NEURAL NETWORKS
MACHINE LEARNING

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CHAPTER VIII

Data Clustering and Self-Organizing Feature Maps

CHAPTER VI : *Data Clustering &Self-Organizing Feature Maps*

Introduction

- Self organizing feature maps (SOFM) - also called Kohonen feature maps - are a special kind of neural networks that can be used for clustering tasks.

- The goal of clustering is to reduce the amount of data by categorizing or grouping similar data items together.

- Since SOFM learn a weight vector configuration without being told explicitly of the existence of clusters at the input, then it is said to undergo a process of self-organised or unsupervised learning. This is to be contrasted to supervised learning, such as the delta rule or backpropagation where a desired output had to be supplied.

- In this chapter first clustering is introduced and then K means clustering algorithm is presented. Next, SOFM is explained in detail together with its training algorithm and its usage for clustering. Finally, the relation between SOFM and K-means clustering is explained.

8.1. Clustering methods

- The goal of clustering is to reduce the amount of data by categorizing or grouping similar data items together.

- Clustering methods can be divided into two basic types: hierarchical and partitional clustering. Within each of the types there exists a wealth of subtypes and different algorithms for finding the clusters.

8.1.1 Hierarchical Clustering

- Hierarchical clustering proceeds successively by either merging smaller clusters into larger ones, or by splitting larger clusters.
- The clustering methods differ in the rule by which it is decided which two small clusters are merged or which large cluster is split.
- The end result of the algorithm is a tree of clusters called a dendrogram, which shows how the clusters are related.
- By cutting the dendrogram at a desired level a clustering of the data items into disjoint groups is obtained.

8.1.2 Partitional Clustering

- Partitional clustering, on the other hand, attempts to directly decompose the data set into a set of disjoint clusters.
- Typically, in clustering algorithms, there exist a global criteria that involve minimizing some measure of dissimilarity in the samples within each cluster, while maximizing the dissimilarity of different clusters.
- A commonly used partitional clustering method, K-means clustering will be discussed in some detail since it is closely related to the SOM algorithm.

CHAPTER VI : *Data Clustering &Self-Organizing Feature Maps*

8.2. The K-Means Clustering Algorithm

- In K-means clustering the criterion function is the average squared distance of the data items $\mathbf{u}^k$ from their nearest cluster centroids,

$$E = (1/P)\sum_{i=1}^{P} \left\|\mathbf{u}^i - \mathbf{m}_{c(\mathbf{u}^i)}\right\|^2 \qquad (8.2.1)$$

where c($\mathbf{u}^i$) is the index of the centroid (mean of the cluster) that is closest to $\mathbf{u}^i$ and P is the number of samples.

- One possible algorithm for minimizing the cost function begins by initializing a set of K cluster centroids denoted by $\mathbf{m}^i$, $i=1..K$.

- The positions of the $\mathbf{m}^i$ are then adjusted iteratively by first assigning the data samples to the nearest clusters and then recomputing the centroids.

- The iteration is stopped when E does not change markedly any more.

8.2.1 The algorithm:

- Suppose that we have P example feature vectors $\mathbf{u}^i \in R^N$, $i=1..P$ and we know that they fall into K compact clusters, $K < P$.
- Let $\mathbf{m}^i$ be the mean of the vectors in Cluster-*i*.
- If the clusters are well separated, we can use a minimum-distance classifier to separate them.
- That is, we can say that $\mathbf{u}$ is in cluster C^k if $\| \mathbf{u} - \mathbf{m}^k \|$ is the minimum of all the K distances.
- This suggests the following algorithm for finding the *K* means:

8.2.1 The algorithm:

Given $\mathbf{u}^i \in R^N$, i=1..P

1. Make initial, i.e. t=0, guesses for the means $\mathbf{m}^k(0)$ for cluster C^k, $k=1..K$

2. Use the means $\mathbf{m}^k$, $k=1..K$ to classify the examples $\mathbf{u}^i$, $i=1..N$ into clusters $C^k(t)$ such that

$$\mathbf{u}^i \in C^k \quad \textit{where} \quad k = \arg\min_j \left\| \mathbf{u}^i - \mathbf{m}^j \right\|$$

3. Replace $\mathbf{m}^k$, $k=1..K$ with the mean of all of the examples for cluster C^k

4. Repeat steps 2 and 3 until there are no changes in any mean $\mathbf{m}^k$, $k=1..K$

$$\mathbf{m}^k(t+1) = \frac{1}{card(C^k(t))} \sum_{\mathbf{u}^i \in C^k(t)} \mathbf{u}^i$$

where $card(C^k(t)$ is the cardinality of cluster C^k (i.e number of elements in that cluster) at iteration t

8.2.1 The algorithm:

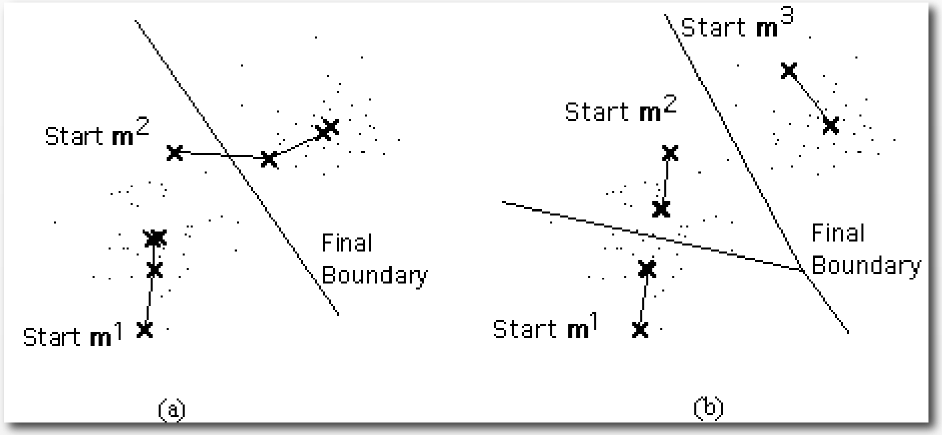


Figure 8.1 Means of the clusters move to the center of the clusters as the algorithm iterates a) *K*=2 b) *K*=3

8.2.1. The algorithm

- The results depend on the metric used to measure $||\mathbf{x} - \mathbf{m}^i||$.

- A potential problem with the clustering methods is that the choice of the number of clusters may be critical: quite different kinds of clusters may emerge when *K* is changed.

8.2.2 Initilization of the centroids:

- Furthermore good initialization of the cluster centroids may also be crucial.
- In the given algorithm, the way to initialize the means was not specified.
- One popular way to start is to randomly choose *K* of the examples.
- The results produced depend on the initial values for the means, and it frequently happens that suboptimal partitions are found.
- It can happen that the set of examples closest to $\mathbf{m}^k$ is empty, so that $\mathbf{m}^k$ cannot be updated.
- The standard solution is to try a number of different starting points.

8.3. Self Organizing Feature Maps

- Self-Organizing Feature Maps (SOFM) also known as Kohonen maps or topographic maps were first introduced by von der Malsburg (1973) and in its present form by Kohonen (1982).

- SOM is a special neural network that accepts *N*-dimensional input vectors and maps them to the Kohonen (competition) layer, in which neurons are organized in an *L*-dimensional lattice (grid) representing the feature space.

- Such a lattice characterizes a relative position of neurons with regards to its neighbours, that is their topological properties rather than exact geometric locations. In practice, dimensionality of the feature space (i.e.Kohonen layer lattice) is often restricted by its visualisation aspect and typically is *L* = 1, 2 or 3.

- The objective of the learning algorithm for the SOFM neural networks is formation of the feature map which captures of the essential characteristics of the N-dimensional input data and maps them on the typically 1-D or 2-D feature space.

8.3.1 Network structure

- The structure of a typical SOM network for $L=2$ is shown in Figure 8.2. It has N input nodes and m-by-m output nodes. Each output node j in the SOFM network has a connection from each input node i and w_{ij} denotes the connection weight between them.

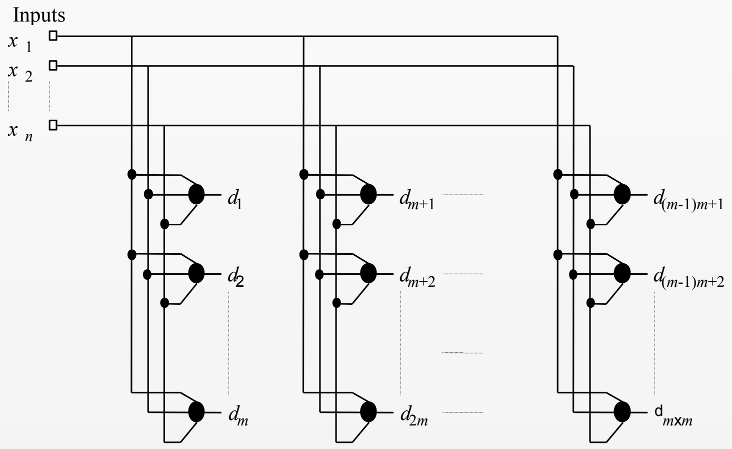
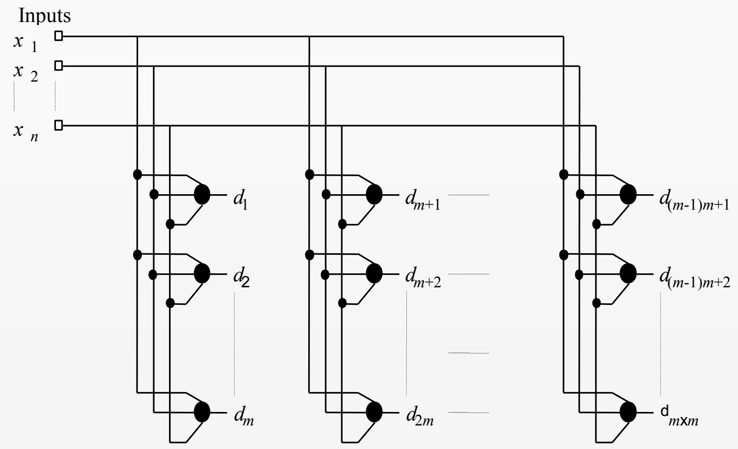


Figure 8.2 Network topology of the SOM

8.3.1 Network structure



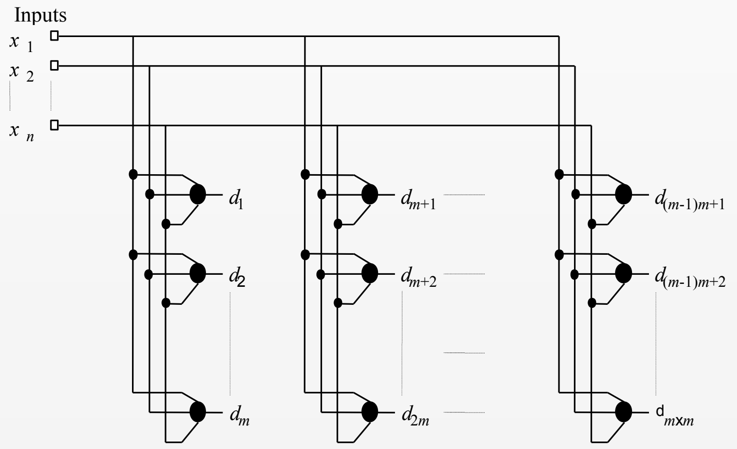
- The weights of the connections from the input neurons to a single neuron in the competition layer are interpreted as a reference vector in the input space.

- That is, a SOFM basically represents a set of vectors in the input space: one vector for each neuron in the competition layer.

8.3.1 Network structure

- A SOFM is trained with a method that is called competition learning: When an input pattern is presented to the network, that neuron in the competition layer having the reference vector closest to the input pattern is determined,

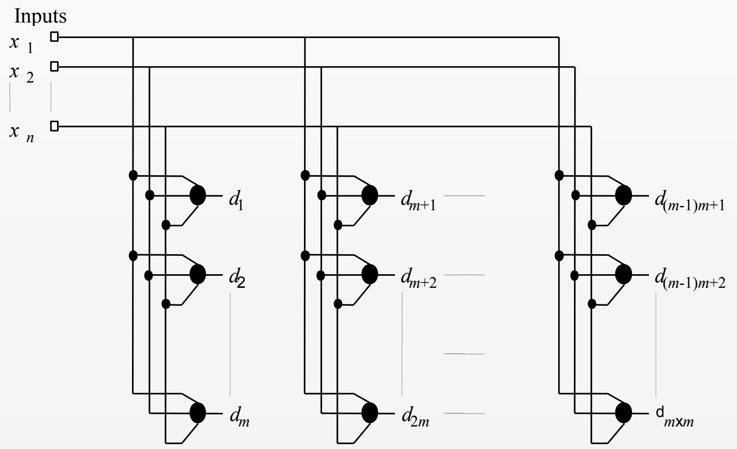
- This neuron is called the winner neuron and it is the focal point of the weight changes.



8.3.1 Network structure

- In pure competition only the weights of the connections leading to the winner neuron are changed. However, generally commpetition is used together with cooperation, such that the connections leading to the neurons in the neighbourhood of the winner are also updated

- The changes are made in such a way that the reference vector represented by these weights is moved closer to the input pattern.



8.3.1 Network structure

- During training the weigts are updated according to the formula

$$w_{ij}(t+1) = w_{ij}(t) + \eta(t)(\mathrm{u_i} - \mathrm{w_{ij}})N(j,t) \tag{8.3.1}$$

where w_{ij} is the i^{th} component of the weight vector $\mathbf{w}_j$ of the neuron n_j, and and u_i is the i^{th} component of the pattern $\mathbf{u}^{\mathrm{k}}$ applied at the input layer, $\eta(t)$ is the learning rate and $N(j,t)$ is the neighborhood function which is changing in time

- The learning algorithm captures two essential aspects of the map formation, namely, competition and cooperation between neurons of the output lattice.

8.3.2 Competition

- Competition determines the winning neuron d_{win}, whose weight vector is the one closest to the applied input vector.

- For this purpose the input vector $\mathbf{u}$ is compared with each weight vector $\mathbf{w}_j$ from the weight matrix $\mathbf{W}$ and the index of the winning neuron n_{win} is established considering the following formula.

$$n_{win} = \arg\min_{j} \left\| \mathbf{u} - \mathbf{w}_j \right\| \qquad (8.3.2)$$

8.3.3 Cooperation

- In SOFMs, not only the weights of the connections to the winner neuron are adapted.
- Rather, there is a neighborhood relation defined on the competition layer which indicates which weights of other neurons should also be changed.
- This neighborhood relation is usually represented as a (usually two-dimensional) grid, the vertices of which are the neurons. This grid most often is rectangular or hexagonal.
- During the learning process, the weights of all neurons in the competition layer that lie within a certain radius around the winner neuron with respect to this grid are also adapted, although the strength of the adaption may depend on their distance from the winner neuron.
- The effect of this learning method is that the grid, by which the neighborhood relation on the competition layer is defined, is "spread out" over the region of the input space that is covered by the training patterns.

8.3.3 Cooperation

- All neurons n_j located in a topological neighbourhood of the winning neurons n_{win} will have their weights updated usually with a strength $\mathrm{N}(j)$ related to their distance $\mathrm{d}(j)$ from the winning neuron, where $\mathrm{d}(j)$ can be calculated using the formula

$$d(j) = \left\| \mathrm{pos}(n_j) - \mathrm{pos}(n_{win}) \right\| \qquad (8.3.3)$$

where $\mathrm{pos}(.)$ is the position of the neuron in the lattice.

The city-block distance (L1 norm) or Euclidian distance (L2 norm) can be used as norm.

In general Lp norm of a vector Z is given formula

$$\|Z\|_p = (\sum_{i=1}^{N} |Z_i|^p)^{1/p}$$

8.3.4 Neighbourhood Function

- In its simplest form, a neighbourhood is rectengular (threshold neighbourhood)

$$N(j,t) = \begin{cases} 1 & d(j) \le D(t) \\ 0 & d(j) > D(t) \end{cases} \qquad (8.3.4)$$

  where $N(j,t)$ is used instead of $N(j)$ since $D(t)$ is a threshold value decreased via a cooling schedule as training progresses.

- For this neighbourhood function the distance is determined considering the distance in the lattice in each dimension, and the one having the maximum value is chosen as $d(j)$.

- For $L=2$, $N(j)$ corresponds to a square around n_{win} having side $\text{length}=2D(t)+1$.

8.3.4 Neighbourhood Function

- When threshold neghbourhood is used, the weights of all neurons within this square are updated with N(j)=1, while the others remaining unchanged.
- As the training progresses, this neighbourhood gets smaller and smaller, resulting in that only the neurons very close to the winner are updated towards the end of the training.
- The training ends as remains no more neuron in the neighbourhood.

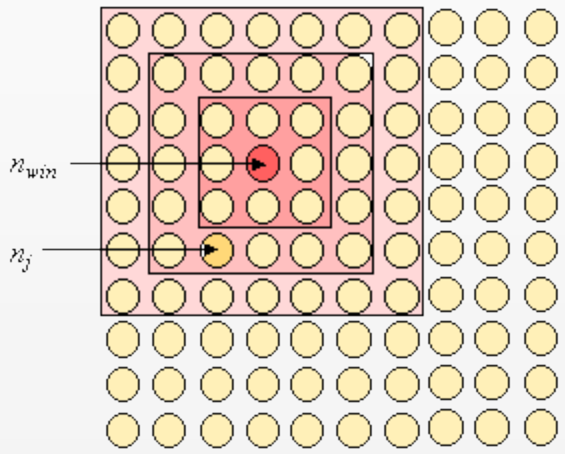


Figure 8.3. Threshold neighbourhood, narrowing as training progresses

8.3.4 Neighbourhood Function

- Usually, the neighbourhood function, N(*j*), is chosen as an L-dimensional Gausssian function:

$$N(j,t) = \exp\left(\frac{-d(j)^2}{2\sigma(t)^2}\right) \qquad (8.3.5)$$

where σ^2 is the variance parameter specifying the spread of the Gaussian function and it is decreasing as the training progresses as training progresses.

- Example of a 2-D Gaussian neighbourhood function is given in Figure 8.4.

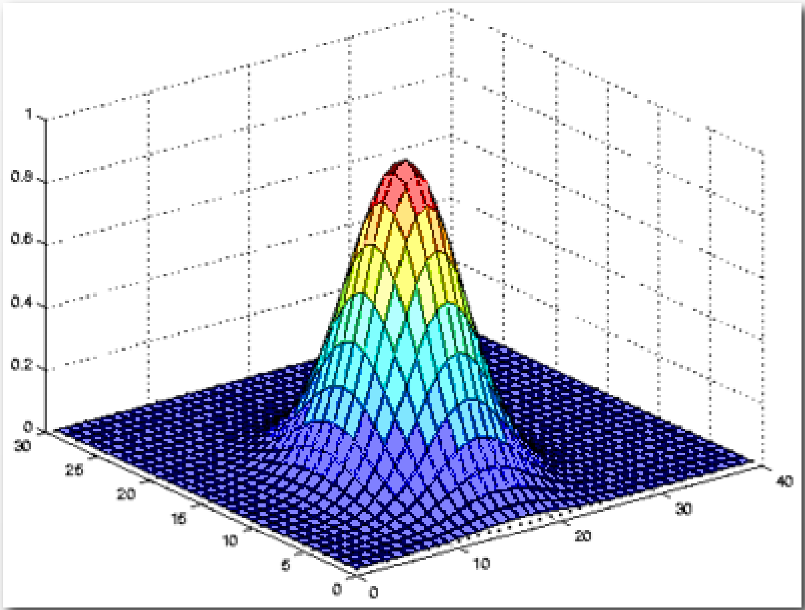


Figure 8.4. 2-D Gaussian neighbourhood function for a 40 ×30 neuronal lattice

8.3.5 Training SOFM

- There are two phases of operation in SOM: the training phase and the clustering phase.
- In the training phase, the network finds an output node such that the Euclidean distance between the current input vector and the weight set connecting the input units to this output unit is minimum.
- This node is called the winner and its weights and the weights of the neighboring output units of the winner are updated so that the new weight set is closer to the current input vector.
- The effect of update for each unit is proportional to a neighborhood function, which depends on the unit’s distance to the winner unit. This procedure is applied repeatedly for all input vectors until weights are stabilized. The choice of the neighborhood function, the learning rate, and the termination criteria are all problem dependent.
- The clustering phase is simple once the training phase is completed successfully. In this phase, after applying the input vector, only the winner unit is determined.

8.3.5 Training SOFM

1. Assign small random values to weights $\mathbf{w}_j = [\, w_{1j}, w_{2j}, \; .... w_{nj}];$

2.Choose a vector $\mathbf{u}^k$ from the training set and apply it as input;

3. Find the winning output node n_{win} by the following criterion:

$$n_{win} = \arg\min_j \left\| \mathbf{u} - \mathbf{w}^j \right\|$$

$\mathbf{w}_j$ is the weight vector connecting input nodes to the output node j;

4. Adjust the weight vectors according to the following update formula:

$$w_{ij}(t+1) = w_{ij}(t) + \eta(t)(\mathrm{u_i} - \mathrm{w_{ij}})N(j,t)$$

where w_{ij} is the i^{th} component of the weight vector $\mathbf{w}_j$, $\eta(t)$ is the learning rate and $N(j,t)$ is the neighborhood function;

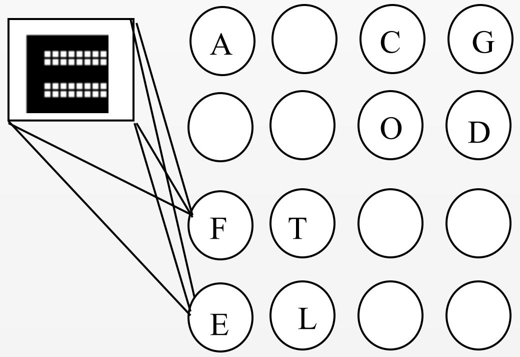
5. Repeat Steps 2 through 4 until no significant changes occur in the weights.

8.3.5 Training SOFM

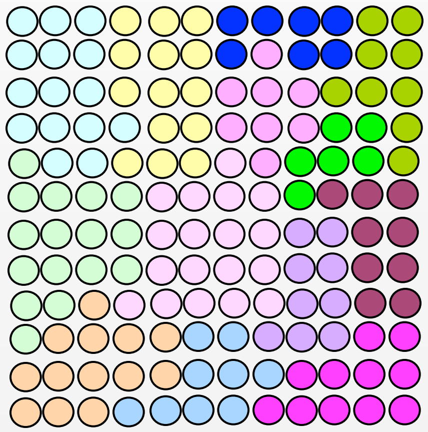
- The learning rate $\eta(t)$ is a decaying function of time; it is kept large at the beginning of the training and decreased gradually as learning proceeds.

- The neighborhood function $N(j,t)$ is a window centered on the winning unit n_{win} found in Step 3. Neighborhood function determines the degree that an output neuron j participates in training. This function is chosen such that the magnitude of weight change decays with increase in distance of the neuron to the winner. This distance is calculated using the topology defined on the output layer of the network. Neighborhood function is usually chosen as rectangular, 2-dimensional Gaussian or Mexican hat windows. Also, the diameter of the neighborhood function decreases in time.

8.3.5 Training SOFM: *effects of number of nodes in K. layer*



Small K: Similar clusters are mapped to neighbouring neurons, each neuron representing one or more clusters



Large K: Similar clusters are mapped to neighbouring neurons again, more than one neurons representing the same clusters

8.3.6 Setting parameters

- Feature map formation is critically dependent on the learning parameters, namely, the learning rate, η, and the spread of the neighbourhood function which is specified by the variance, σ^2 in the Gaussian case. In general, both parameters should be time-varying, but their values are selected experimentally.

- Usually, the trainin phase is seperated into two sub phases
  - Ordering phase
  - Convergence phase

8.3.6 Setting parameters

Usually, the trainin phase is seperated into two sub phases

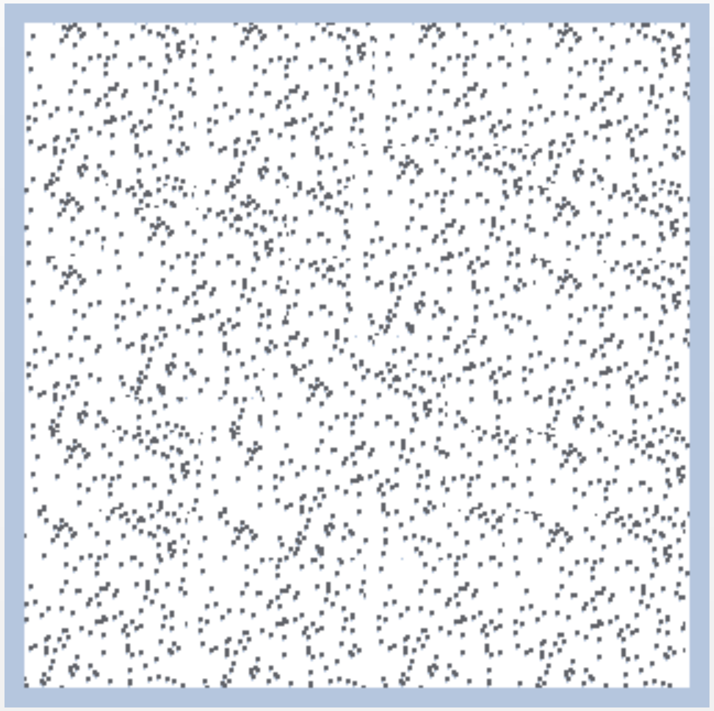
- Ordering phase (say, 1000 iterations):
  - The learning gain stay close to unity during this phase of the algorithm which can last for,
  - The spread of the neighbourhood function should initially include all neurons for any winning neuron and it should be slowly reduced to eventually include only the winner

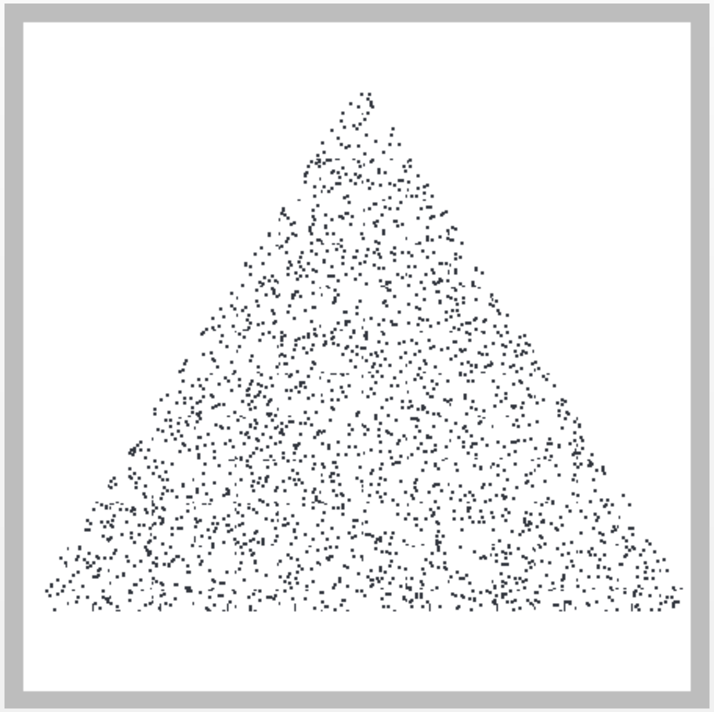
- Convergence phase (say, another 1000 iterations):
  - The learning gain initially should have the value assigned in the ordering phase and then it should be reduced slowly to reach the value of, say, 0.1.
  - The neighbourhood function should include only the winning neuron.

8.3.7 Topological mapping

- In SOFM the neurons are located on a discrete lattice.
- In training not only the winning neuron but also its neighbors on the lattice are allowed to learn.
- This is the reason why neighboring neurons gradually specialize to represent similar inputs, and the representations become ordered on the map lattice.
- As the training progresses, the winning unit and its neighbors adapt to represent the input even better by modifying their reference vectors towards the current input.
- This topological map also reflect the underlying distribution of the input vectors as it is illustraded in the figures 8.5 and 8.6.

8.3.7 Topological mapping





8.4. SOFM versus K-means clustrering

- Rigorous mathematical treatment of the SOFM algorithm has turned out to be extremely difficult in general (Kangas, 1994; and Kohonen, 1995). In the case of a discrete data set and a fixed neighborhood kernel, however, there exists an error function for the SOFM, [Kohonen, 1991, Ritter and Schulten, 1988] which is:

$$E = \sum_k \sum_{u^i \in C_k} \alpha_{c_k} \left\| \mathbf{u}^i - \mathbf{m}^k \right\|^2 \qquad (8.4.1)$$

- The weight update rule of the SOFM, corresponds to a gradient descent step in minimizing the above error function

8.4.1 Relation to K-means clustering.

Remember

$$E = (1/P)\sum_{i=1}^{P} \left\| \mathbf{u}^i - \mathbf{m}_{c(\mathbf{u}^i)} \right\|^2 \quad (8.2.1)$$

$$E = \sum_{k} \sum_{u^i \in C_k} \alpha_{c_k} \left\| \mathbf{u}^i - \mathbf{m}^k \right\|^2 \quad (8.4.1)$$

- The cost function of the SOFM, Equation (8.4.1), closely resembles Equation (8.2.1), which the K-means clustering algorithm tries to minimize. The difference is that in the SOFM the distance of each input from all of the reference vectors (instead of just the closest one) is taken into account, **weighted by the neighborhood kernel N.**

- Thus, the SOFM functions as a conventional clustering algorithm if the width of the neighborhood kernel is zero.