture and learning.
- SOM visualizations.
- SOM evaluation.

Competitive Learning

- Nature inspired.
- No arbiter needed – unsupervised learning.
- Individuals (units, neurons) learn from examples.
- System **self-organizes**.
- Now we are going to apply this to **cluster analysis**.

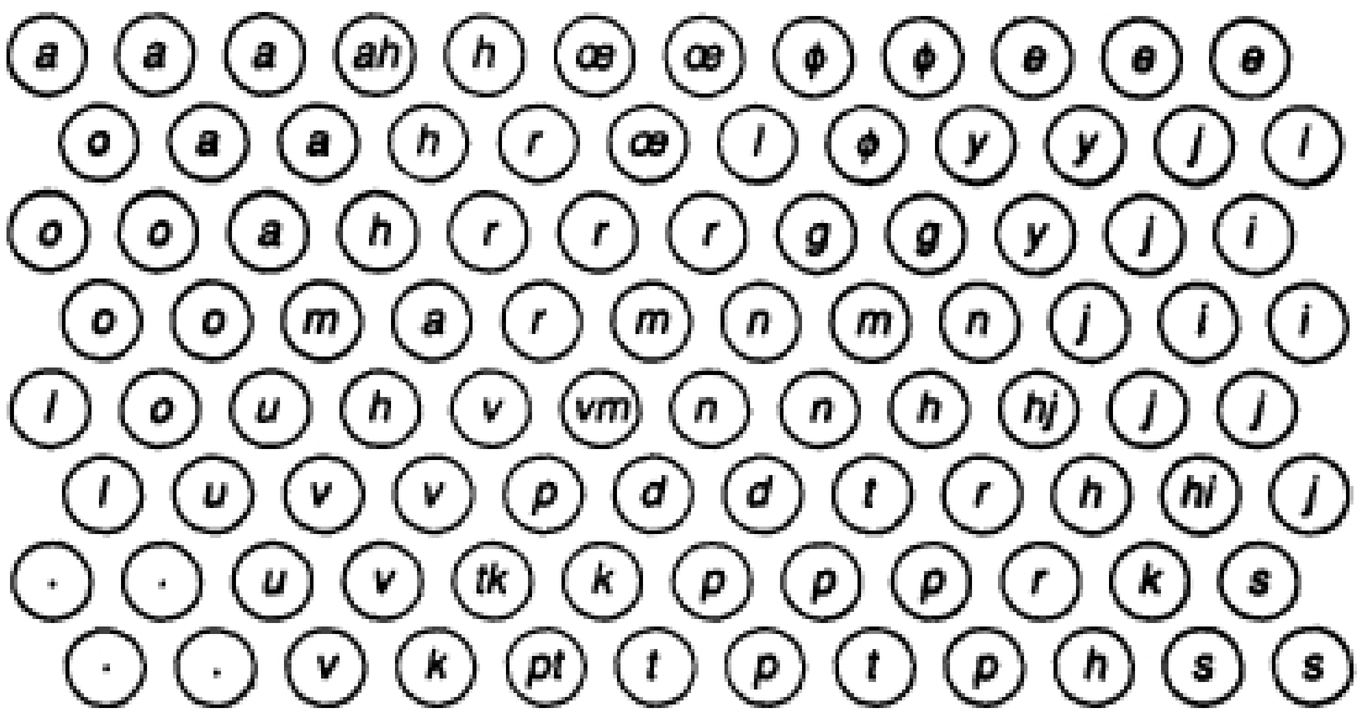
SOM

- SOM = Self Organizing Maps.
- Prof. Teuvo Kohonen, Finsko,

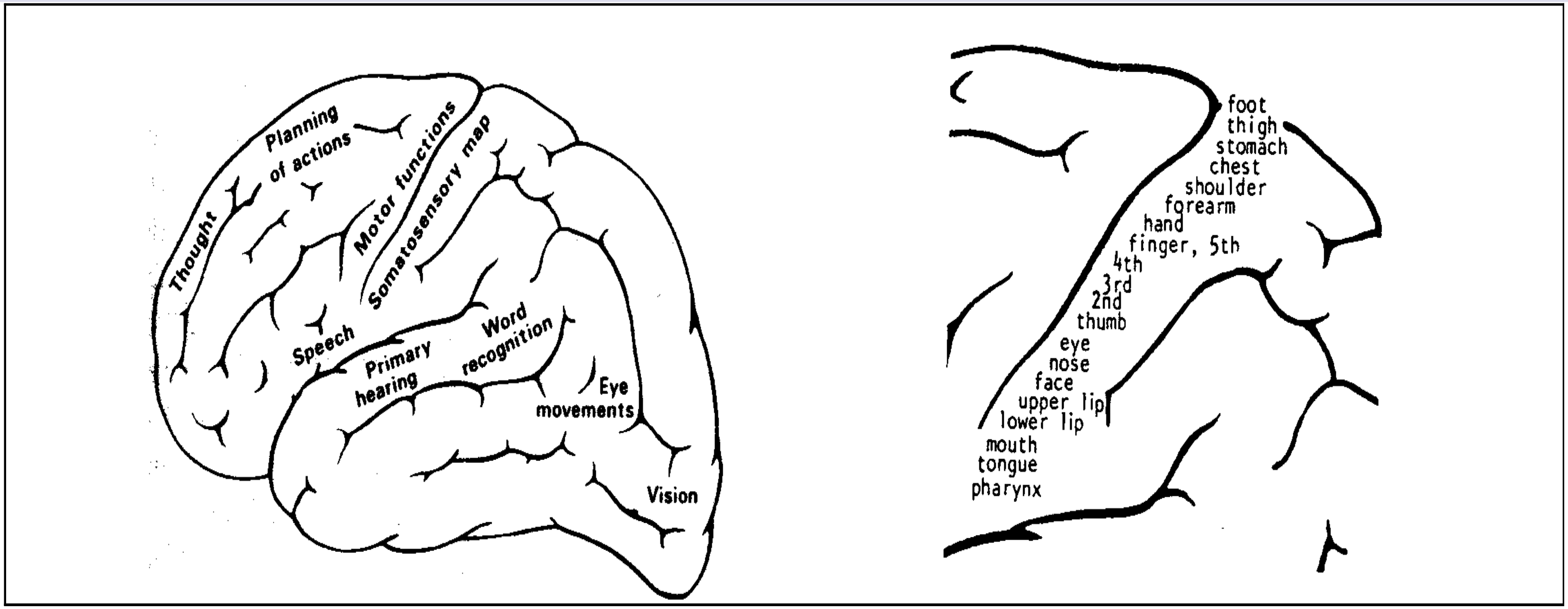
  TU Helsinki, 1981, several thousands scientific publications since...

SOM – Kohonen's Application

- Original application: phonetic “typewriter”:
  - Finish language.

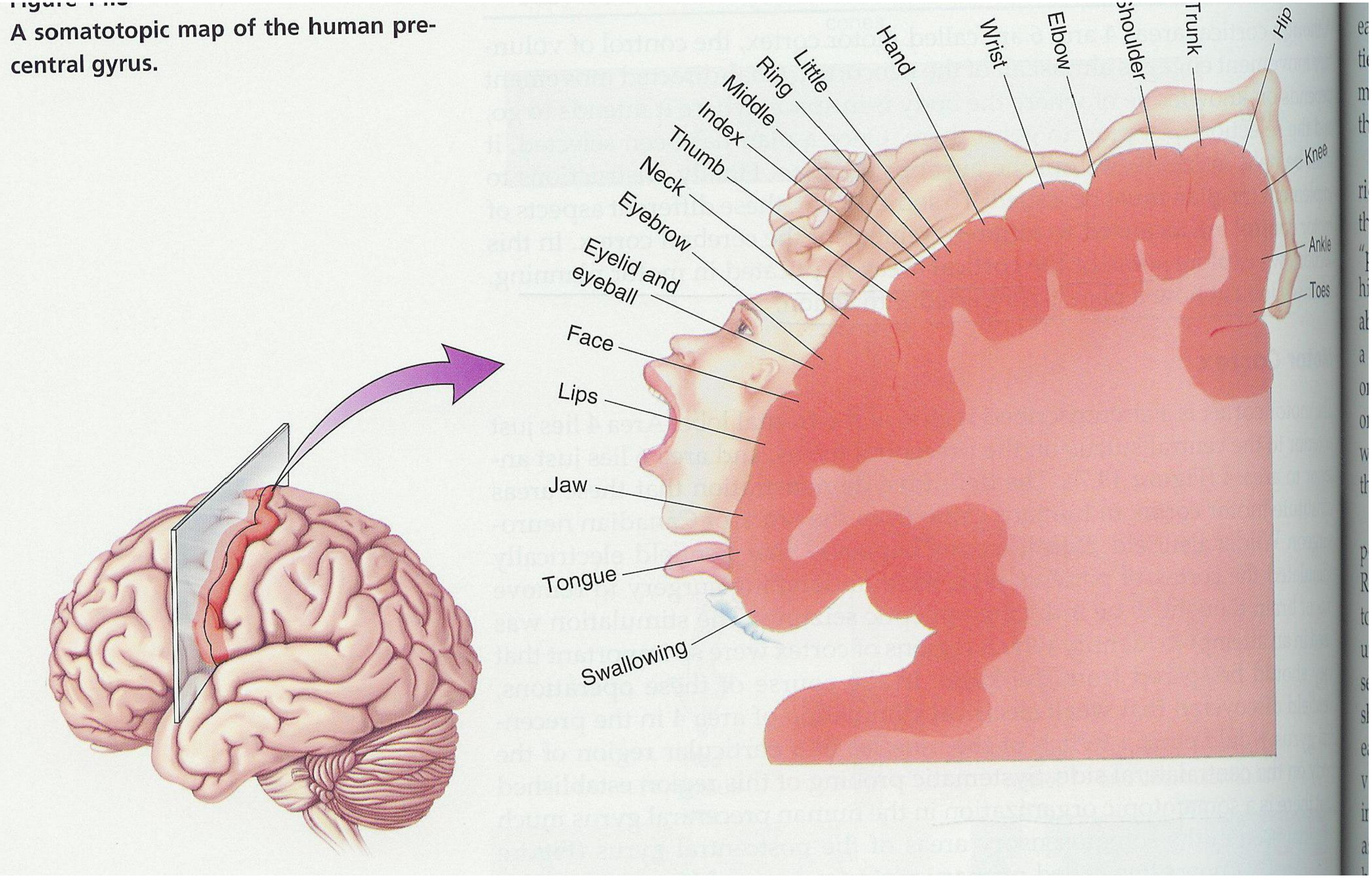


SOM Inspiration



- Brain represents the world in a **topological way**.
- Exterior spatial relations are mapped to similar spatial relations in the brain:
  - i.e. signals from hand and arm are processed nearby.

SOM Inspiration II



Bear, Connors & Paradiso (2001). *Neuroscience: Exploring The Brain*. Pg. 474.

SOM Overview

- Single layer, feed-forward.
- Unsupervised, **self-organization**.
- No output, instead **Winner-takes-all**.
- Used for **cluster analysis**.
- Performs **vector quantization**.
- Not a classifier!
  - But can be simply transformed into one by adding another layer.

What is Self-Organization?

- Self-organization of a system is a process which leads to a rise of a quality of its inner configuration while not using any information from outside.
- Self-organization clears up relationships between parts of a system.

What is Cluster Analysis

- Assignment of a set of observations into subsets (clusters).
- A measure of similarity is defined:
  - observations in the same cluster are similar,
  - observations between two clusters are dissimilar.
- Classic cluster analysis works with $\boldsymbol{R}^n$ input space observations.

See: http://en.wikipedia.org/wiki/Cluster_analysis

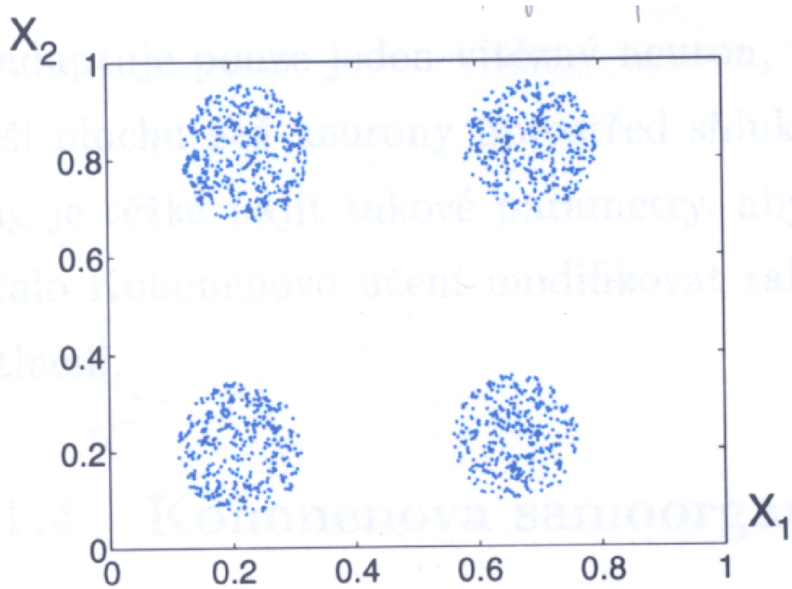
What is Vector Quantization

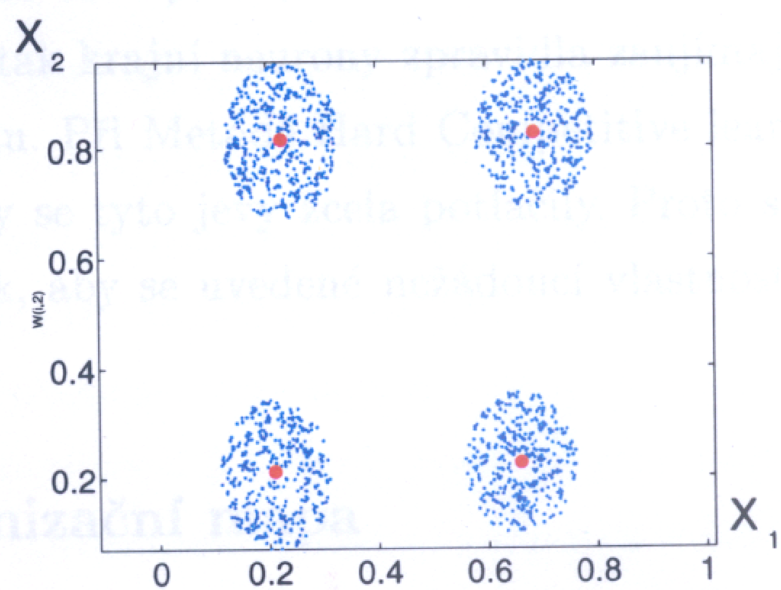
The goal of Vector Quantization is to approximate the probability density $p(x)$ of real input vectors $\boldsymbol{x} \in \boldsymbol{R}^n$ distribution using finite number of representatives $\boldsymbol{w}_i \in \boldsymbol{R}^n$.

The representative vectors tend to drift there where the data is dense, while there tends to be only a few of them where data is sparsely located. In this manner, the net tends to approximate the probability density of the input data. *Hollmen '96*

Vector Quantization Example

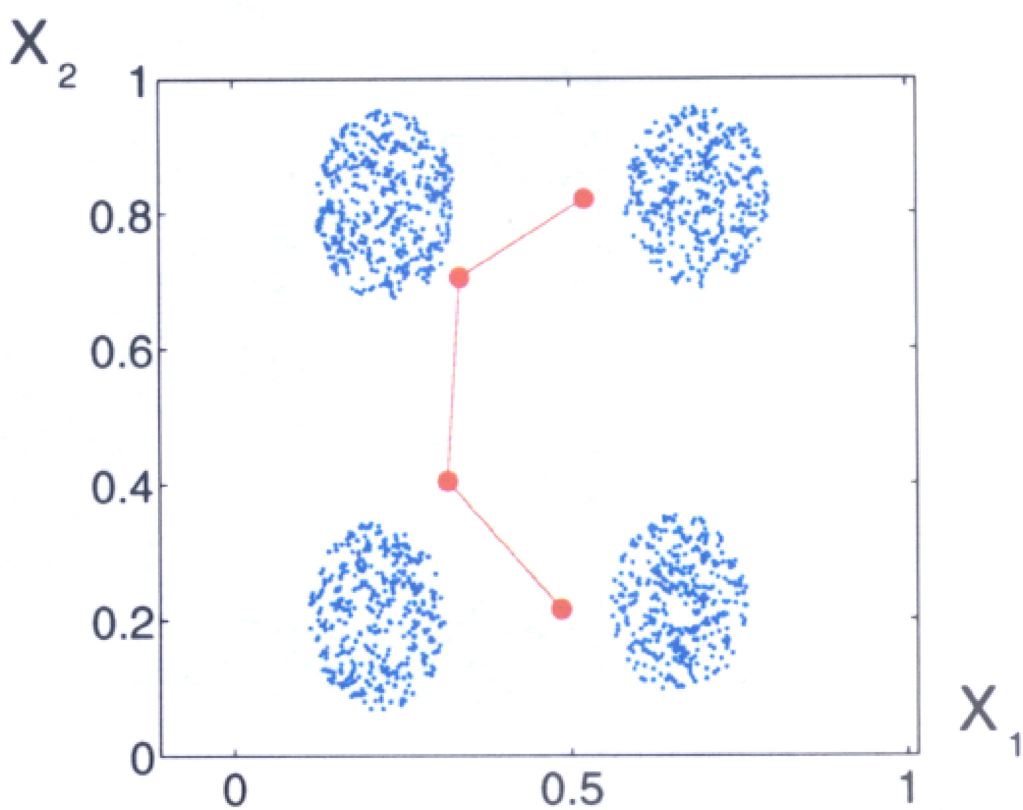
Blue points are the input vectors.





Red points are the representatives.

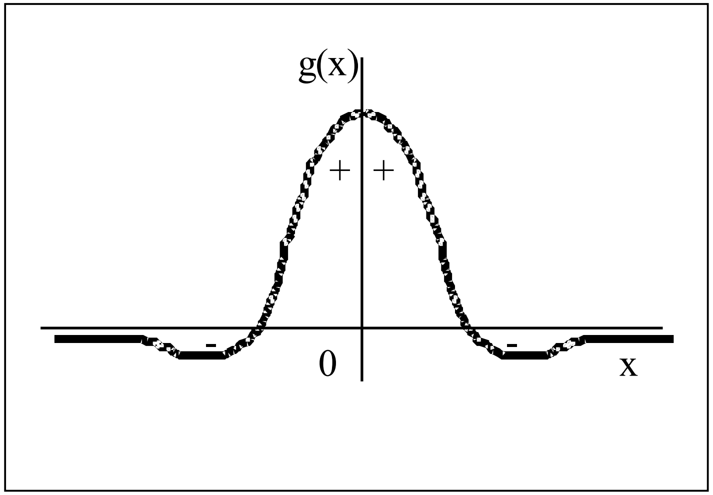
VQ by SOM



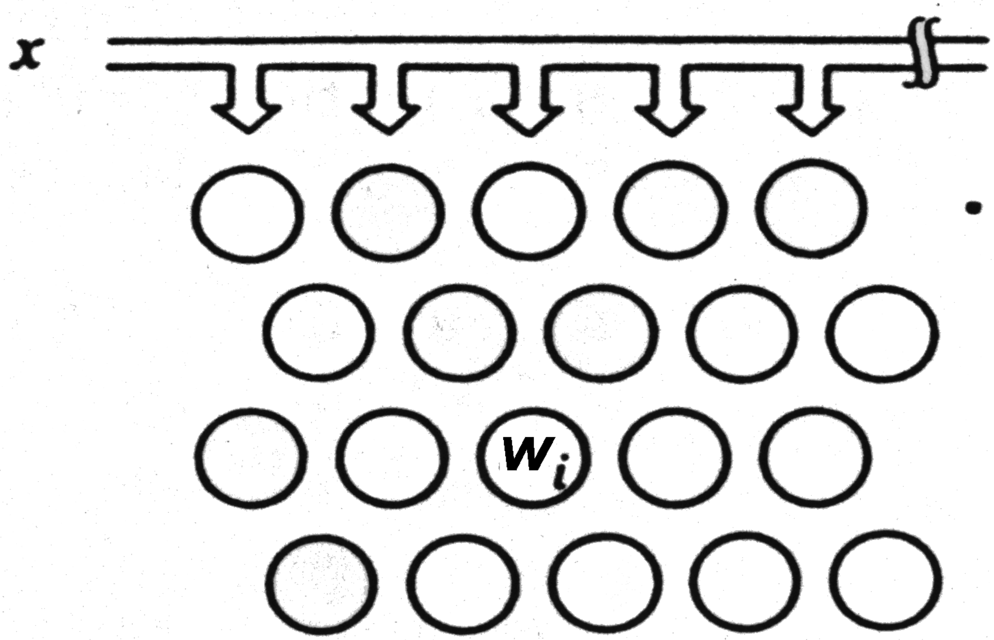
1D SOM of 4 neurons

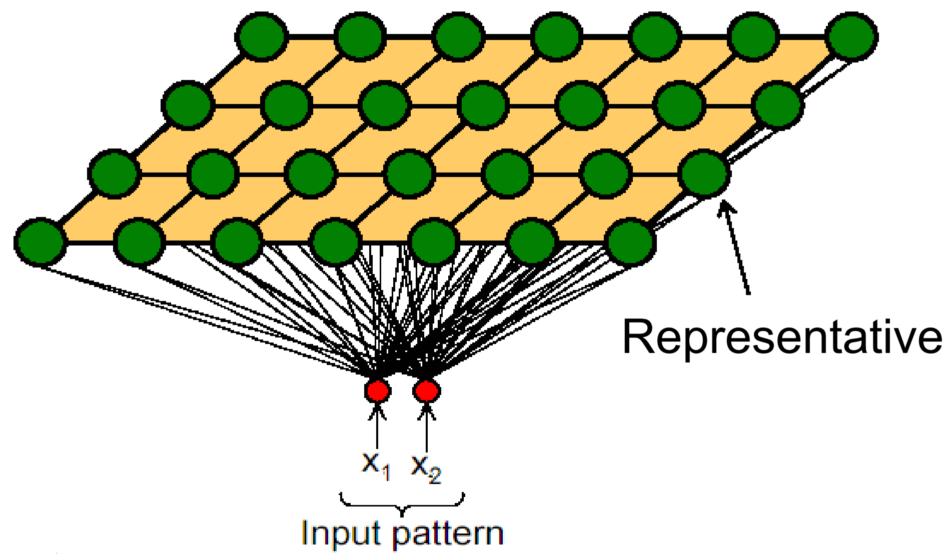
Why the Different Result?

- SOM works with neighbourhood.
- Representatives influence each other.
- They form “elastic”:
  - chain for 1D SOM,
  - mesh for higher dimensions.



SOM Architecture 1/3





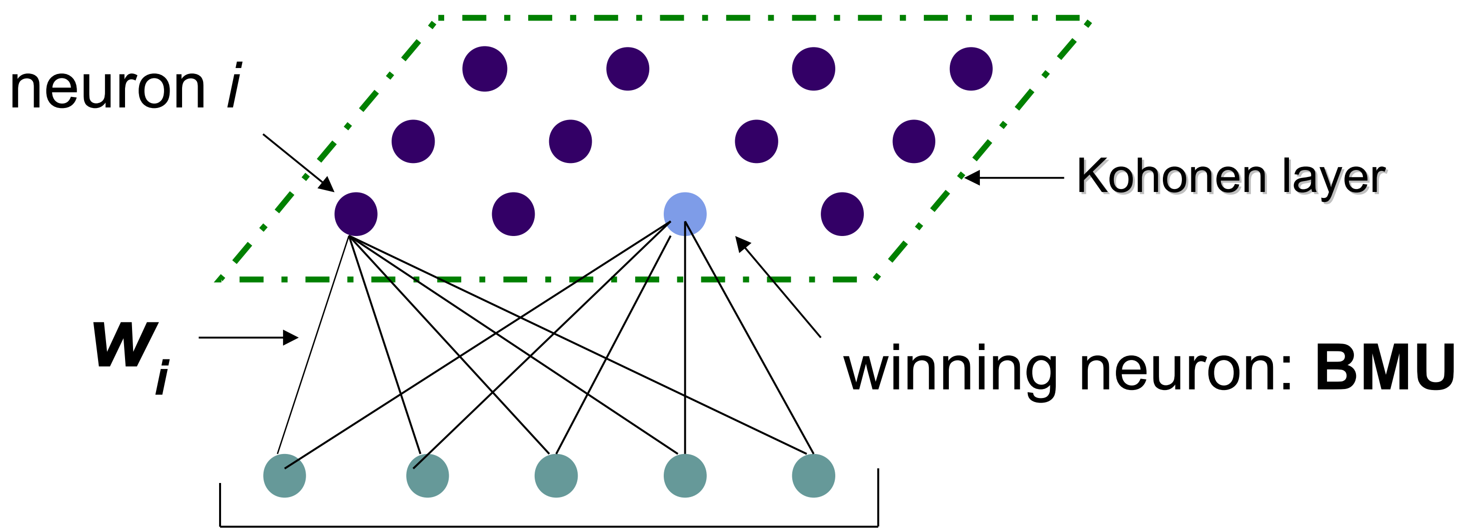
Typically: 2D mesh of representatives (neurons)

SOM Architecture 2/3

- Arrangements:
  - 1D linear quite often,
  - 2D mesh most frequently,
  - 3D (and higher dimensions) exceptionally – problematic visualization.
- The arrangement defines **neighbourhood** of a neuron.
- Kohonen suggests: rectangular SOM!

SOM Architecture 3/3

- Input vector ***x*** has a dimension *N*.
- Each neuron has a weight vector ***w*** of the same dimension *N*.
- Weight vectors of all neurons are compared to ***x***.
- The most similar is chosen → BMU (Best Matching Unit).
- BMU becomes a representative of vector ***x***.



SOM Neuron 1/2

Evaluates the similarity of input vector ***x*** and weight vector $\boldsymbol{w}_i$.

Similarity: i.e. Euclidean

The most similar neuron to a input vector is chosen (BMU):

$$j^* = \underset{i}{\operatorname{argmin}} \left\{ \| x - w_i \| \right\},$$

SOM neuron is a representative of a cluster.

SOM Neuron 2/2

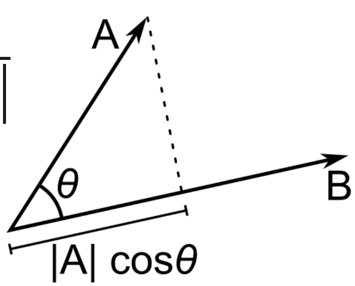
- Note, we don't have to use Euclidean distance.
- We can use directional similarity expressed by the dot product:

$$j^* = \arg\max_i \left\{ x^T(t)\, w_i(t) \right\}.$$

Why max here?

Note:

$$\cos\theta = \frac{A.B}{|A||B|}$$



http://en.wikipedia.org/wiki/Dot_product

Learning SOM

- Initialization (random weights).
- Apply input pattern $\boldsymbol{x} = (x_1, x_2, \ldots x_N)$.
- Compute distances.
- Select BMU – neuron j.
- Adjust weights for all neurons i:

$$w_i(t+1) = w_i(t) + \eta_{ij}(t)\left[x(t) - w_i(t)\right]$$

Neighbourhood function

- Continue with next pattern.

Example

$$\boldsymbol{X} = \begin{bmatrix} 0.52 \\ 0.12 \end{bmatrix}$$

$$\boldsymbol{W}_1 = \begin{bmatrix} 0.27 \\ 0.81 \end{bmatrix} \qquad \boldsymbol{W}_2 = \begin{bmatrix} 0.42 \\ 0.70 \end{bmatrix} \qquad \boldsymbol{W}_3 = \begin{bmatrix} 0.43 \\ 0.21 \end{bmatrix}$$

$$d_1 = \sqrt{(x_1 - w_{11})^2 + (x_2 - w_{21})^2} = \sqrt{(0.52 - 0.27)^2 + (0.12 - 0.81)^2} = 0.73$$

$$d_2 = \sqrt{(x_1 - w_{12})^2 + (x_2 - w_{22})^2} = \sqrt{(0.52 - 0.42)^2 + (0.12 - 0.70)^2} = 0.59$$

$$d_3 = \sqrt{(x_1 - w_{13})^2 + (x_2 - w_{23})^2} = \sqrt{(0.52 - 0.43)^2 + (0.12 - 0.21)^2} = 0.13$$

The third vector is the winner (BMU).

Example contd.

Let's move the neuron closer to the input pattern: $w_{ij}(t+1) = w_{ij}(t) + \eta(t)\left[x_i(t) - w_{ij}(t)\right]$

$$\Delta w_{13} = \eta(t)(x_1 - w_{13}) = 0.1(0.52 - 0.43) = 0.01$$

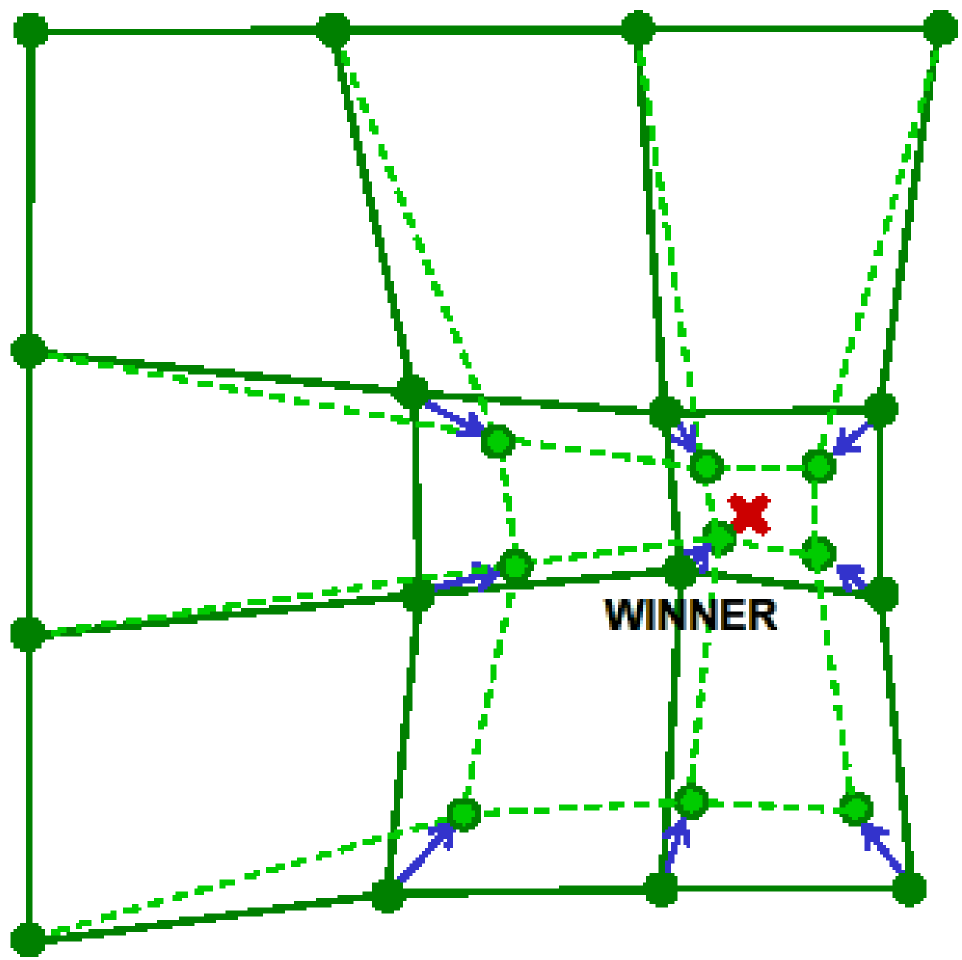
$$\Delta w_{23} = \eta(t)(x_2 - w_{23}) = 0.1(0.12 - 0.21) = -0.01$$

$$W_3(t+1) = W_3(t) + \Delta W_3(t) = \begin{bmatrix} 0.43 \\ 0.21 \end{bmatrix} + \begin{bmatrix} 0.01 \\ -0.01 \end{bmatrix} = \begin{bmatrix} 0.44 \\ 0.2 \end{bmatrix}$$

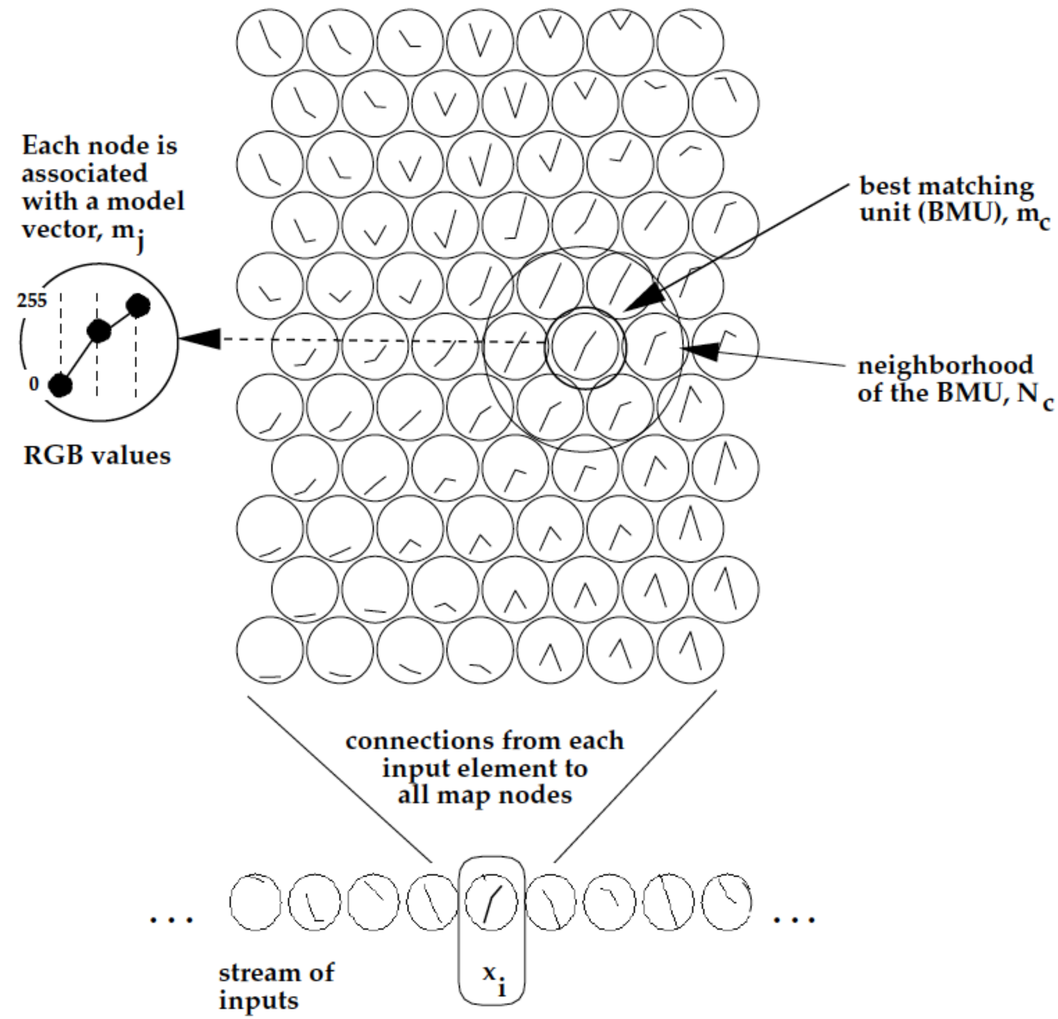
We adjusted only BMU weights.

Here, the winner takes all.

What About Updating Also Neurons in the Neighbourhood?

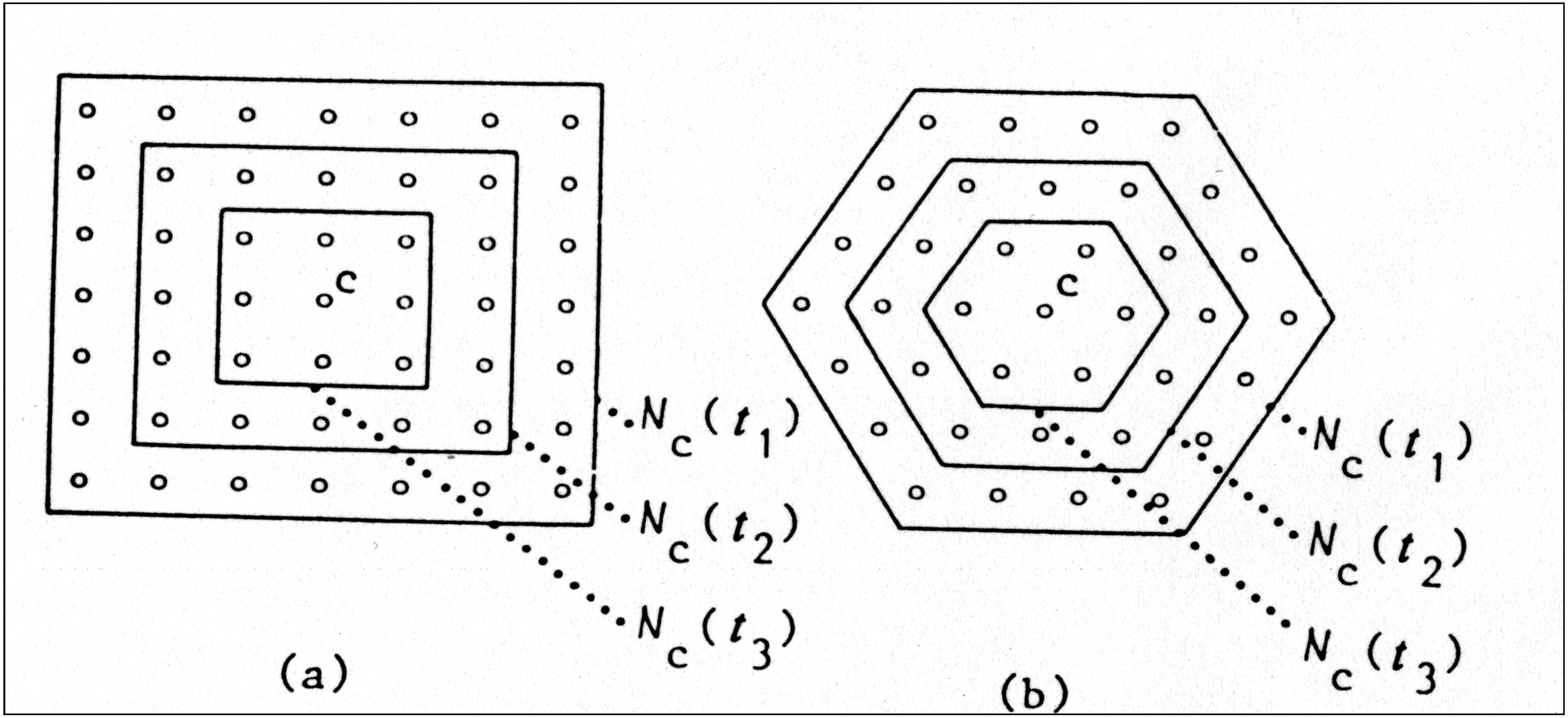


Neighbourhood for SOM



Timo Honkela (Description of Kohonen's Self-Organizing Map)

Common Neighbourhoods



square hexagonal

T. Kohonen: Self Organizing Maps

Learning SOM II

- The neighbourhood plays important role when learning SOM:
  - topological arrangement,
  - neighbour distances.
- Neighbourhood changes in time:
  - its "diameter" decreases (to zero).
- The change is realised by neighbourhood function $\eta(t)$.

Gaussian Neighbourhood

- Neighbourhood function for neuron *i*.

$$\eta_{ij^*}(t) = \alpha(t) . \exp\left(-\frac{\|r_{j^*} - r_i\|^2}{2\sigma^2(t)}\right)$$

- Where j^* is the BMU,
  r the position of neuron in map,
  and function $\alpha(t)$: learning rate.
- The exp expression represents neighbourhood shape.

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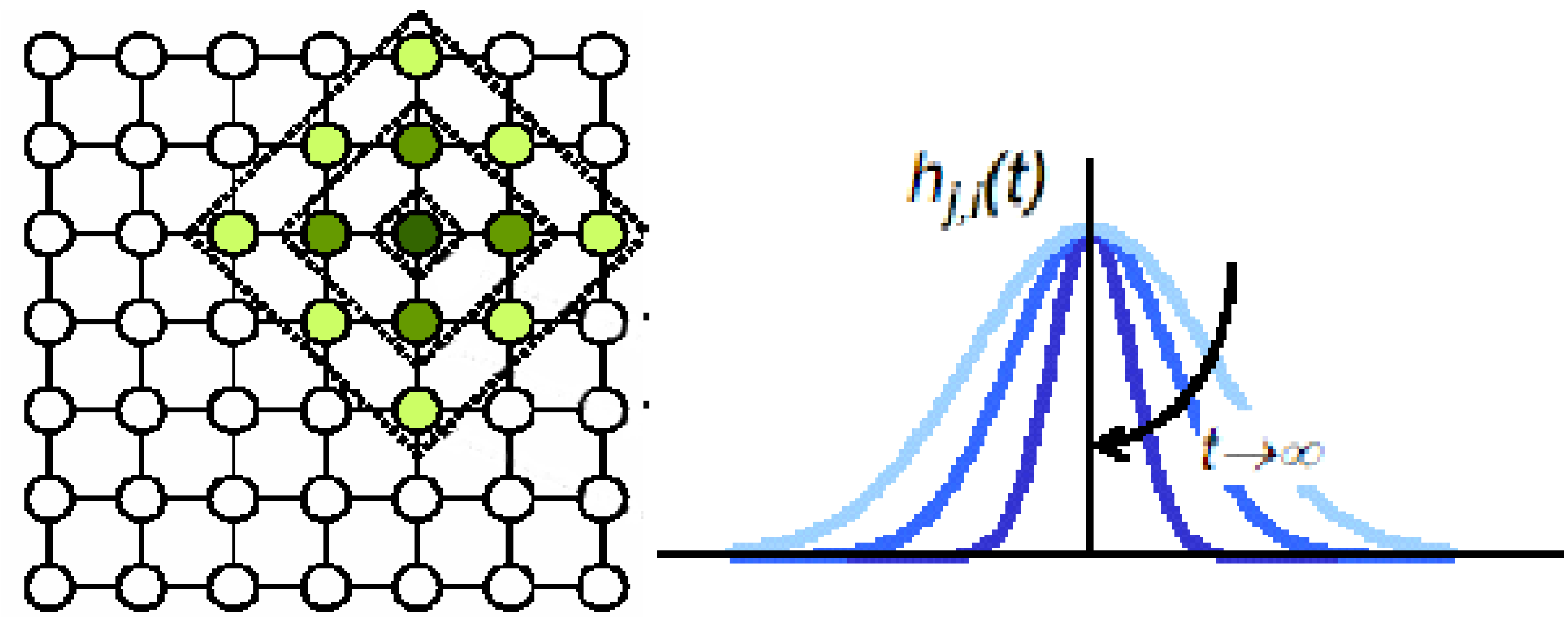
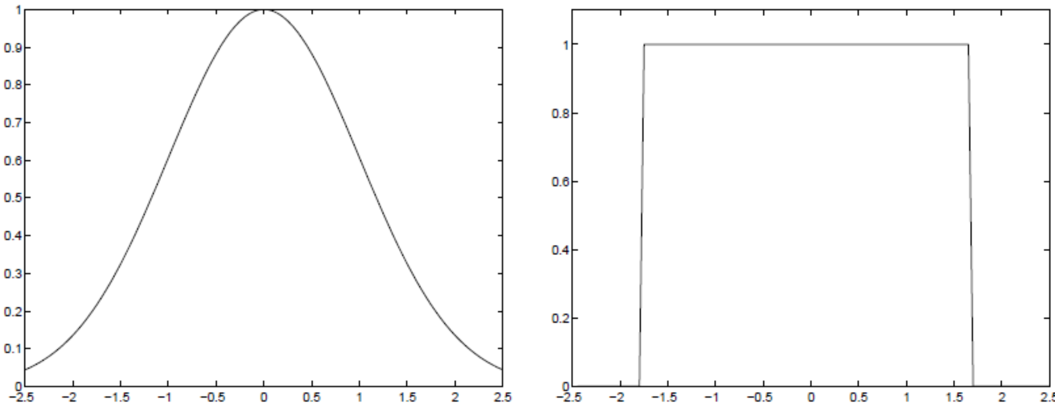
Gaussian Neighbourhood



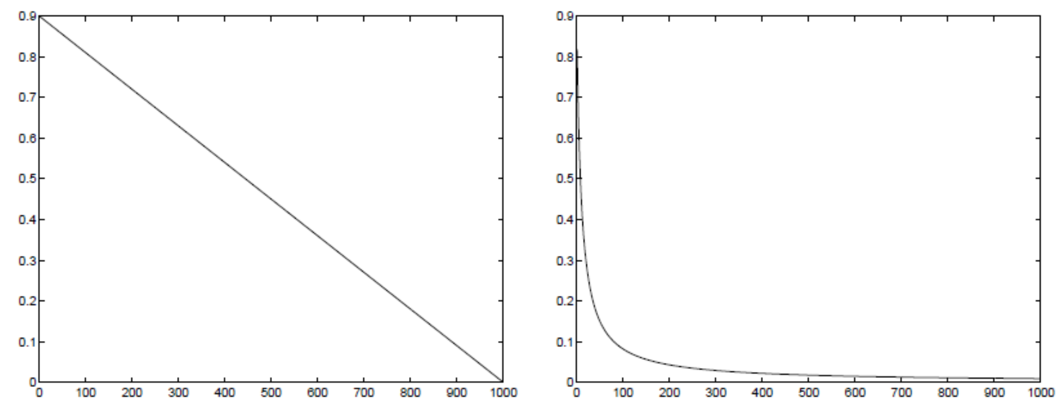
Distance related learning

Neighbourhood Related Functions



(a) (b)

Figure 2.6: Neighborhood function values



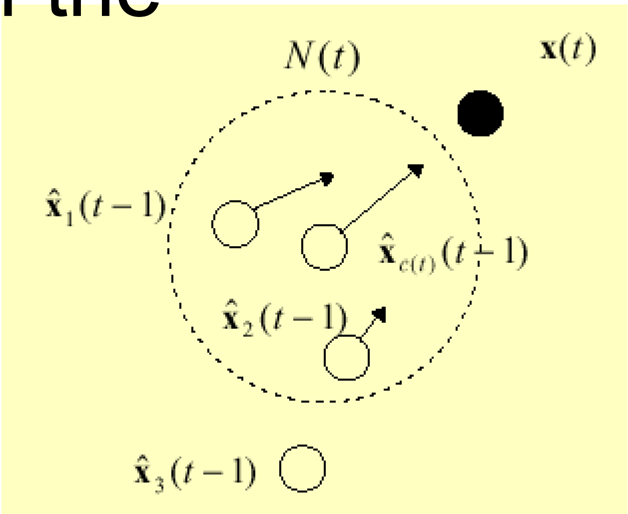
(a) (b)

Figure 2.7: Learning rates as functions of time

Hollmen '96, MSc.

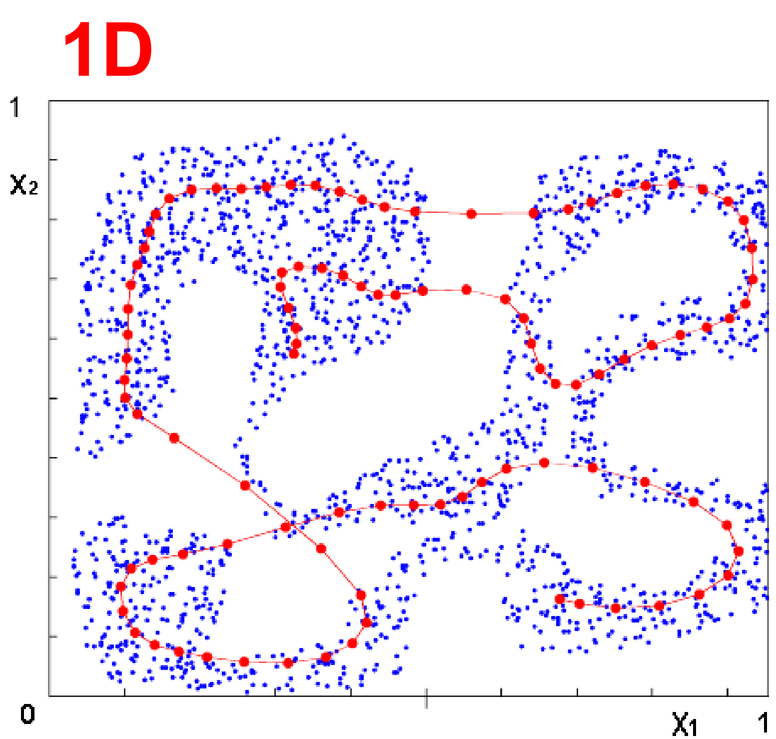
Learning Process

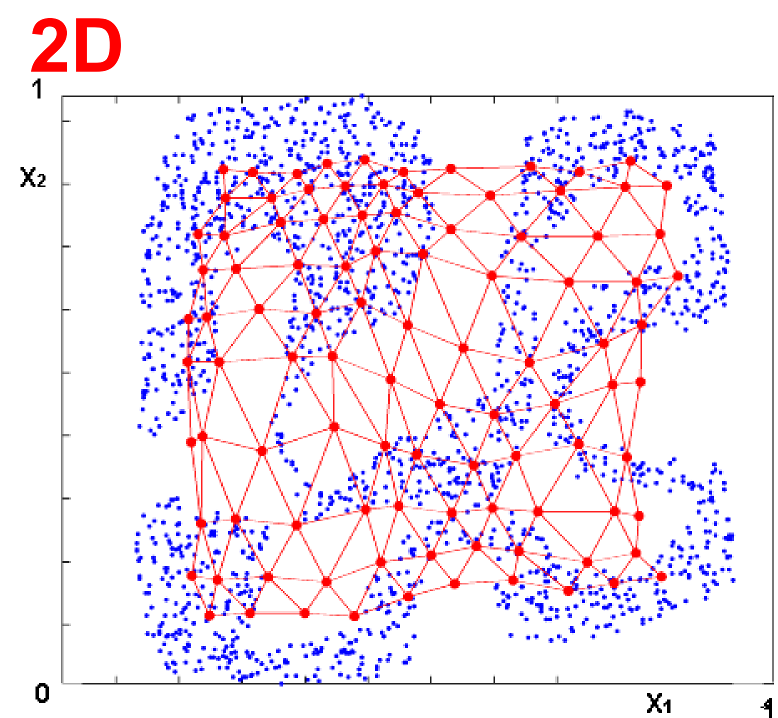
- During the learning the BMU (and its neighbours) is adapted to get closer to the input pattern which have caused its activation.
- Neurons are moving towards the input pattern.
- What influences the magnitude of the approach?



SOM Applications

- To visualize data.
- To cover the input space by representatives.





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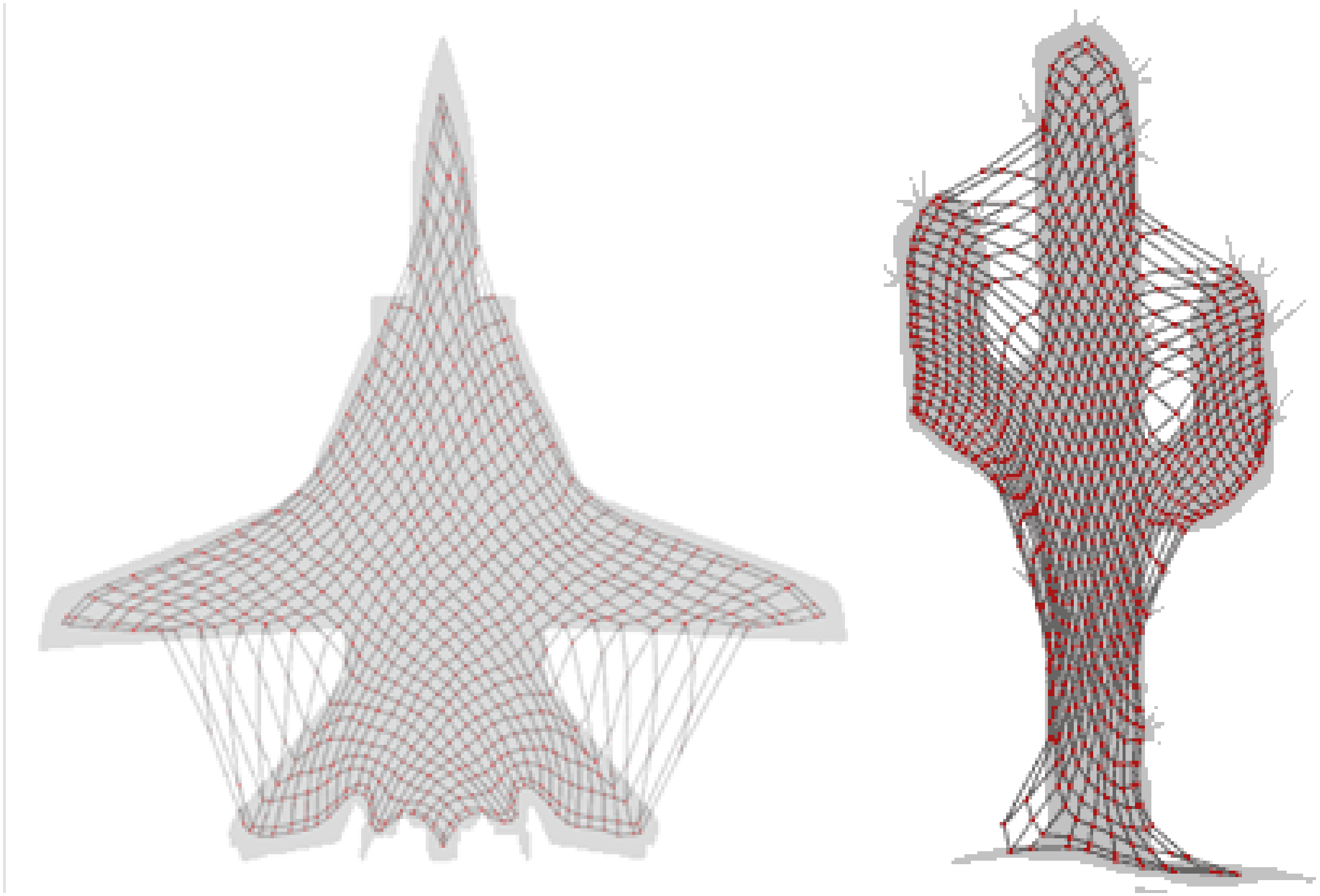
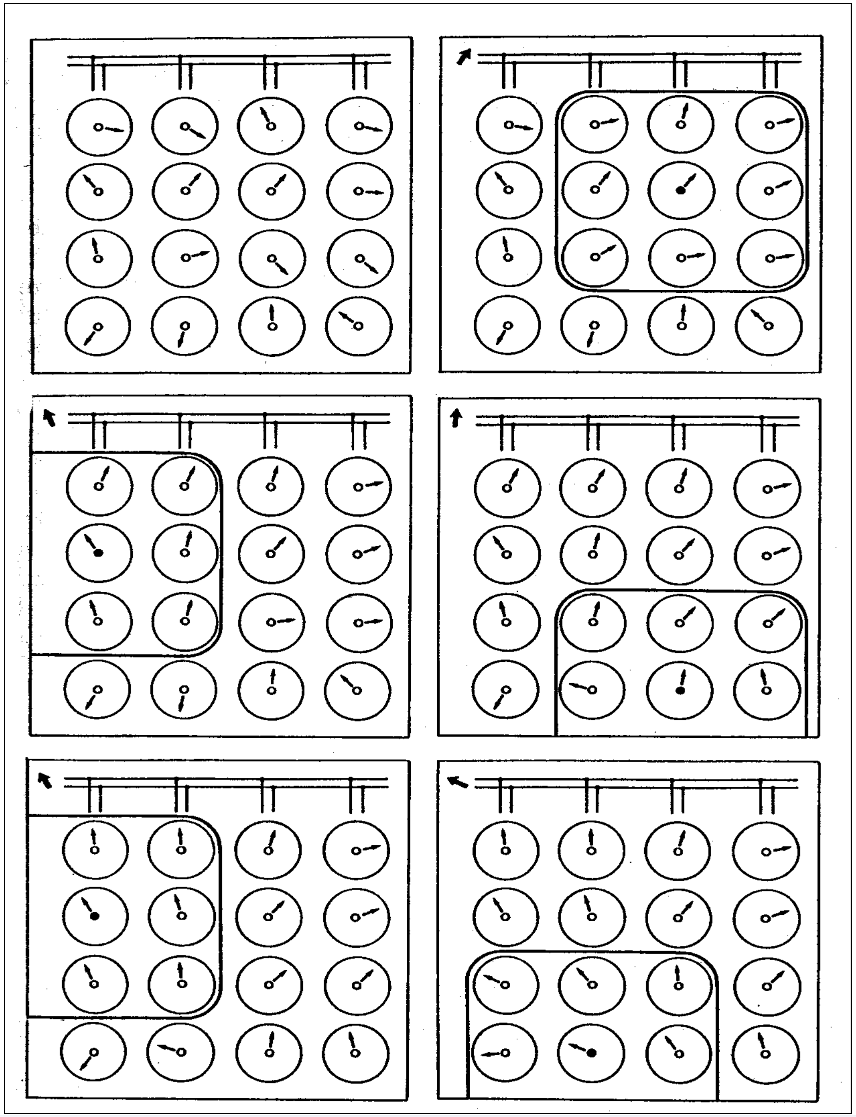
Or …



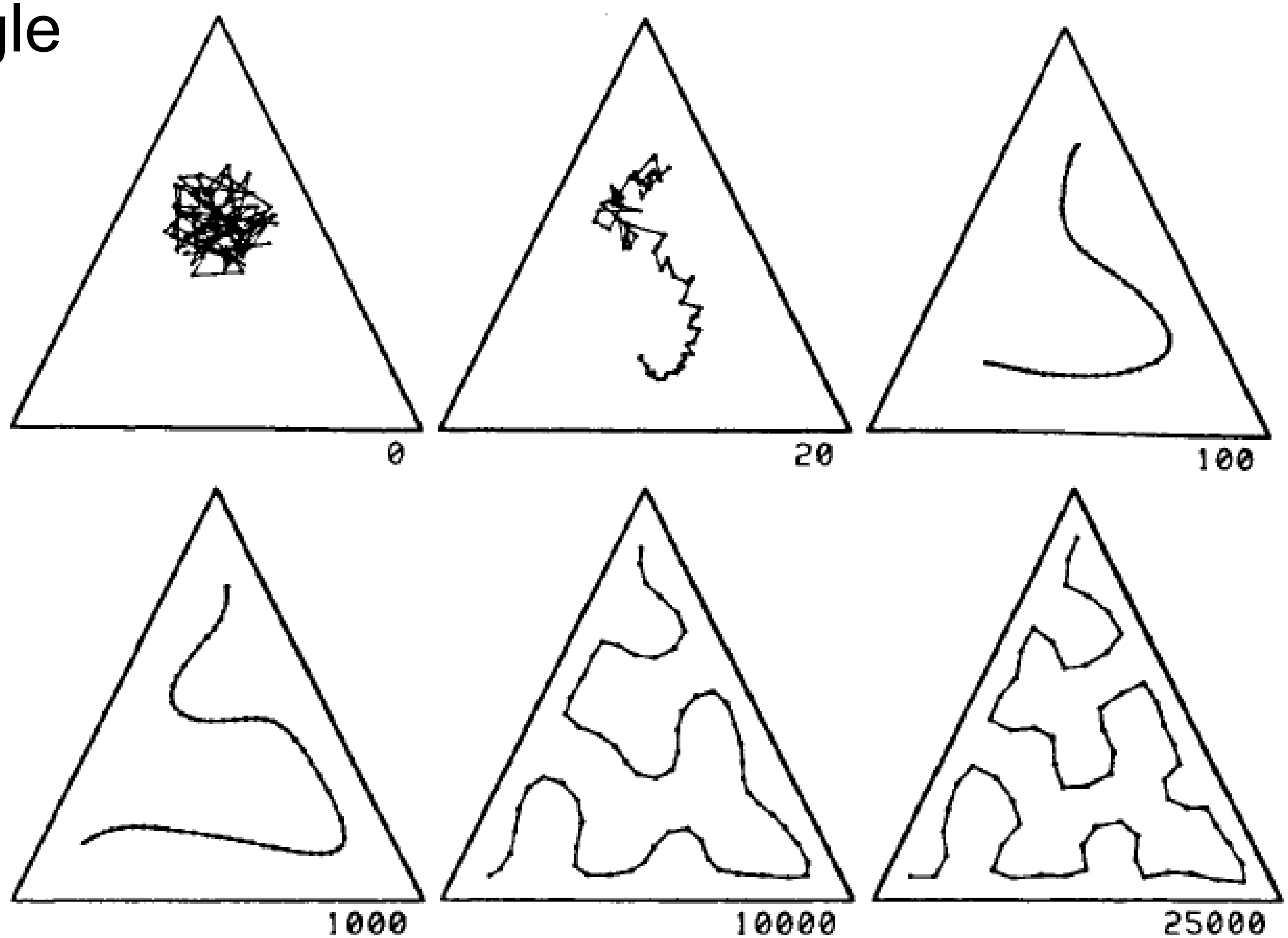
Slide by Johan Everts

Example: Learning Dot-Product SOM



More Examples

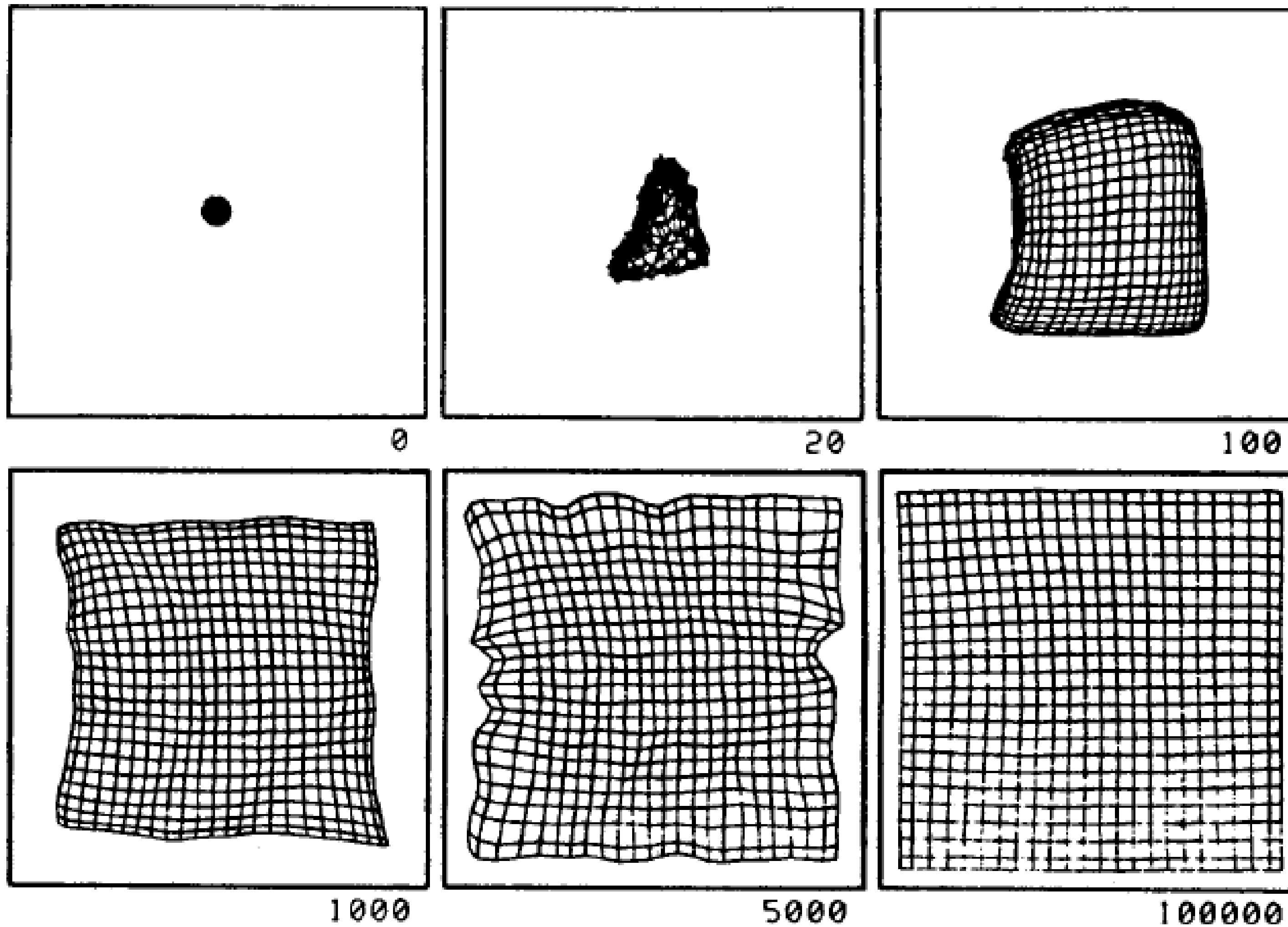
Covering a triangle by 1D SOM.



T. Kohonen: Self Organizing Maps

More Examples contd.

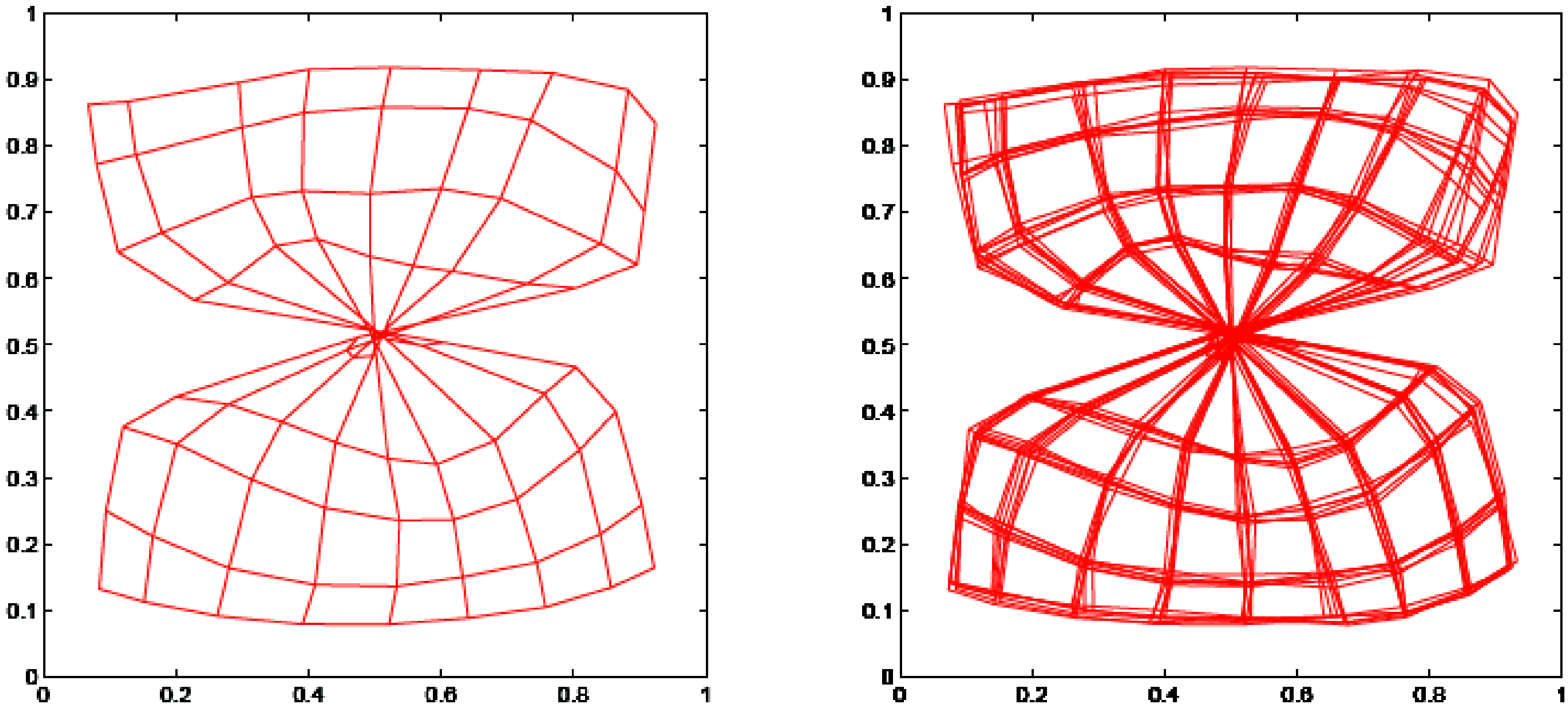
Covering a square by 2D SOM.



T. Kohonen: Self Organizing Maps

Possible Problem: Knots

- This problem is not likely to be corrected by further learning if the *plasticity* is low:



Rojas: Neural Networks - A Systematic Introduction

What is the Cause?

- There are many:
  - Random initialization of weights → we are unable the change bad initial orientation of vectors.
  - Choice of a neighbourhood function.
  - Scheduling of neighbourhood modification in time.
  - Input data of course...

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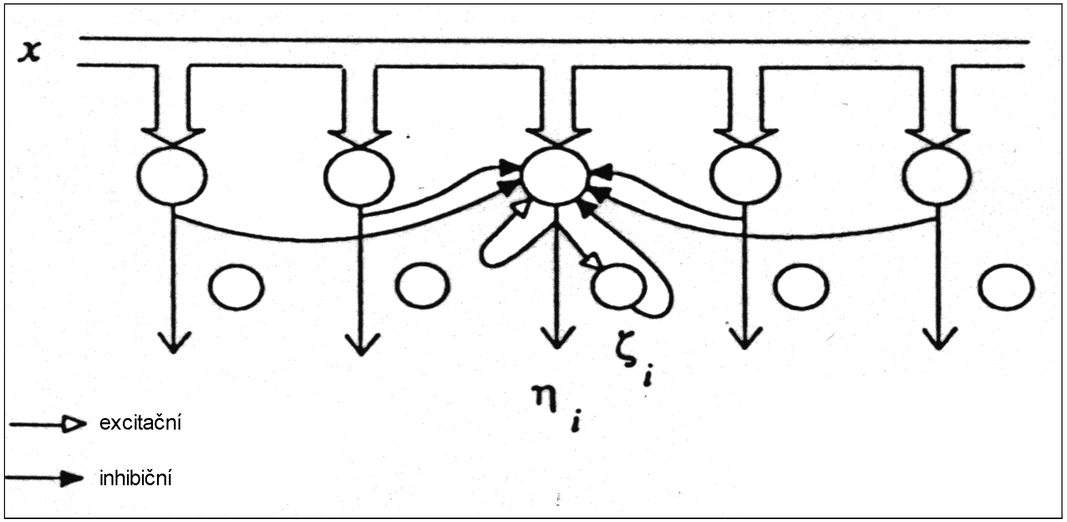
What Can Help?

- Same weights for all neurons initially → each neuron has a same chance to represent a pattern.
- Add random noise to input patterns at start.
- Lateral inhibition...

Lateral Inhibition

- When choosing the BMU we do not pick isolated winner.
- The choice does not depend on an activation of a single neuron but also on activity of its neighbours...



Lateral Inhibition II

$$I_j = I_j^l + I_j^f = d_j + \sum_k g_{jk} I_k$$

j-th neuron response

local response

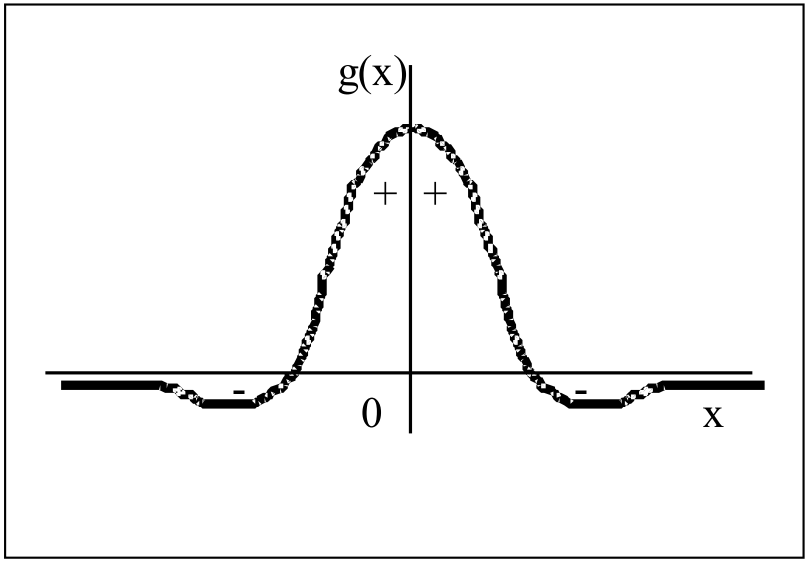
neighbourhood response

distance from input vector

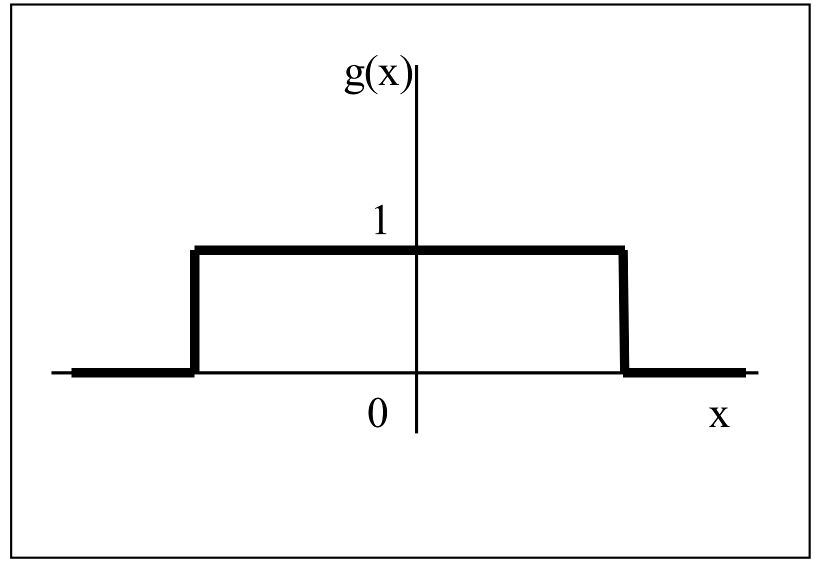
neighbours

lateral inhibition interaction

Lateral Inhibition Functions



biological



simplified

SOM Visualization

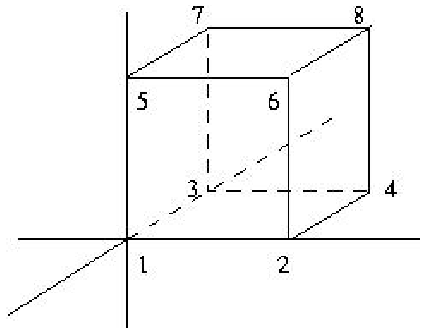
- How to visualize representatives?
- Weight dimension = input vector dimension.
- How to show in 2D?
  - U-matrix,
  - P-matrix,
  - PCA (linear projection),
  - Sammon's projection (non-linear).

U-matrix (UMAT)

- Visualizes distances between neurons:
  - Dark coloring between neurons → large distance.
  - Light → close in input space.
- Dark gaps separate clusters.
- Neuron colour reflects the distance of its weight vector to all other weight vectors, again:
  - dark → large distance,
  - light → close distance.

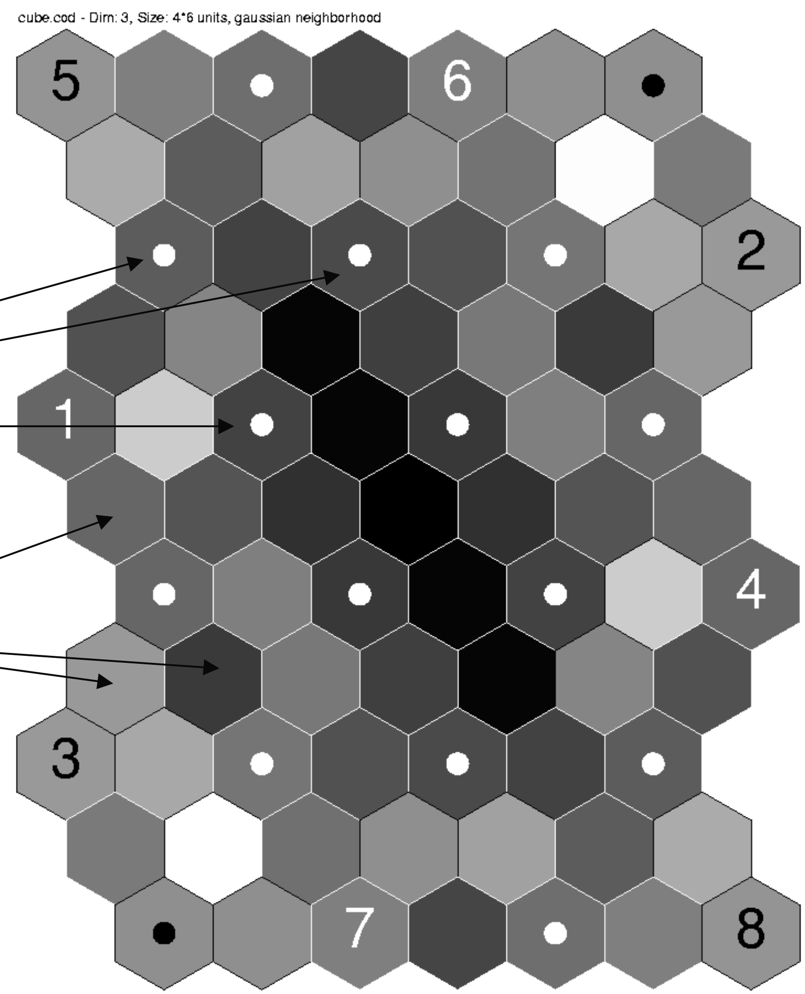
U-matrix Example

data



neurons

distance between adjacent neurons



P-matrix (Pareto Density Estimation)

- Shows the number of input space vectors which belong to a sphere centered in the neuron's weight vector.
- Visualizes data density.
- Neurons with high value belong to “dense” areas of input space.
- Neurons with low value are “lonesome”.
- Valleys separate clusters (“plateaus”).

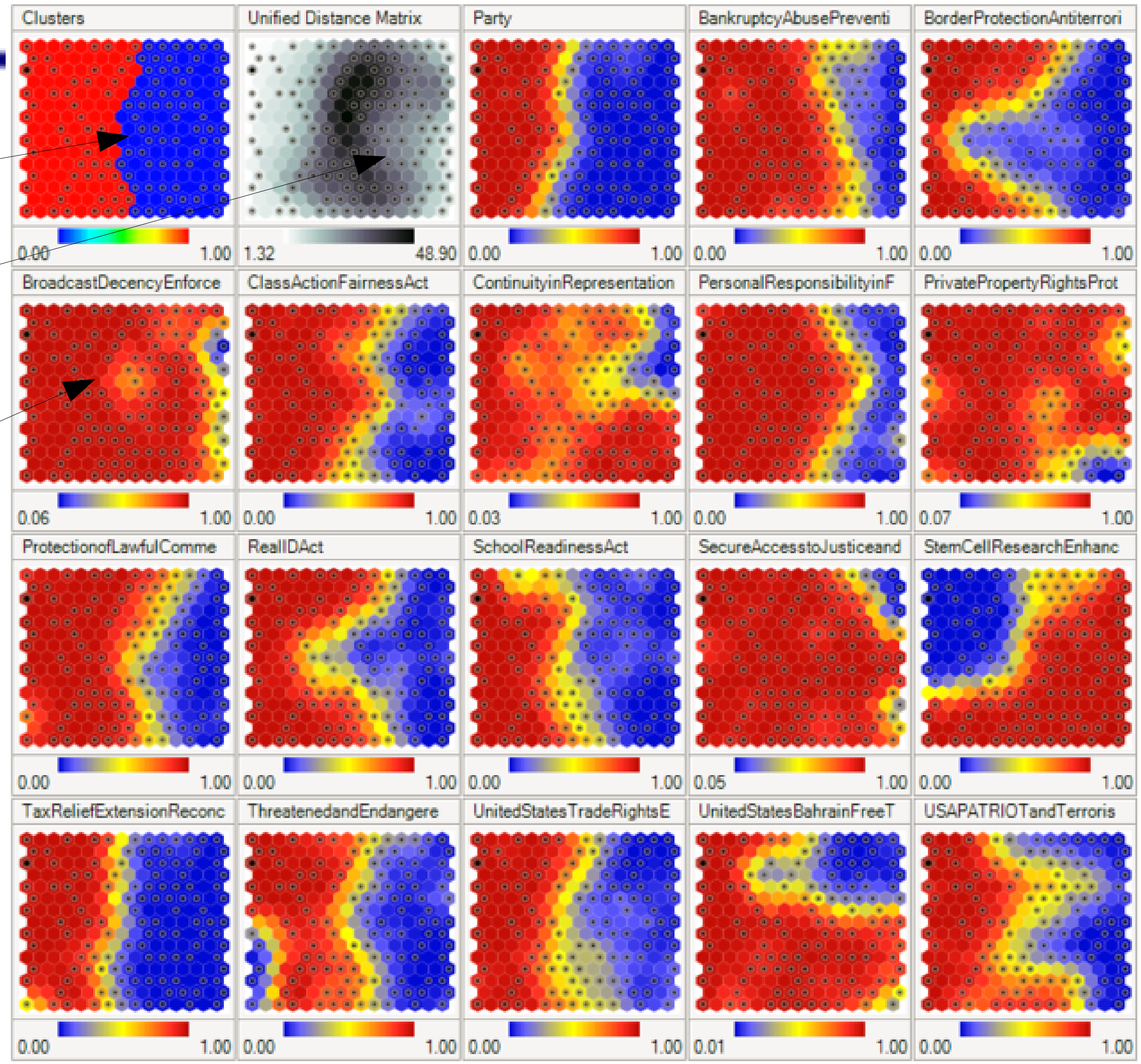
Feature Plots

clustering

UMAP

feature plot shows a value of a single component (feature) of a weight vector

can be used to check if two components correlate



http://en.wikipedia.org/wiki/Self-organizing_map

Drawbacks of UMAT, PMAT

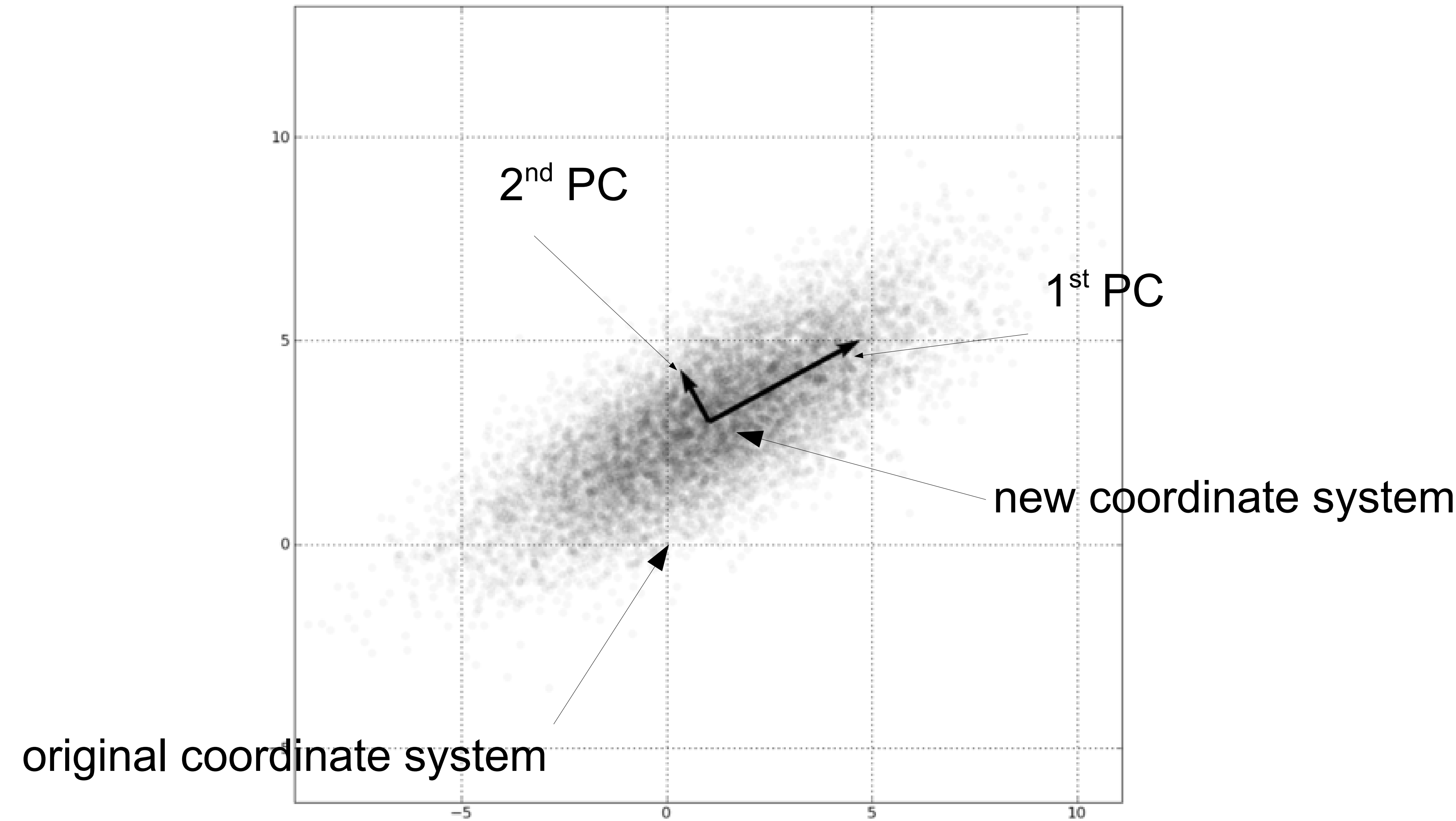
- Only distances between neighbours.
- New learning on the same data may give different results: (i.e. 90 degrees rotation)
- Not intuitive.

- **How can we show high-dimensional data in 2D(3D) keeping notion of original distances?**

PCA

- Principal Component Analysis.
- Linear transformation to a new coordinate system such that:
  - 1st coordinate (principal component) → greatest variance by any projection of the data
  - 2nd coordinate → 2nd greatest variance
  - etc.
- Dimension reduction → use only *N* first coordinates, **throw the rest away**...

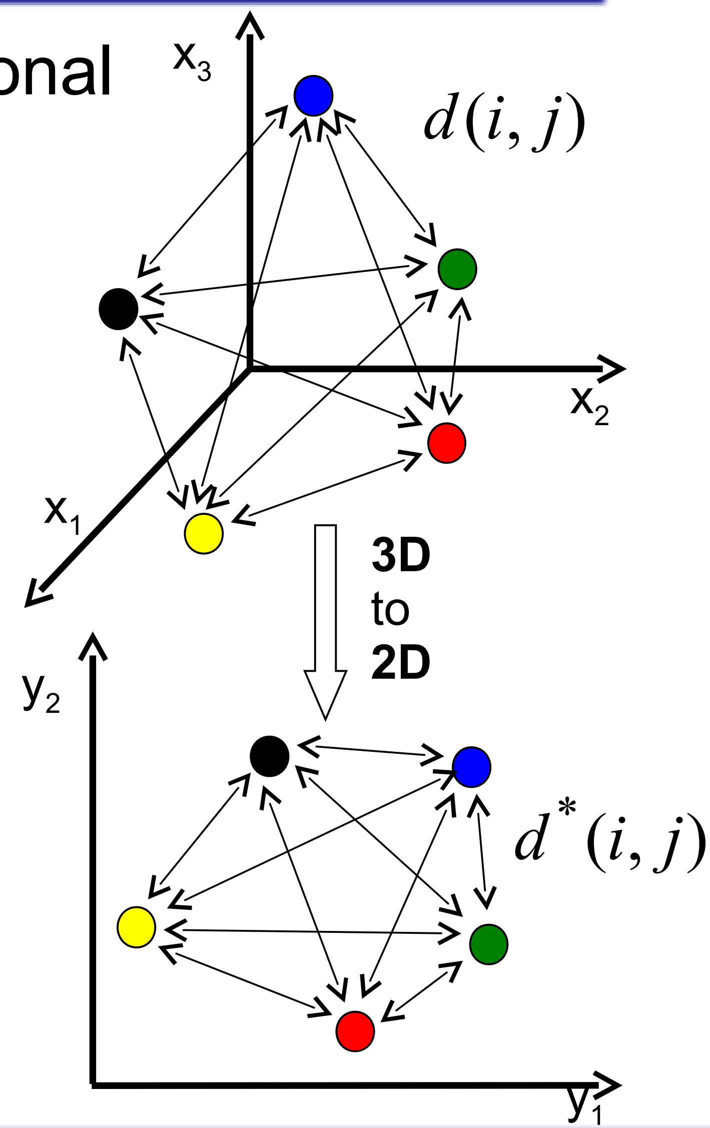
Principal Components Example



http://en.wikipedia.org/wiki/Principal_component_analysis

Sammon's Projection

- Non-linear reduction of higher-dimensional space to lower-dimensional space.
- Tries to preserve distances.



energy function → low for similar distances in both spaces.

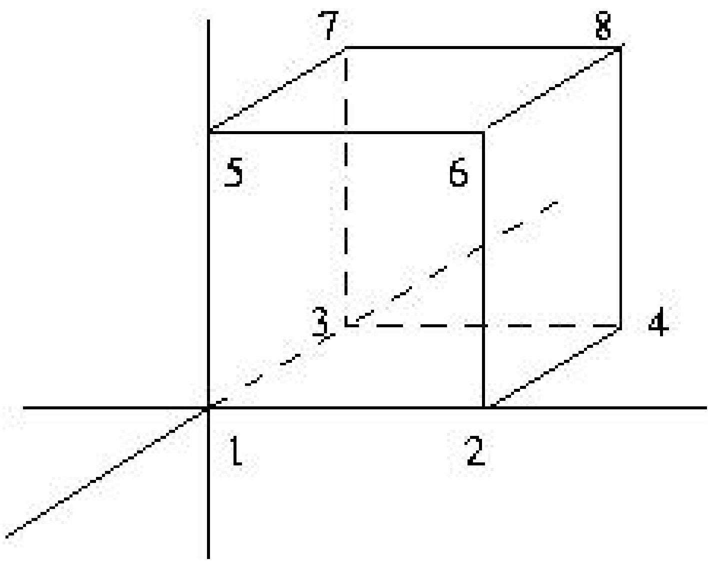
distance in high dim. space

distance in low dim. space

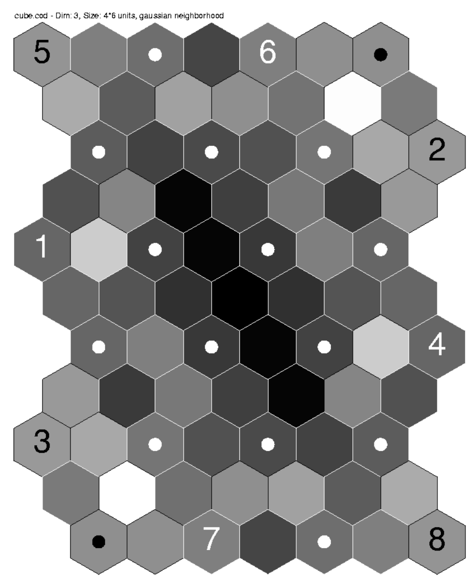
$$E=\frac{1}{\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} d(i,j)}\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{\left(d(i,j)-d^*(i,j)\right)^2}{d(i,j)}$$

- Energy function is a subject to minimization (originally using gradient descent).

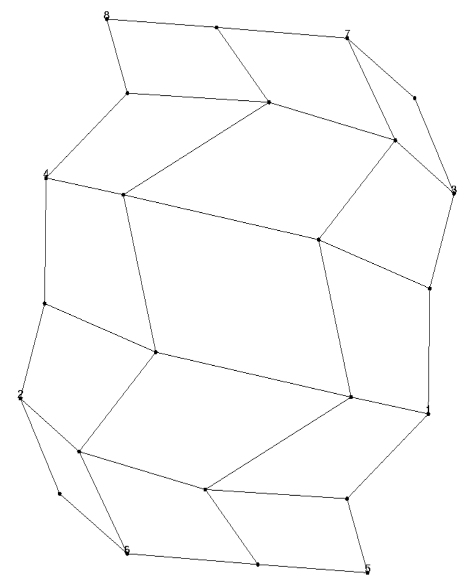
Standard SOM Visualizations



UMAT



Sammon
neuron weights projected to 2D, neighbours connected

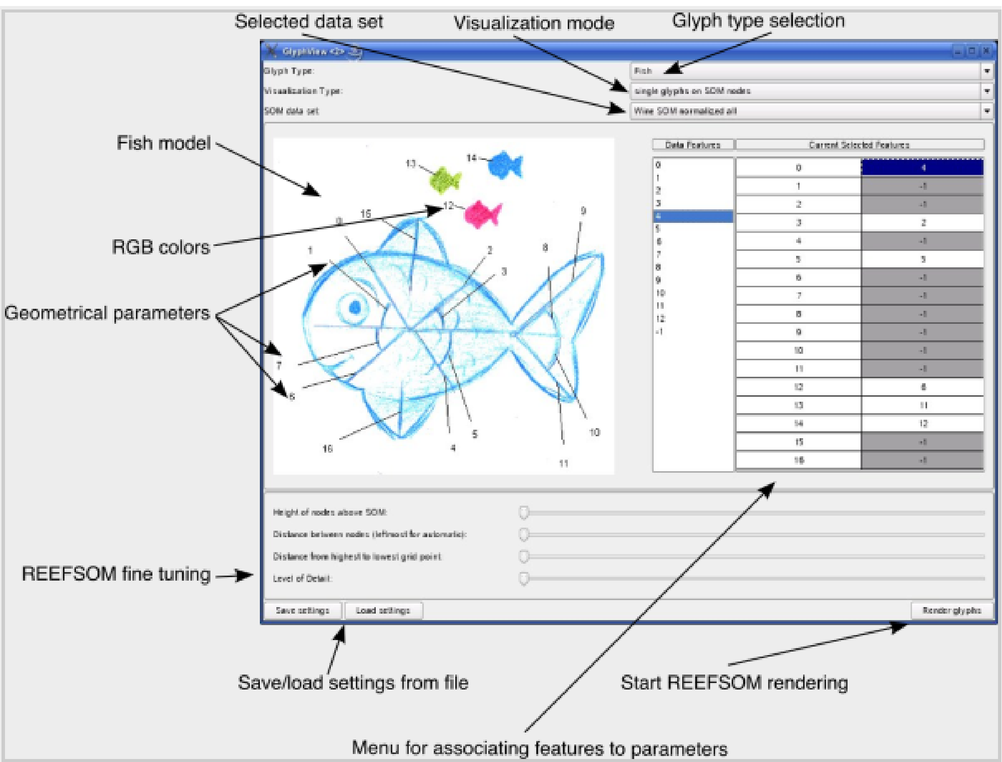


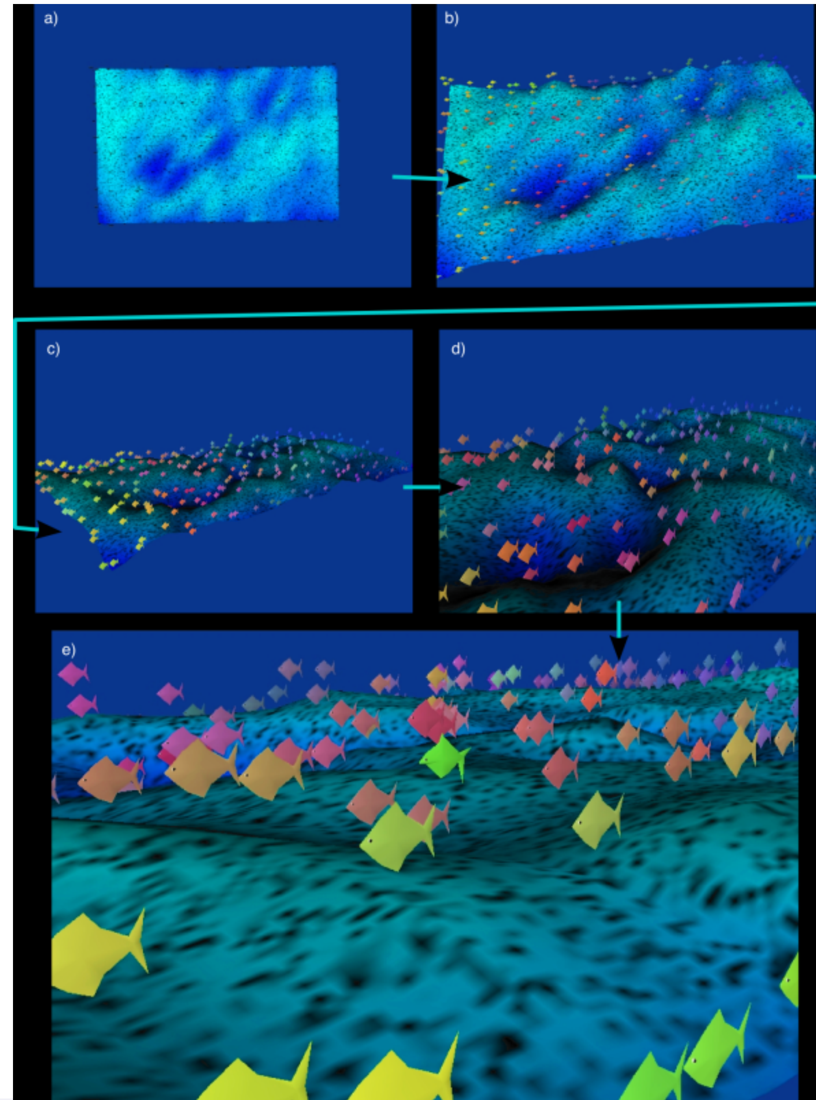
SOM Applications

- Detection of similar images.
- http://www.generation5.org/content/2007/kohonenImage.asp

ReefSOM

- SOM visualization for non-experts.
- UMAT + glyphs.
- http://www.brains-minds-media.org/archive/305





SOM Evaluation

- VQ – vector quantization, more input vectors mapped into a single neuron → **quantization error or distortion**.
- Compression of an input space dimension.
- Preserves data topology – neighbour vectors (from an input space) are mapped to neighbour neurons (in the mesh) → **topographic error**.

SOM Quantization Error & Distortion

- Quantization Error → average distance between input vector and its BMU (computed over all input vectors).
  - precision of mapping.
- Distortion → count with neighbours:

$$E=\sum_{i\in N}\sum_{j\in I}\eta_{i,bmu(j)}\|w(i)-x(j)\|^2$$

neurons

input vectors

Energy function again!

Topographic Error of SOM

- # of input vectors, for which the winner (BMU) and the second best neuron are not adjacent in the mesh.

Next Lecture

- Universal approximation.
- Kolmogorov's theorem.
- RBF networks.
- GMDH networks.