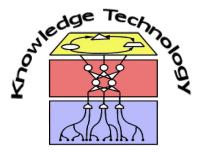
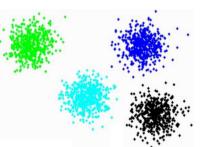
Knowledge Management and Intelligent Assistive Systems

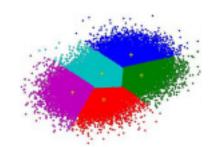
Lecture 8
Clustering and Selforganizing Networks



http://www.informatik.uni-hamburg.de/WTM/



What is Cluster Analysis?

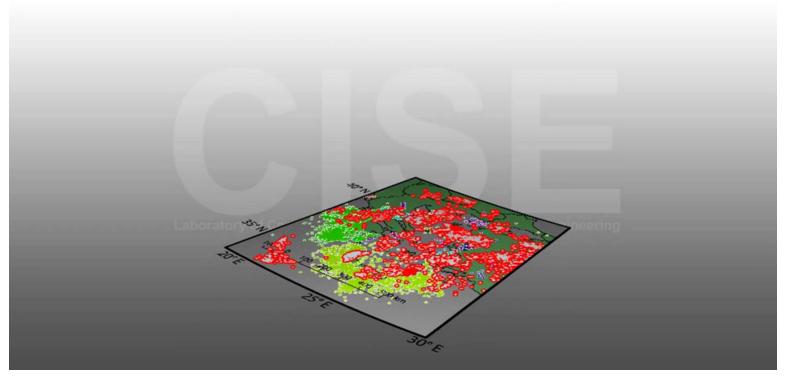


- Cluster: A group of data objects
 - similar (or related) to one another within the same group
 - dissimilar (or unrelated) to the objects in other groups
- Cluster analysis
 - Finding similarities between data according to their characteristics and grouping similar data objects into clusters
- Unsupervised learning: no predefined classes
- Typical applications
 - As a stand-alone tool to get insight into data distribution
 - As a preprocessing step for other algorithms

Clustering for Data Understanding and Applications

- Biology: taxonomy of living things: class, family, genus and species
- Information retrieval: document clustering
- Marketing: help marketers discover distinct customer groups, and develop targeted marketing programs
- Land use: similar land use in an earth observation database
- City-planning: identifying groups of houses according to their house type, value, and geographical location
- Climate: understanding earth climate, find patterns of atmospheric similiarities
- Earth-quake studies: observed earth quake epicenters should be clustered along continent faults

Spatiotemporal Clustering of Earthquakes in Greece



http://www.teicrete.gr

Quality: What Is Good Clustering?

- A good clustering method will produce high quality clusters
 - high intra-class similarity: cohesive within clusters
 - low inter-class similarity: distinctive between clusters
- The quality of a clustering method depends on
 - the similarity measure used by the method
 - its implementation, and
 - its ability to discover the hidden patterns

Measure the Quality of Clustering

Dissimilarity/Similarity metric

- Similarity is expressed in terms of a distance function, e.g. metric: d(i, j)
- The definitions of distance functions are usually different for interval-scaled, boolean, categorical, or vector variables
- Weights may be associated with different variables based on applications and data semantics
- Quality of clustering:
 - A (separate) "quality" function measures the "goodness" of a clustering process
 - It is hard to set thresholds for "similar enough" for data points or "good enough" for the clustering

Typical Requirements

- Scalability
- Incremental clustering and insensitivity to input order
- High dimensionality
- Ability to deal with different types of attributes
- Ability to deal with noisy data
- Discovery of clusters with arbitrary shape
- Constraint-based clustering
- Domain knowledge to determine input parameters
- Interpretability and usability

Major Clustering Approaches (1)

Partitioning approach

- Construct various partitions and then evaluate them by some criterion, e.g., minimizing the sum of squared errors
- Typical methods: k-means, k-medoids, CLARANS

Hierarchical approach

- Create a hierarchical decomposition of the set of data (or objects) using some criterion
- Typical methods: Diana, Agnes, BIRCH, CAMELEON

Density-based approach

- Based on connectivity and density functions above threshold
- Typical methods: DBSCAN, OPTICS, DenClue

Major Clustering Approaches (2)

Grid-based approach

- multiple-level granularity structure, finite number of cells
- Typical methods: STING, WaveCluster, CLIQUE

Model-based

- A model is hypothesized for each of the clusters and tries to find the best fit of that model to each other
- Typical: Gaussian Mixture Models, EM, SOM, COBWEB

Frequent pattern-based

- Based on the analysis of frequent patterns
- Typical methods: p-Cluster

Instance-based

 Typical method: K-nearest neighbors — classify a data point by the majority vote of its K closest neighbour points

Data Matrix and Dissimilarity Matrix

Data matrix

 n data points with p dimensions

$$\begin{bmatrix} x_{11} & \cdots & x_{1f} & \cdots & x_{1p} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{i1} & \cdots & x_{if} & \cdots & x_{ip} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{n1} & \cdots & x_{nf} & \cdots & x_{np} \end{bmatrix}$$

Dissimilarity matrix

- Registers the distances between the n data points
- A triangular matrix

$$\begin{bmatrix} 0 & & & & & \\ d(2,1) & 0 & & & \\ d(3,1) & d(3,2) & 0 & & \\ \vdots & \vdots & \vdots & & \\ d(n,1) & d(n,2) & \dots & \dots & 0 \end{bmatrix}$$

Reminder: Numeric Data: Minkowski Distance

Minkowski distance: A popular distance measure

$$d(i,j) = \sqrt[h]{|x_{i1} - x_{j1}|^h + |x_{i2} - x_{j2}|^h + \dots + |x_{ip} - x_{jp}|^h}$$

where

 $i = (x_{i1}, x_{i2}, ..., x_{ip})$ and $j = (x_{j1}, x_{j2}, ..., x_{jp})$ are two p-dimensional data objects,

h = order (the distance so defined is also called L-h norm)

- Properties
 - d(i, j) > 0 if $i \neq j$, and d(i, i) = 0 (Positive definiteness)
 - d(i, j) = d(j, i) (Symmetry)
 - $d(i, j) \le d(i, k) + d(k, j)$ (Triangle Inequality)
- A distance that satisfies these properties is a metric

Reminder: Special Cases of Minkowski Distance

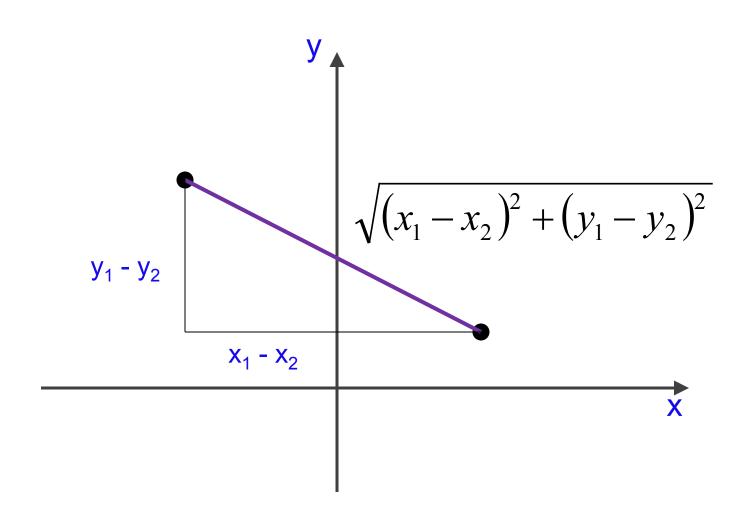
- h = 1: (L₁ norm) **Manhattan distance**
 - E.g., the Hamming distance between two binary vectors: the number of bits that are different

$$d(i,j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + \dots + |x_{ip} - x_{jp}|$$

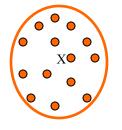
• h = 2: (L₂ norm) **Euclidean distance**

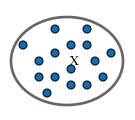
$$d(i,j) = \sqrt{|x_{i1} - x_{j1}|^2 + |x_{i2} - x_{j2}|^2 + \dots + |x_{ip} - x_{jp}|^2}$$

Euclidean Distance



Distance between Clusters





- Single link: smallest distance between an element in one cluster and an element in the other, i.e., dist(K_i, K_j) = min(t_{ip}, t_{jq})
- Complete link: largest distance between an element in one cluster and an element in the other, i.e., dist(K_i, K_i) = max(t_{ip}, t_{iq})
- Average: avg distance between an element in one cluster and an element in the other, i.e., dist(K_i, K_i) = avg(t_{io}, t_{iq})
- Centroid: distance between the centroids of two clusters, i.e., dist(K_i, K_j) = dist(C_i, C_j)
- Medoid: distance between the medoids of two clusters, i.e., dist(K_i, K_j) = dist(M_i, M_j)
 - Medoid: a chosen, centrally located object in the cluster (whose dissimilarity to all other objects in the cluster is minimal)

Centroid, Radius and Diameter of a Cluster (for numerical data sets)

- Centroid: the "center of mass" of a cluster (has minimal average Euclidean distance) $C_m = \frac{\sum_{i=1}^{N} (t_{ip})}{N}$
- Radius: (proportional to) average Euclidean distance from any point of the cluster to its centroid $R_m = \sqrt{\frac{\sum_{i=1}^{N} (t_{ip} c_m)^2}{N}}$

Diameter: average Euclidean distance between all *pairs* of points

in the cluster

$$D_{m} = \sqrt{\frac{\sum_{i=1}^{N} \sum_{j=1}^{N} (t_{ip} - t_{jp})^{2}}{N(N-1)}}$$

Partitioning Algorithms: Basic Concept

Partitioning method: partitioning a database D of n objects into a set of k clusters, minimising sum of squared distance to means m_i

$$E = \sum_{i=1}^{k} \sum_{p \in C_i} (p - m_i)^2$$

- Given k, find a partition of k clusters that optimizes the chosen partitioning criterion
 - Find global optimum: exhaustively enumerate all possible partitions
 - Find a local optimum by heuristic methods:
 - k-means (MacQueen'67):
 Each cluster is represented by its center
 - k-medoids or Partition around medoids (PAM, Kaufman&Rousseeuw'87):
 Each cluster is represented by one of the objects in the cluster

The K-Means Clustering Method

- Given k, the k-means algorithm is as:
 - 1. Partition objects into *k* nonempty subsets
 - Compute the centroids (center of mass / mean point) of the clusters of the current partitioning
 - Assign each object to the cluster with the nearest centroid
 - Go to Step 2; Stop when none of the assignments changed

The k-Means Algorithm

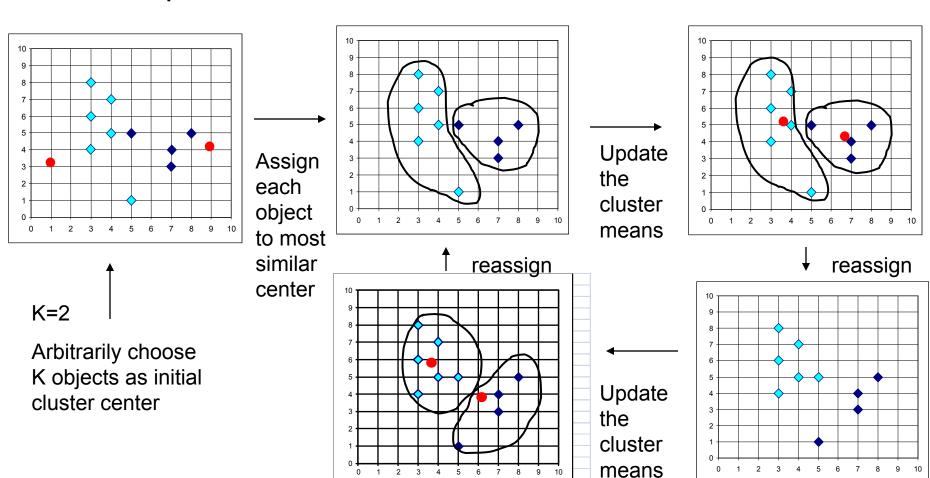
- Initialization
 - Set a value for k
 - Place the k cluster centres μ_i at random positions in input space
- Learning: Repeat ...
 - For each data point x_i
 - Compute distance to each cluster centre
 - Assign data point to nearest cluster centre with distance $d_i = \min_i d(x_i, \mu_i)$
 - For each cluster centre
 - Move position of centre to mean of points in cluster

$$\mu_j = \frac{1}{N_j} \sum_{i=1}^{N_j} x_i$$
 N_j = number of points in cluster j

- until the assignments don't change (then, cluster centres stop moving)
- On-line version: move cluster center only a bit for each data point

The K-Means Clustering Method

Example



Why k-means converges

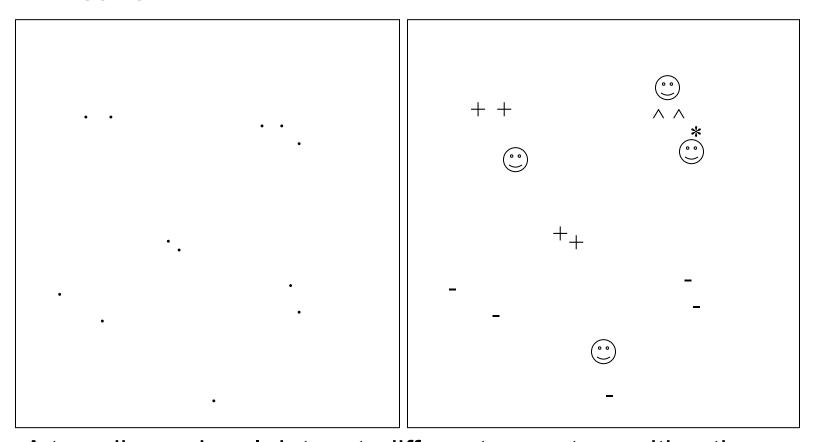
 Whenever an assignment is changed, the sum squared distances of datapoints from their assigned cluster centers is reduced.

 Whenever a cluster center is moved, the sum squared distances of the datapoints from their currently assigned cluster centers is reduced.

 If the assignments do not change in the assignment step, we have converged.

Visualisation of the Clustering

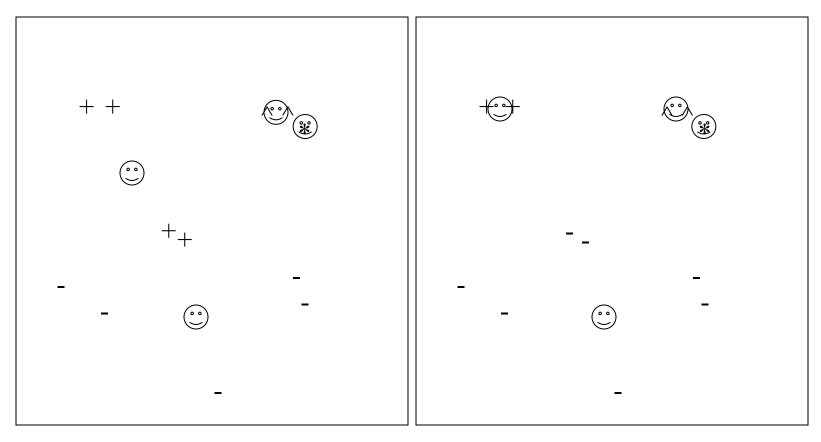
4 means



A two dimensional dataset; different ways to position the centres, one is shown to the right

Visualisation of the Clustering

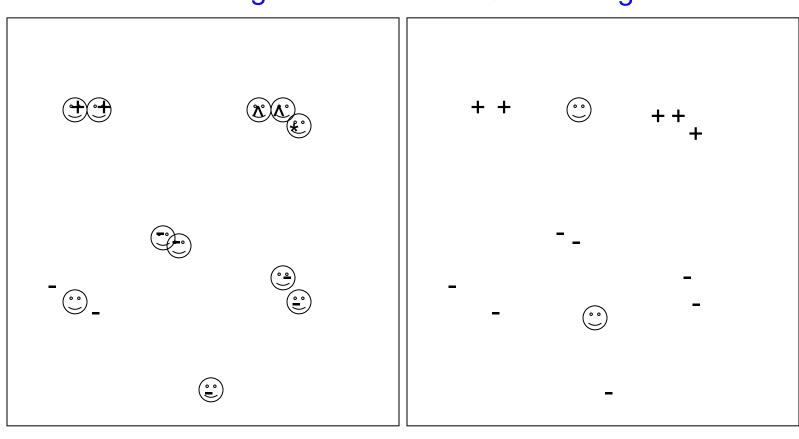
These are local minima solutions



Visualisation of the Clustering

Overfitting

Underfitting



Comments on the *K-Means* Method

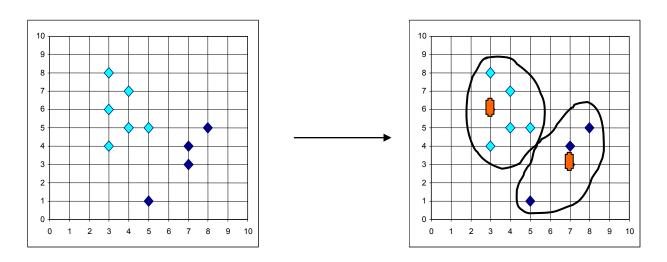
Strength: Relatively efficient: O(tkn). Typically, k, t << n. (n = #objects, k = #clusters, t = #iterations)

Weaknesses

- Need to specify k, the number of clusters, in advance
- Sensitive to noisy data and outliers
- Terminates at a *local* optimum
- Not suitable to discover clusters with non-convex shapes
- Applicable only when mean is defined not for categorical data

Handling Outliers: the K-Medoids Method

- The k-means algorithm is sensitive to outliers!
 - Since an object with an extremely large value may substantially distort the distribution of the data.
- K-Medoids: Instead of taking the mean value of the objects in a cluster as a reference point, medoids can be used, which is the most centrally located object in a cluster.



Example: Object Hypotheses in Natural Scenes using k-means

- In a stereo image pair of a scene, pixels can be clustered based on position, disparity, hue and saturation.
- For object segmentation, if two objects are in close proximity, they are likely to be encapsulated by the same segment.
- If we give the information that a segment covers two objects, k-means (k=2) can find a likely split of that segment.
- Then the object modeling loop is resumed with the new hypotheses.

Object Hypotheses Example

Generating Object Hypotheses in Natural Scenes through Human-Robot Interaction

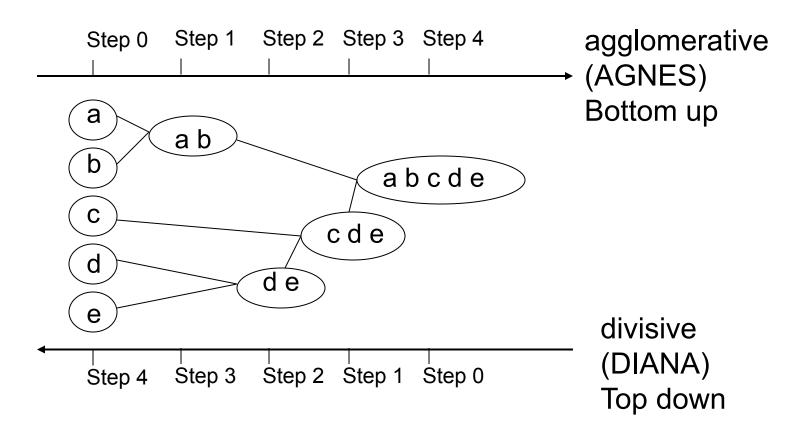
Niklas Bergström, Mårten Björkman, Danica Kragic CSC/KTH Stockholm, Sweden IROS 'I I

Other Typical Partitioning Clustering Methods

- K-Medoids Clustering: Find representative objects (medoids) in clusters
 - PAM (Partitioning Around Medoids, 1987)
 - starts from an initial set of medoids and iteratively replaces one of the medoids by one of the non-medoids if it improves the total distance of the resulting clustering
 - PAM works effectively for small data sets, but does not scale well for large data sets (due to the computational complexity)
 - CLARA (Kaufmann & Rousseeuw, 1990): PAM on samples
 - CLARANS (Ng & Han, 1994): Randomized sampling
- K-Medians Clustering: Find k medians instead of means (minimizes error w.r.t. the 1-norm distance, e.g. Manhatten)

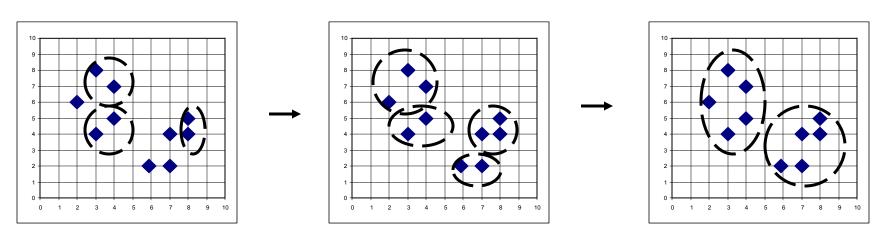
Hierarchical Clustering

 Use distance matrix as clustering criteria. This method does not require the number of clusters k as an input, but needs a termination condition



AGNES (Agglomerative Nesting)

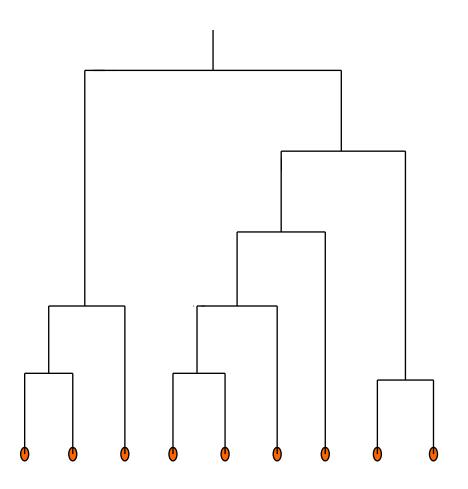
- Introduced in Kaufmann and Rousseeuw (1990)
- Implemented in statistical packages, e.g., Splus
- Use the single-link method and the dissimilarity matrix
- Merge nodes that have the least dissimilarity
- Go on in a non-descending fashion
- Eventually all nodes belong to the same cluster



Dendrogram shows how clusters are merged

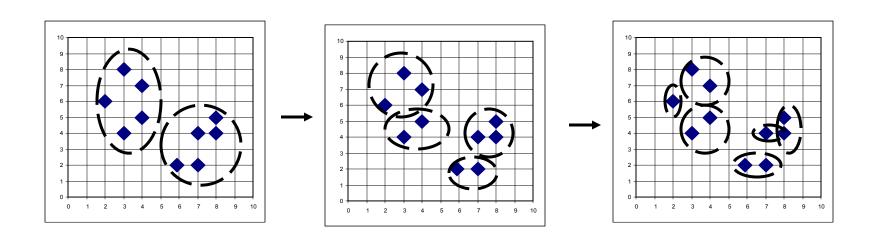
 Decompose data objects into several levels of nested partitioning (tree of clusters), called a dendrogram.

A clustering of the data objects is obtained by cutting the dendrogram at the desired level, then each connected component forms a cluster.



DIANA (Divisive Analysis)

- Introduced in Kaufmann and Rousseeuw (1990)
- Implemented in statistical analysis packages, e.g., Splus
- Inverse order of AGNES: top down
- Eventually each node forms a cluster on its own



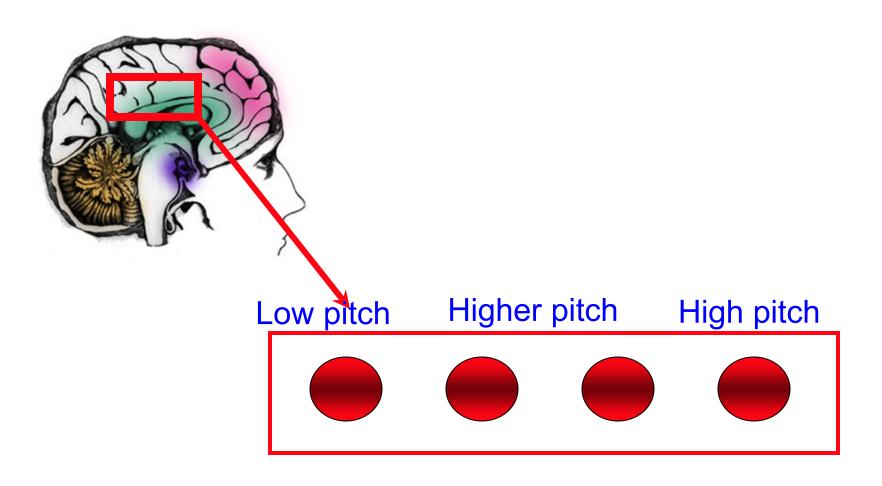
Model-Based Clustering

- What is model-based clustering?
 - Assumption: a cluster is generated by a model such as a probability distribution
 - A model (e.g., Gaussian distribution) is determined by a set of parameters
 - Task: optimize the fit between the given data and some mathematical model by learning the parameters of the model
- Typical statistical methods
 - Gaussian Mixture Models, EM (Expectation maximization), AutoClass
- Typical neural network methods
 - SOM (Self-Organizing Feature Map)

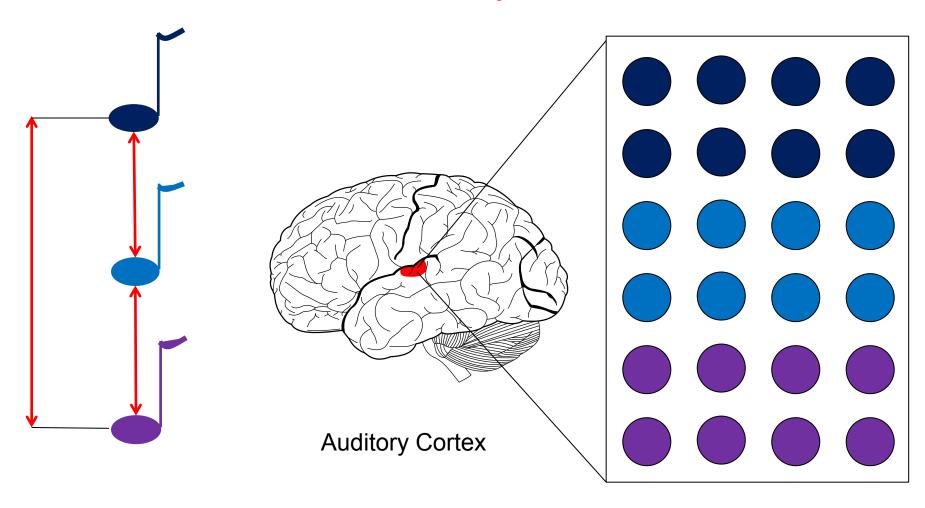
Neural Network Approaches

- Neural network approaches
 - Represent each cluster with an exemplar (a neuron), acting as a "prototype" of the cluster
 - New objects are assigned to the cluster whose exemplar is the most similar according to some distance measure
- Typical methods
 - SOM (Self-Organizing feature Map)
 - Competitive learning
 - Neurons compete in a "winner-takes-all" fashion for the object currently being presented

Feature Maps



Feature Maps: How are Signals Mapped into the Auditory Cortex?



Different sound signals

Activated Neurons

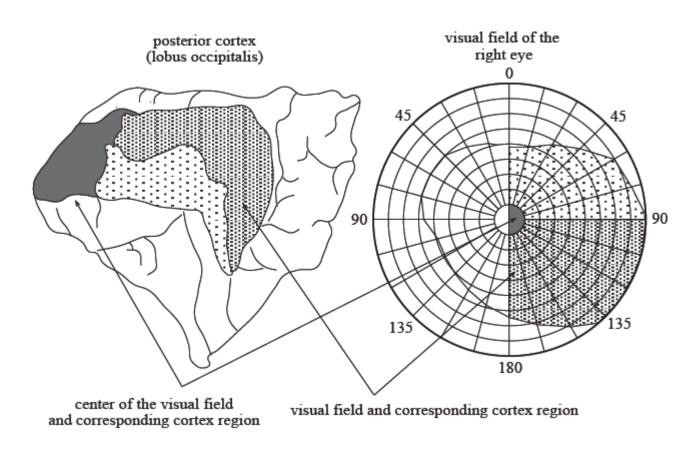
Feature Maps

- Sounds that are similar ('nearby in input space') excite neurons that are near to each other (in `output space')
- Sounds that are very different excite neurons that are a long way off

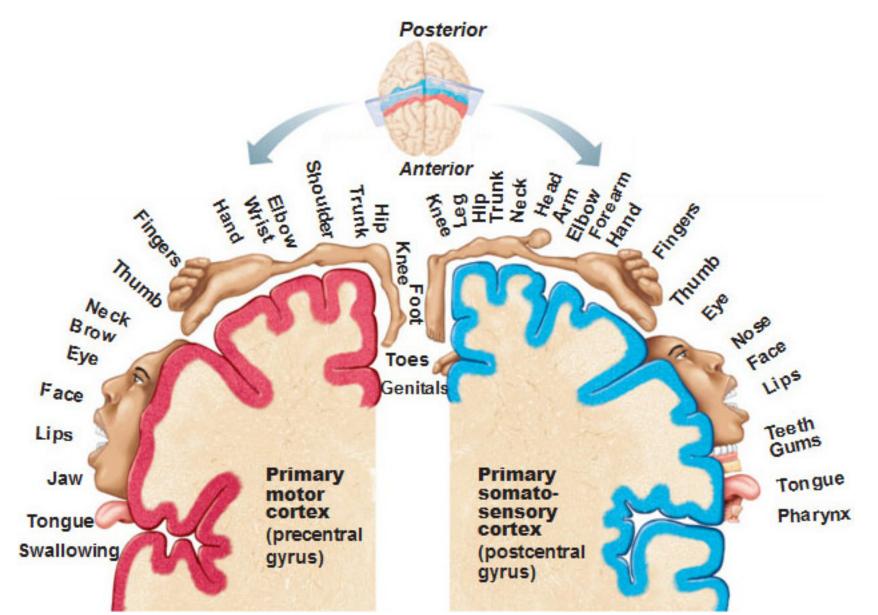
- This is known as topology preservation
- The ordering of the inputs is preserved
 - If possible (perfectly topology-preserving)

Mapping of visual Field to Cortex

 Neighboring visual fields processed by neighboring cortex regions; fovea is large

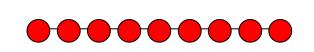


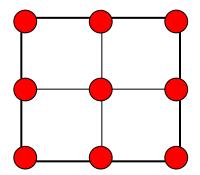
Mapping of effectors and sensors to Cortex



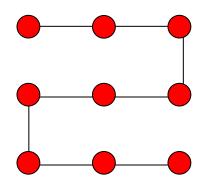
Topology Preservation in 2D

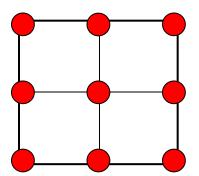
Network Topology





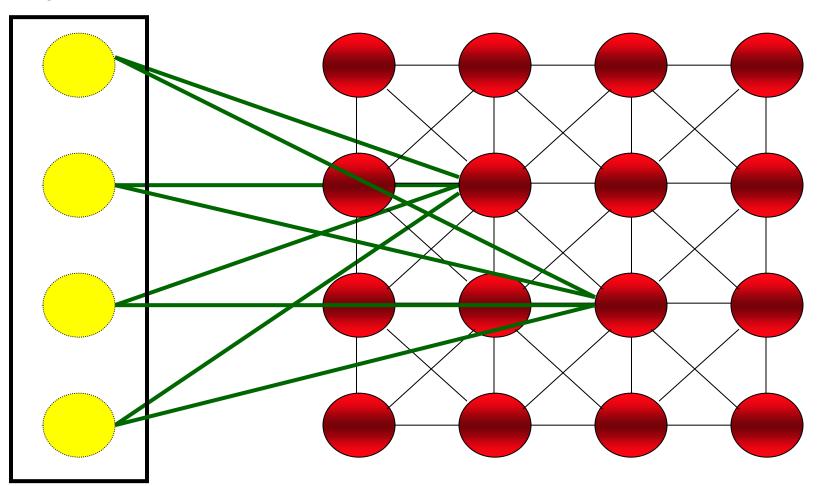
Network Representation of Input Space





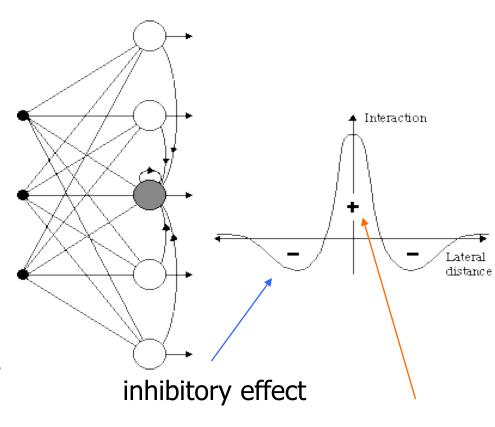
The Self-Organising Map

Inputs



Mexican hat function

- The Mexican hat function represents the relationship between the distance from the winning neuron and the strength of "connections" within the Kohonen layer
- Near neighbourhood short range lateral excitation area has strong positive effect
- Remote neighbourhood has a weak negative inhibitory effect
- → leads to WTA behaviour (competitive network!)



excitatory effect

Neuron Connections?

- We do not actually need the inhibitory connections
 - Just use a neighbourhood of positive connections

- How large should this neighbourhood be?
 - Early in learning, network is unordered
 - Big neighbourhood: similar input vectors excite neurons far apart
 - They will also learn similarly and form clusters in input space
 - Later on, just fine-tuning network
 - Small neighbourhood: similar input vectors excite neurons closer together

Everybody Needs Good Neighbours

Generate a neighbourhood size function

Pick the nodes that are in the neighbourhood

Decrease the neighbourhood each epoch

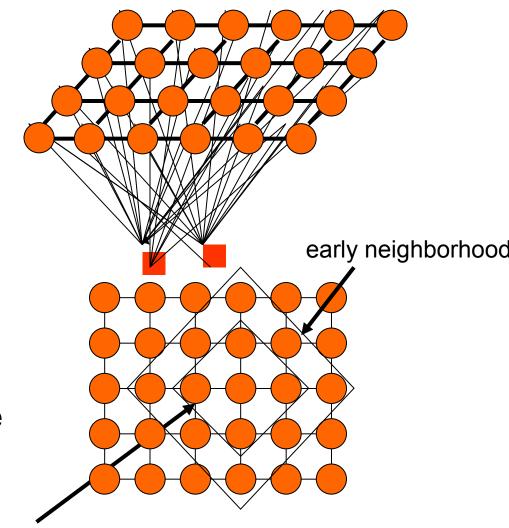
Do the same for the learning rate

Self-Organizing Feature Map (SOM)

- SOMs, also called topological ordered maps, or Kohonen Self-Organizing Feature Map (KSOMs)
- It maps the points in a high-dimensional source space into a 1D,
 2D (most typical) or 3D target space; distances and proximity relationships (i.e., topology) are preserved as much as possible
- Similar to k-means: cluster centers tend to lie in a lowdimensional manifold in the feature space
- Clustering is performed by having several units competing for the current object
 - The unit whose weight vector is closest to the current object wins
 - The winner and its neighbors learn by having their weights adjusted
- SOMs mimic some aspects of competitive processing in the brain
- Useful for visualizing high-dimensional data

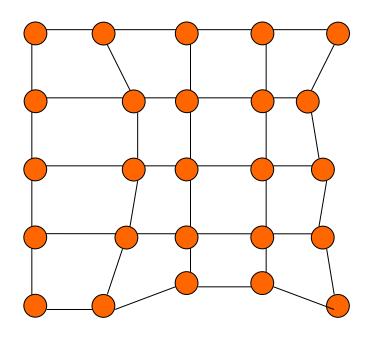
Self organizing maps

- The activation of the neuron is spread in its direct neighborhood
 - neighbors become sensitive to the same input patterns
- The size of the neighborhood is initially large but reduced over time during training as the network neurons become more specialized

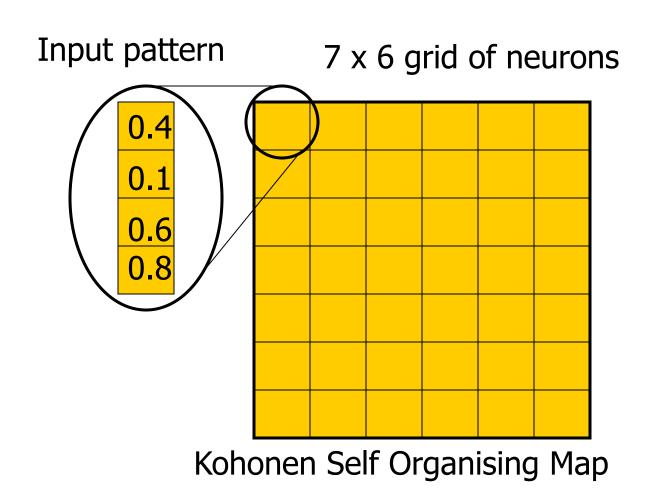


Adaptation

- During training, the "winner" neuron and its neighborhood adapts to make their weight vector more similar to the input pattern that caused the activation
- The neurons are moved closer to the input pattern
- The magnitude of the adaptation is controlled via a learning parameter which decays over time



SOM Architecture Overview



SOM 'Cost Function'

K-means:

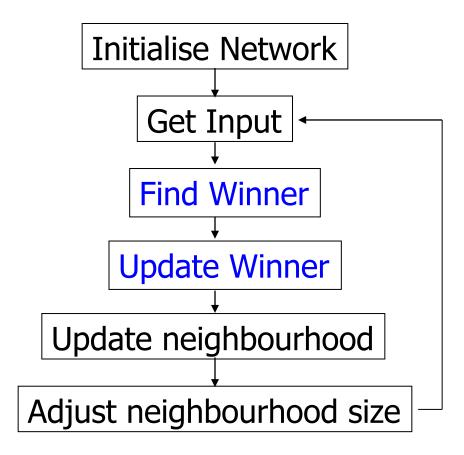
$$E = \sum_{i=1}^{k} \sum_{p \in C_i} (p - m_i)^2$$

SOM:

$$E = \sum_{i=1}^{k} \sum_{p \in C_i} \sum_{j=1}^{k} h(|i-j|) (p-m_j)^2$$

neighbourhood activation function h

SOM Algorithm



The Self-Organising Map Algorithm

- The weight vectors are randomly initialised
- Input vectors are presented to the network
 - Determine best matching neuron n_b with the minimal Euclidean distance between input x and weight vector w

$$n_b = \min_{j} \left\| x - w_j^T \right\|$$

• The winning node and neighbours have weight vector moved closer to the input (with learning rate $\eta(t)$)

$$w_j^T \leftarrow w_j^T + \eta(t) \cdot \left(x - w_j^T\right)$$

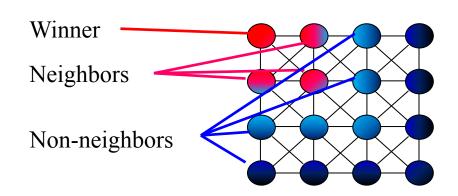
 Over time, the network self-organises so that the input topology is preserved

Neighborhood Function Preserves Topology

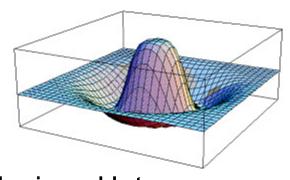
The neighborhood function $h(n_b, t)$ determines the degree of weight vector change of the neighbors

$$w_j^T \leftarrow w_j^T + \eta(t) \cdot h(n_b, t) \cdot (x - w_j^T)$$

- Mostly: Gaussian function rarely: Mexican Hat function
- Width decreases during training
 (→ implicit decrease of learning rate)
- May decrease to zero (→ k-means)







Mexican Hat (Difference of Gaussian)

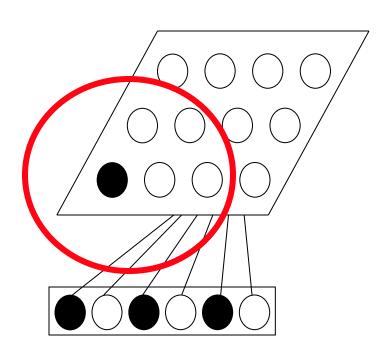
Self-Organization

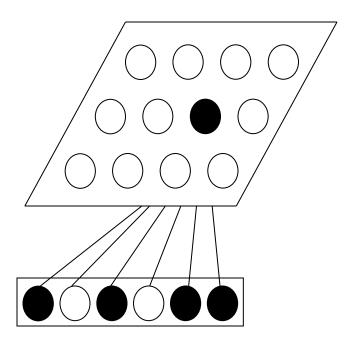
- Global ordering from local interactions
 - Each neuron sees its neighbors
 - The whole network becomes ordered

Understanding self-organization is part of complexity science

The Self-Organizing Map

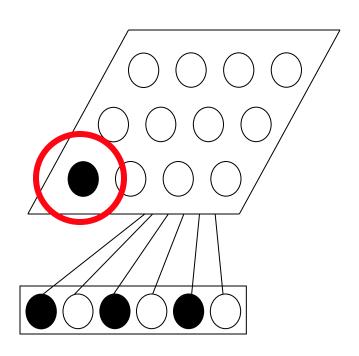
Before training (large neighbourhood)

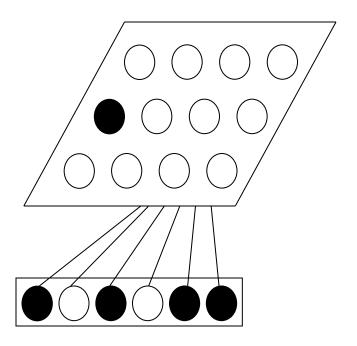




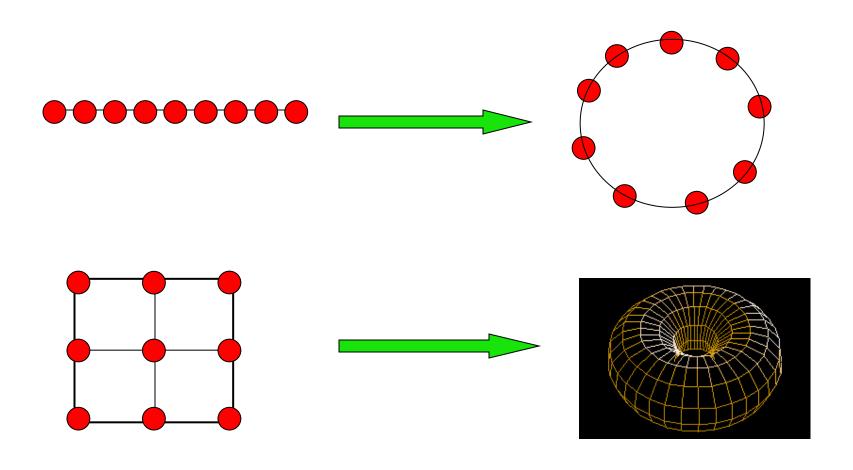
The Self-Organizing Map

After training (small neighbourhood)

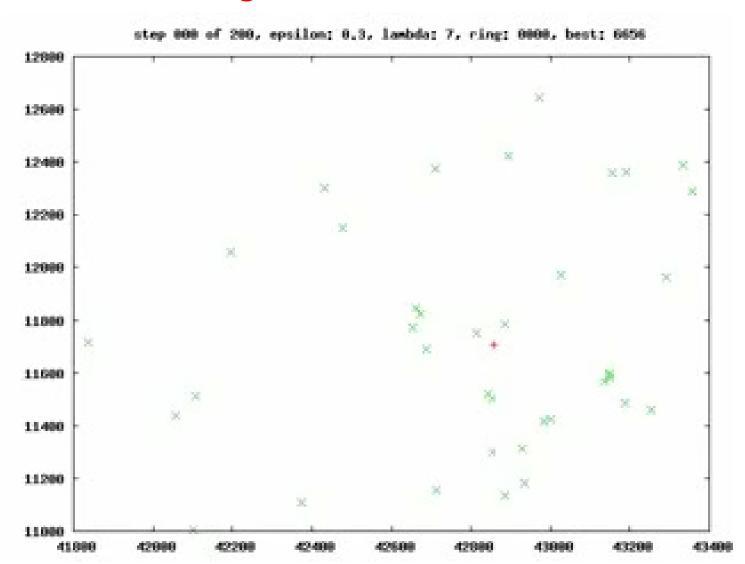




Boundary Conditions: No Neurons at the End of the Map



1D Ring-Form SOM for the Travelling Salesman Problem



Network Size

- We have to predetermine the network size
- Big network
 - Each neuron can in principle represent exact features
 - → not much generalisation
 - Large neighbourhood interaction keeps network `small'
- Small network
 - Too much generalization
 - → no differentiation
- Experiments to identify most suitable size

Batch Learning

- Need all the data to start with
 - Run for many iterations

- Can therefore order neurons to begin with
 - Principal components of data

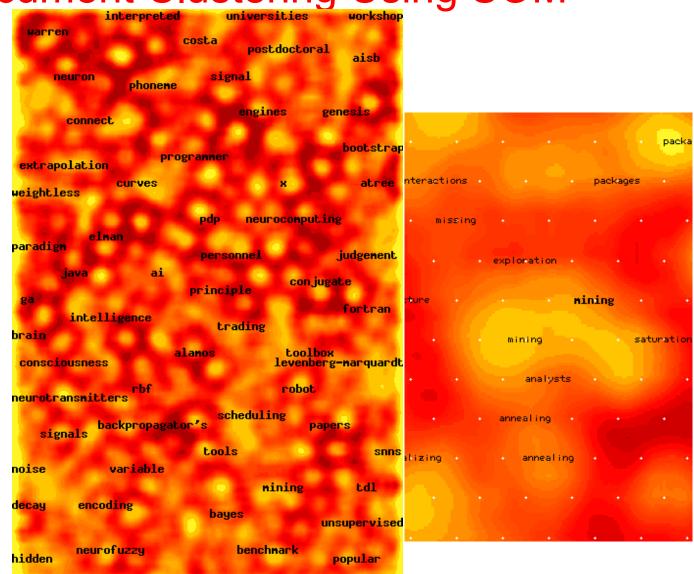
- For on-line learning there are other algorithms
 - Fritzke's 'Growing Neural Gas'
 - Marsland's 'Growing When Required' network

Web Document Clustering Using SOM

signoid

validation

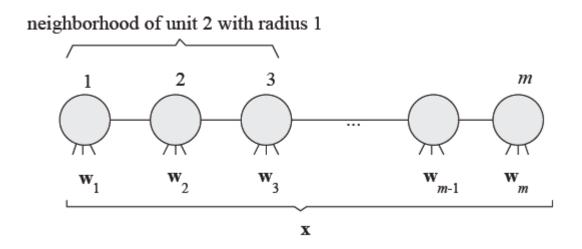
- The result
 of SOM
 clustering of
 12088 Web
 articles
- The picture on the right: drilling down on the keyword "mining"



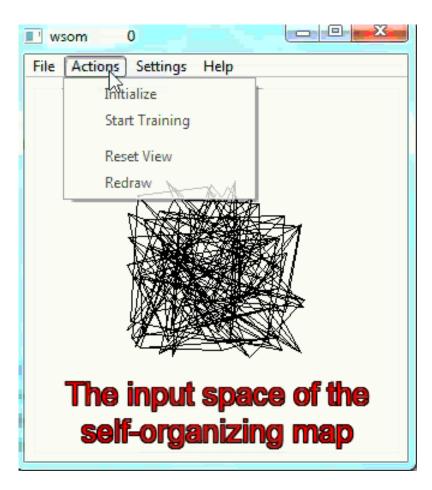
Examples: One-dimensional Lattice of Kohonen Elements

Units are arranged in sequence

 Each unit learns to specialize for different regions of input space [Rojas]



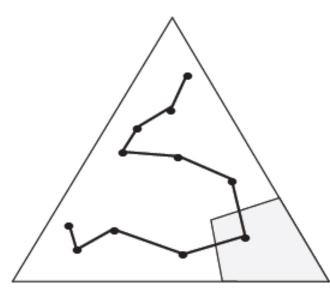
SOM Demo



[http://www.borgelt.net/somd.html]

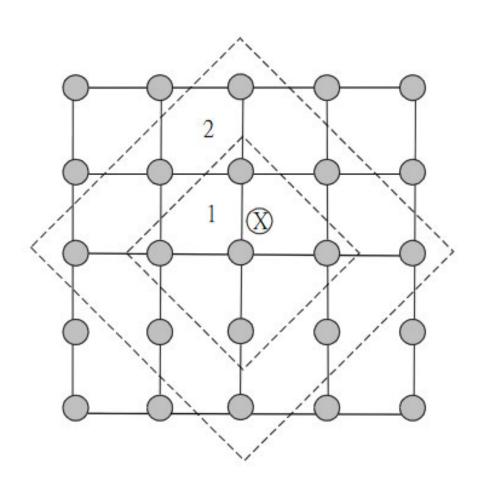
Map of a Triangular Region

 Triangular input domain is mapped to a smaller number of one-dimensional representative units



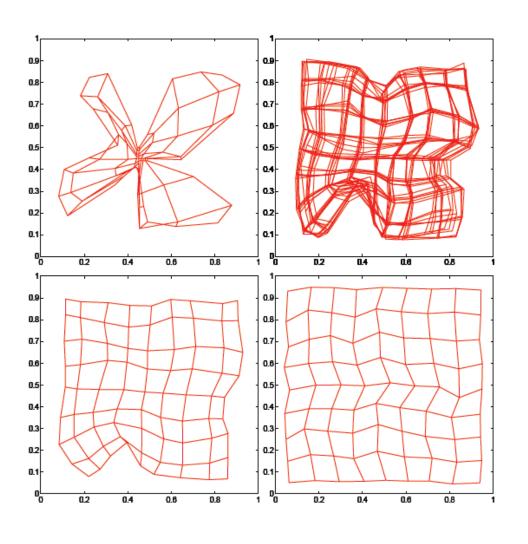
Unit with strongest excitation for shaded region

Example of SOM Neighborhood



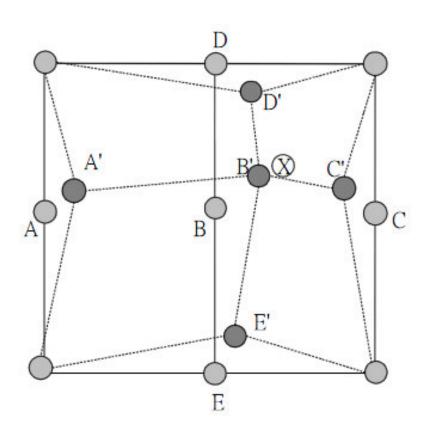
The input vector is represented as X.
Units in neighbourhood 1 are more active than those in neighbourhood 2.

Good Fit of dimensions: Mapping a Square with a 2-dimensional Lattice



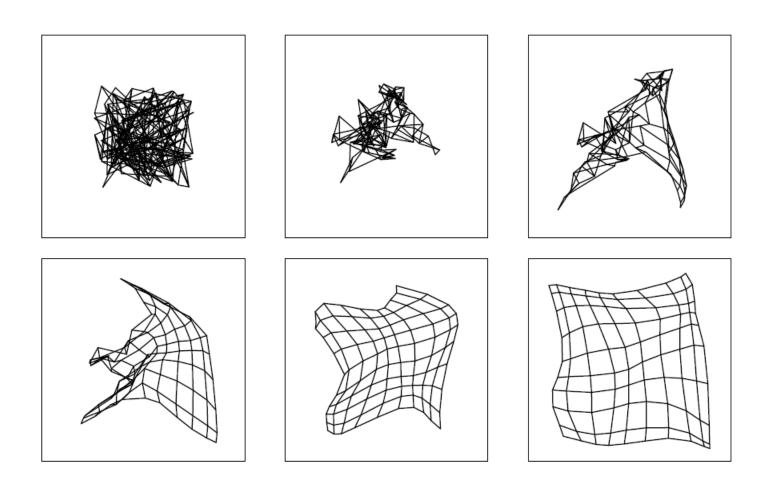
- Upper right with some overlapped learning iterations
- Results for 100, 1000, 5000, 10000 iterations (Kohonen 1984)

Influence by Pre-Defined Topology

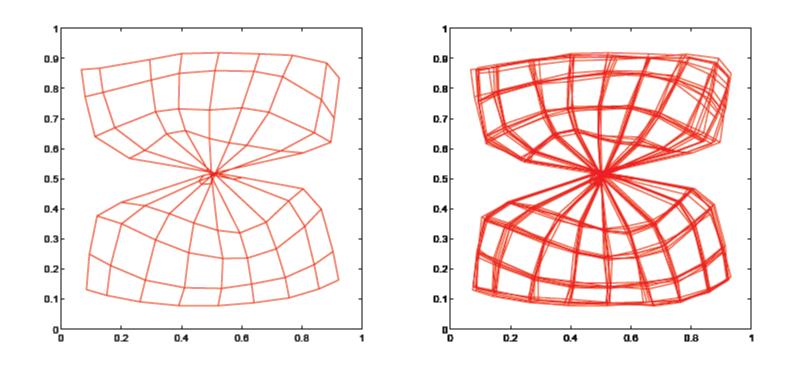


- The winner B and its neighbors such as A, C, D and E move towards the input vector X
- Modified units are shown as dark circles

Unfolding of a 2-D Map in a 2-D Data Space

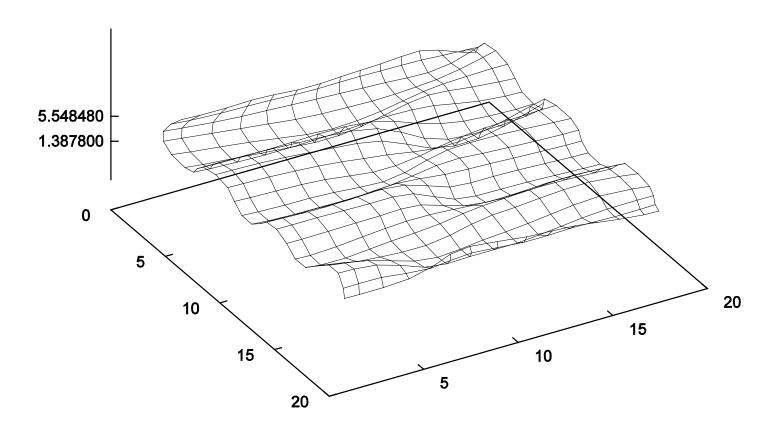


Planar Network with a Knot



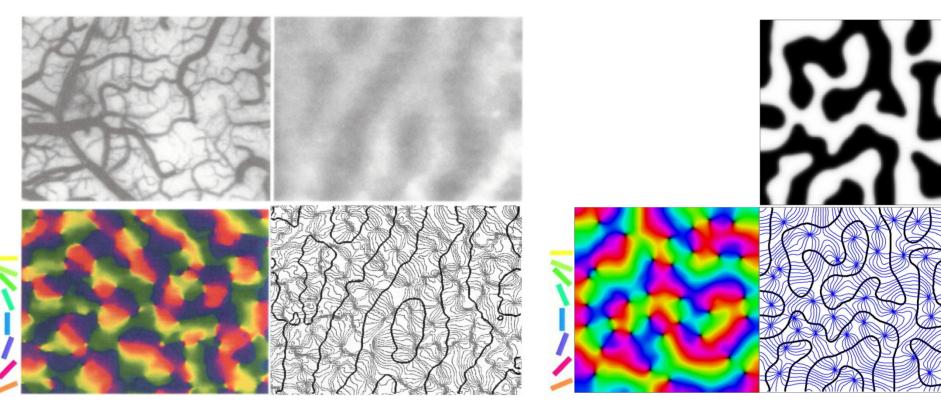
State difficult to correct

Unfolding of a 2-D Map in a 3-D Data Space



Example Application: V1 Maps

ocular dominance



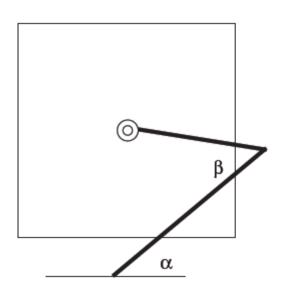
orientation preference

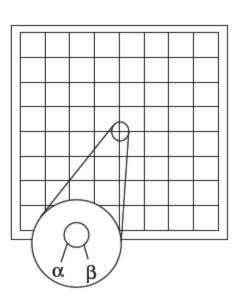
Obermayer, Blasdel. .. Orientation and Ocular Dominance Columns in Monkey .. Jneurosci, 1993

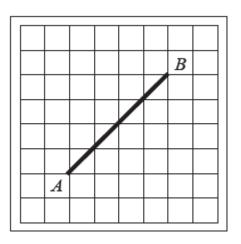
Goodhill . Theoretical Modelling to .. Neural Map Development. Neuron, 2007

Learning Simple Inverse Kinematics

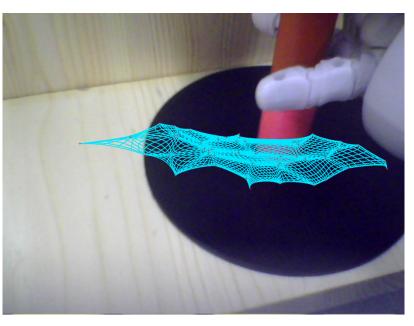
- Mapping the configuration space of a robot arm using 2dimensional network
- For one point only one parameter combination; many paths from A to B







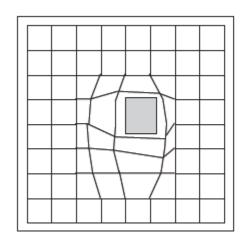
Learning Simple Inverse Kinematics

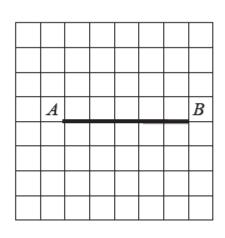


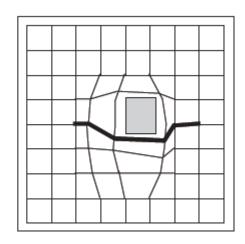


Learning Obstacles in Work Area

- Kohonen network charts configuration space avoiding the obstacles
- Moving the arm from A to B avoids the obstacle





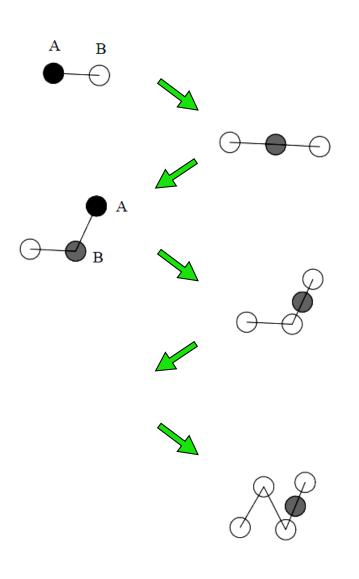


Existing Neural Clustering models

- Static Models (fixed number of units): Competitive Learning (CL), Self-Organizing Map (SOM), Neural Gas (NG)....
- Dynamic Models (variable number of units): Growing Grid (GG), Growing Cell Structure (GCS), Growing Neural Gas (GNG), Grow When Required (GWR), etc.
- Hierarchical Models: Multilayered Self-Organising Feature Maps (M-SOM), Growing Hierarchical Self-Organizing Map (GHSOM), etc.

But there are several shortcomings for them in a nonstationary environment.

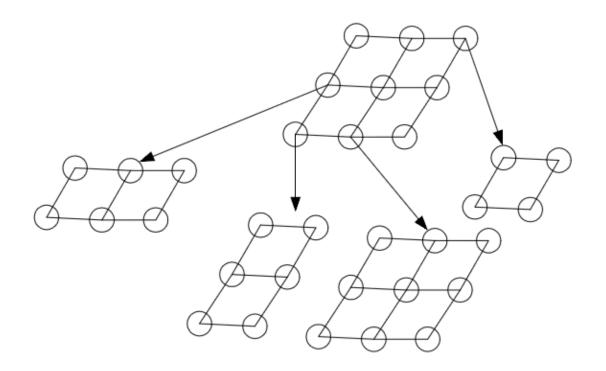
Growing Processes for DASH Model (Growing Neural Gas – GNG Fritzke)



- GNG adds unit after every predefined period.
- Units are represented as circles.
- Circle A indicates unit with biggest error
- Circle B indicates neighbor with biggest error for Circle A.
- The grey circle is the new unit at each stage.

Growing Hierarchical SOM

(Rauber et al)



A sub-map **grows** from a unit whose error is greater than a pre-defined proportion of the expected unit error

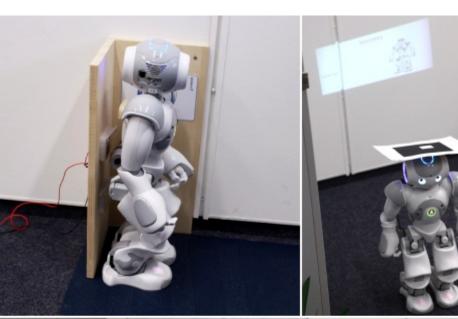
Dynamical SOM for Dynamical Knowledge Acquisition Over Time



Shortcomings of static Models in a non-stationary Environment

- Pre-defined number of units
- Pre-defined topology (mostly a grid)

- Pre-defined training length
- A decaying learning rate (e.g. SOM, CL, NG, GG, GSOM, Snet-SOM, M-SOM, GHSOM)



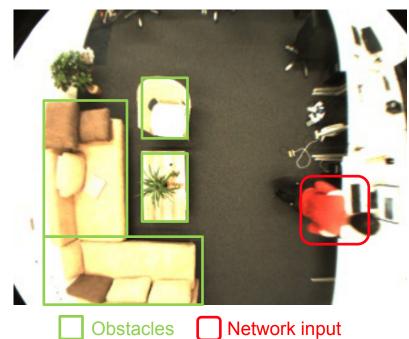


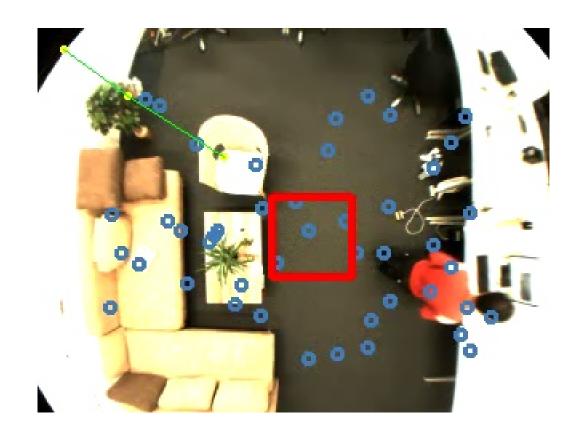




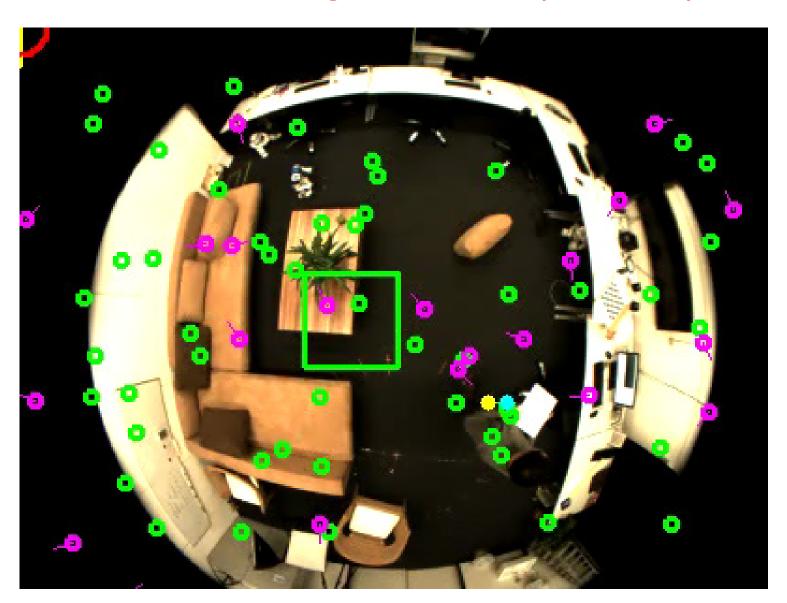


- Map the topological structure of a room using growing neural gas for robot navigation
- Since the person's movement can show the free space in the room, we use the detected position of a person as the network input





- Blue dots are particles for person detection
- Red bounding box shows the estimated position of the target person
- Yellow dots are the neurons of the growing neural gas and the green lines are the connections



Summary

- Cluster analysis groups objects based on their similarity and has wide applications
- Measure of similarity can be computed for various types of data
- Clustering algorithms can be categorized into partitioning methods, hierarchical methods, density-based methods, grid-based methods, and model-based methods
- Outlier detection and analysis are very useful for fraud detection, etc. and can be performed by statistical, distance-based or deviation-based approaches
- There are still lots of research issues on cluster analysis