A Survey of Kernel Clustering Methods

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Outline

- Unsupervised Learning and Clustering
- Types of clustering algorithms
- Clustering Algorithms

Partitioning Methods
(in Euclidean Space)

- K-Means
- Self Organizing Maps(SOM)
- Neural Gas
- Fuzzy C-Means
- Probabilistic C-Means

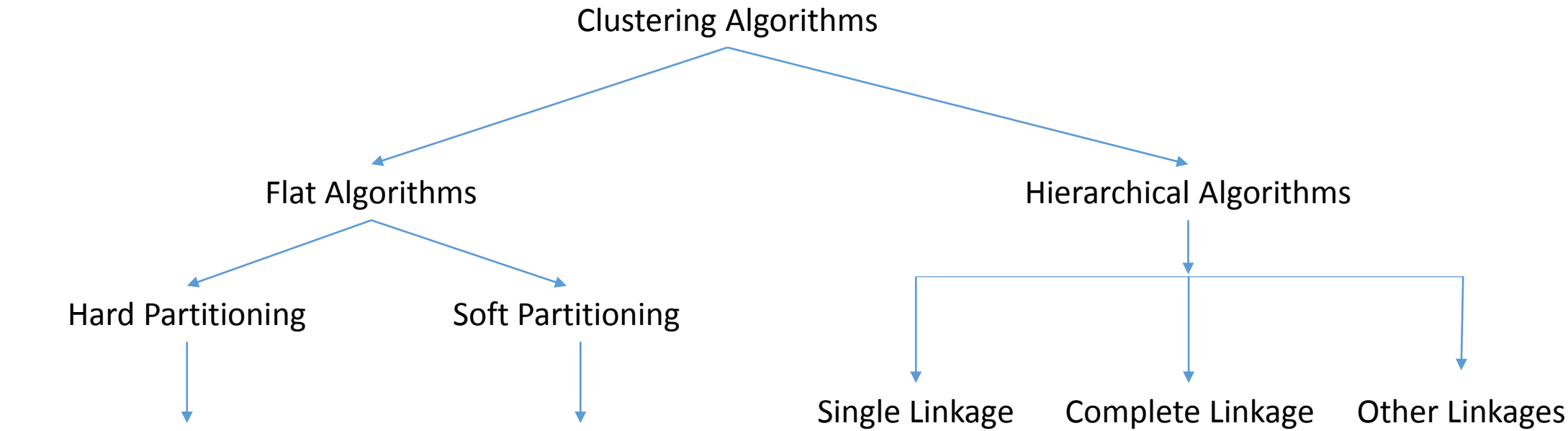
Kernel Clustering Methods

- Kernel K-Means
- Kernel SOM
- Kernel Neural Gas
- Kernel Fuzzy C-Means
- Kernel Probabilistic C-Means
- One class SVMs and Support Vector Clustering

Unsupervised Learning And Clustering

- Supervised learning - human effort involved
  - Example: Learning conditional distribution P(Y|X), X: features, Y: classes
- Unsupervised learning - no human effort involved
  - Example: learning distribution P(X), X: features
- Definition: **Clustering** is the task of grouping a set of objects in such that objects in the same group are more similar to each other than to those in other groups

Types of Clustering Algorithms



Examples:
- K-Means
- Self Organizing maps
- DBSCAN

Examples:
- Expectation Maximization
- Fuzzy Clustering Methods

K-means

- Objective: Minimize the empirical quantization error E(X)

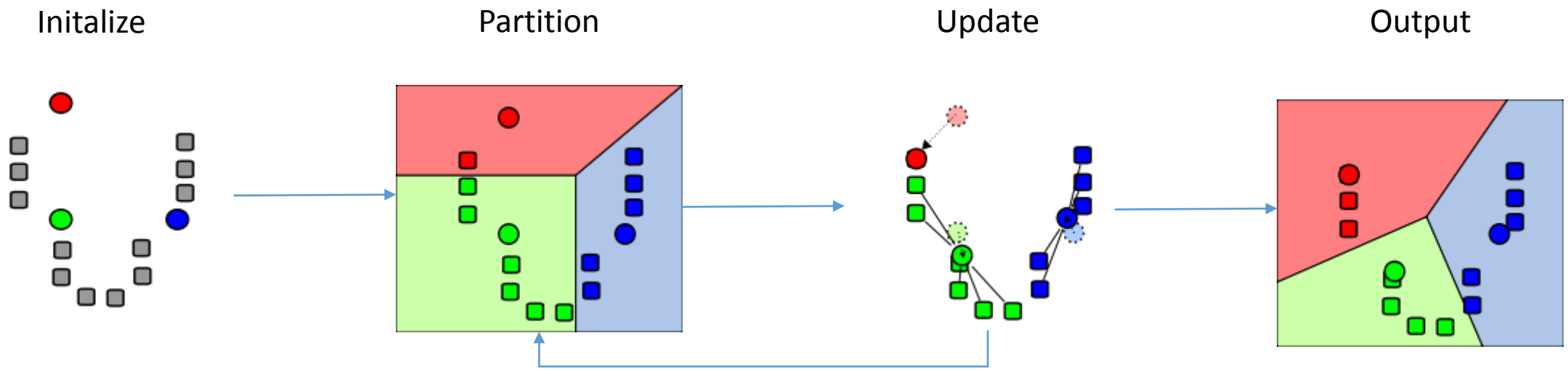
$$E(X) = \frac{1}{2n} \sum_{i=1}^{k} \sum_{\mathbf{x} \in \pi_i} \| \mathbf{x} - \mathbf{v}_i \|^2$$

- Algorithm:
    1. choose the number *k* of clusters;
    2. initialize the codebook *V* with vectors randomly picked from *X*;
    3. compute the Voronoi set *i* associated to the code vector $\mathbf{v}_i$;
    4. move each code vector to the mean of its Voronoi set

$$\mathbf{v}_i = \frac{1}{|\pi_i|} \sum_{\mathbf{x} \in \pi_i} \mathbf{x}$$

    5. return to step 3 if any code vector has changed otherwise
    6. return the codebook.

K-means Vizualization



Source: http://en.wikipedia.org/wiki/K-means_clustering

Kernel Clustering Basics

- Mercer Kernels:
  - Polynomial: $K^{(\mathrm{p})}(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i \cdot \mathbf{x}_j)^p, \quad p \in \mathbb{N}$
  - Gaussian: $K^{(\mathrm{g})}(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}\right), \quad \sigma \in \mathbb{R}$
- Distances in kernel space can be computed by using the distance kernel trick

$$\begin{aligned}
&\|\Phi(\mathbf{x}_i) - \Phi(\mathbf{x}_j)\|^2 \\
&= (\Phi(\mathbf{x}_i) - \Phi(\mathbf{x}_j)) \cdot (\Phi(\mathbf{x}_i) - \Phi(\mathbf{x}_j)) \\
&= \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_i) + \Phi(\mathbf{x}_j) \cdot \Phi(\mathbf{x}_j) - 2\Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j) \\
&= K(\mathbf{x}_i, \mathbf{x}_i) + K(\mathbf{x}_j, \mathbf{x}_j) - 2K(\mathbf{x}_i, \mathbf{x}_j)
\end{aligned}$$

- First map the data set *X,* into kernel space by computing the Gram Matrix, *K,* where each element k_{ij} is the dot product in kernel space.

$\Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_i)$ using $\|\Phi(\mathbf{x}_i) - \Phi(\mathbf{x}_j)\|^2 = k_{ii} + k_{jj} - 2k_{ij}$

Kernel K-means

- The Voronoi region and Voronoi Set in the feature space are redefined as: $R_i^{\Phi} = \{\mathbf{x}^{\Phi} \in \mathscr{F} | i = \arg\min_j \|\mathbf{x}^{\Phi} - \mathbf{v}_j^{\Phi}\|\}$ and $\pi_i^{\Phi} = \{\mathbf{x} \in X | i = \arg\min_j \|\Phi(\mathbf{x}) - \mathbf{v}_j^{\Phi}\|\}$

- Algorithm:
  1. Project the data set *X* into a feature space F, by means of a nonlinear mapping Φ
  2. Initialize the codebook $V^{\Phi} = (\mathbf{v}_1^{\Phi}, \ldots, \mathbf{v}_k^{\Phi})$ with $\mathbf{v}_i^{\Phi} \in \mathscr{F}$
  3. Compute for each center the set $\mathbf{v}_i^{\Phi}$ the set π_i^{Φ}
  4. Update the code vectors $\mathbf{v}_i^{\Phi}$ in $\mathscr{F}$ $\mathbf{v}_i^{\Phi} = \frac{1}{|\pi_i^{\Phi}|} \sum_{\mathbf{x} \in \pi_i^{\Phi}} \Phi(\mathbf{x})$
  5. Go to step 3 until any $\mathbf{v}_i^{\Phi}$ changes
  6. Return the feature space codebook.

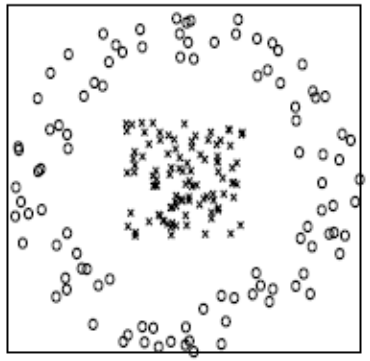
Kernel K-means Continued

- Since Φ is not explicitly known updating the code vectors is not straight forward
- Writing each centroid in Kernel space $\mathbf{v}_j^{\Phi} = \sum_{h=1}^{n} \gamma_{jh} \Phi(\mathbf{x}_h)$ where γ_{jh} is 1 if x_h belongs to the set *j,* zero otherwise.
- Now, $\|\Phi(\mathbf{x}_i) - \mathbf{v}_j^{\Phi}\|^2 = \left\| \Phi(\mathbf{x}_i) - \sum_{h=1}^{n} \gamma_{jh} \Phi(\mathbf{x}_h) \right\|^2$ can be expanded to:

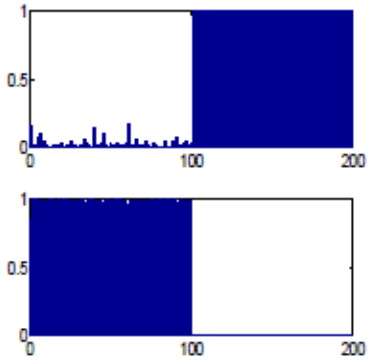
$$\left\| \Phi(\mathbf{x}_i) - \sum_{h=1}^{n} \gamma_{jh} \Phi(\mathbf{x}_h) \right\|^2 = k_{ii} - 2 \sum_{h} \gamma_{jh} k_{ih} + \sum_{r} \sum_{s} \gamma_{jr} \gamma_{js} k_{rs}$$

- Gram Matrix, ideally has a block diagonal structure if the clusters are uniformly dense and hence provide a good way to estimate the number of clusters too

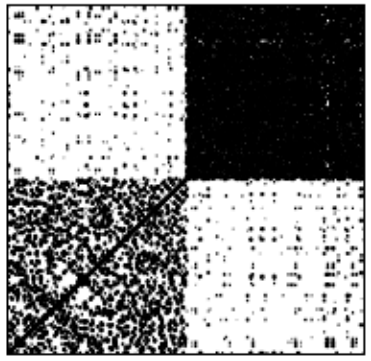
Kernel K-means Examples



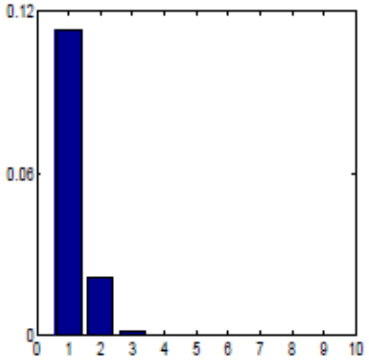
Input Data



Fuzzy Membership After Clustering

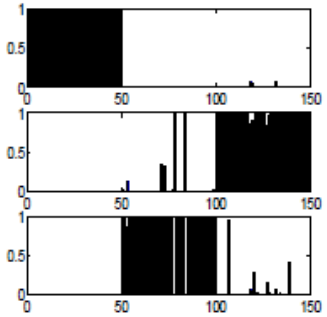


Gram Matrix After Reordering

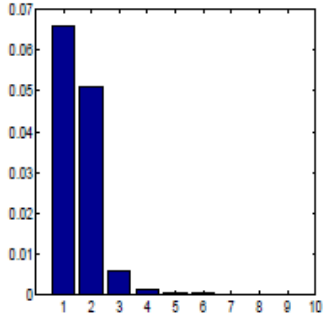


Eigenvalues of Gram Matrix

Iris Data



Performance



Eigenvalues of Gram Mat with RBF = 0.5 showing three major clusters

M. Girolami, Mercer kernel based clustering in feature space, IEEE Trans. Neural Networks 13 (3) (2002) 780–784.

Self Organizing Map(SOM)

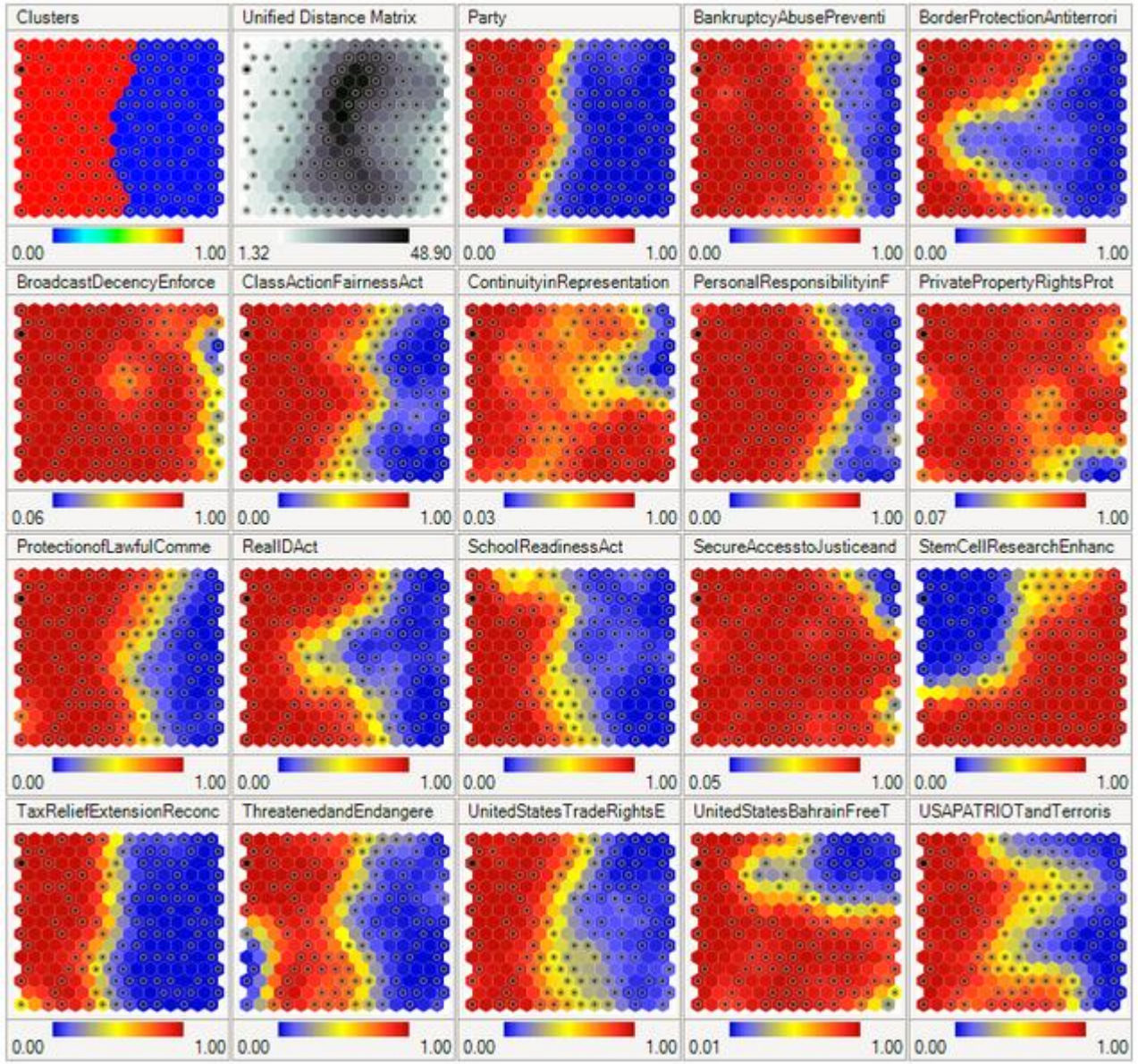
- Code vectors organized on a grid and their adaptation is propagated along the grid
- Some popular metrics for the map include the Manhattan distance where the distance between two elements **r** = (r_1, r_2) and **s** = (s_1, s_2) is:

$$d_{rs} = |r_1 - s_1| + |r_2 - s_2|$$

- Algorithm
  1. Initialize the codebook *V* randomly picking from *X*
  2. Initialize the set *C* of connections to form the rectangular grid of dimension $n_1 \times n_2$
  3. Initialize $t = 0$
  4. Randomly pick an input **x** from *X*.
  5. Determine the winner: $\mathbf{s}(\mathbf{x}) = \arg \min_{\mathbf{v}_j \in V} \|\mathbf{x} - \mathbf{v}_j\|$
  6. Adapt each code vector: $\Delta \mathbf{v}_j = \varepsilon(t) h(d_{rs})(\mathbf{x} - \mathbf{v}_j)$ $h(d_{rs}) = \exp\left(-\frac{d_{rs}^2}{2\sigma^2(t)}\right)$ $\sigma(t) = \sigma_i \left(\frac{\sigma_f}{\sigma_i}\right)^{t/t_{max}}$
  7. Increment *t*
  8. If $t < t_{max}$ go to step 4

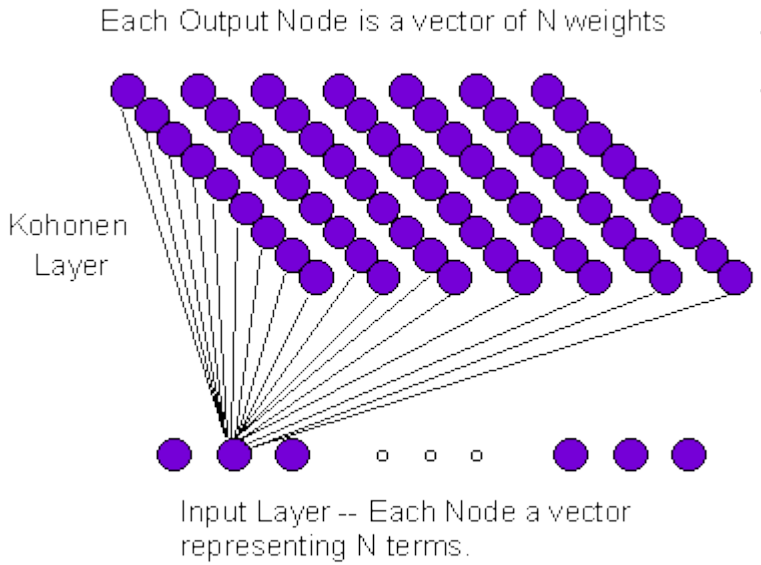
$$\varepsilon(t) = \varepsilon_i \left(\frac{\varepsilon_f}{\varepsilon_i}\right)^{t/t_{max}}$$

SOM Example



A SOM showing U.S. Congress voting patterns. The data were initially distributed randomly on a 2D grid and then clustered. The grey dots show the neurons. The first box shows clustering and, the second distances. The third is a panel shows the party affiliation, red-republican and blue-democrat and the rest are the features, which, in this instance are yes(blue) or no(red) votes.

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



Schematic of A Self Organizing Map

Source: http://cs.oswego.edu/~dschlege/sitev2/courses/468/Cog468%20ASOM%20Presentation.htm

Kernel SOM

- Again the algorithm is adapted by first mapping the points to kernel space.
- The code vectors are defined as: $\mathbf{v}_j^{\Phi} = \sum_{h=1}^{n} \gamma_{jh} \Phi(\mathbf{x}_h)$ (1)
- The winner is computed with:

$$\mathbf{s}(\Phi(\mathbf{x}_i)) = \arg \min_{\mathbf{v}_j^{\Phi} \in V} \|\Phi(\mathbf{x}_i) - \mathbf{v}_j^{\Phi}\| \quad \text{or}$$

$$\mathbf{s}(\Phi(\mathbf{x}_i)) = \arg \min_{\mathbf{v}_j^{\Phi} \in V} \left(k_{ii} - 2 \sum_h \gamma_{jh} k_{ih} \sum_r \sum_s \gamma_{jr} \gamma_{js} k_{rs} \right)$$

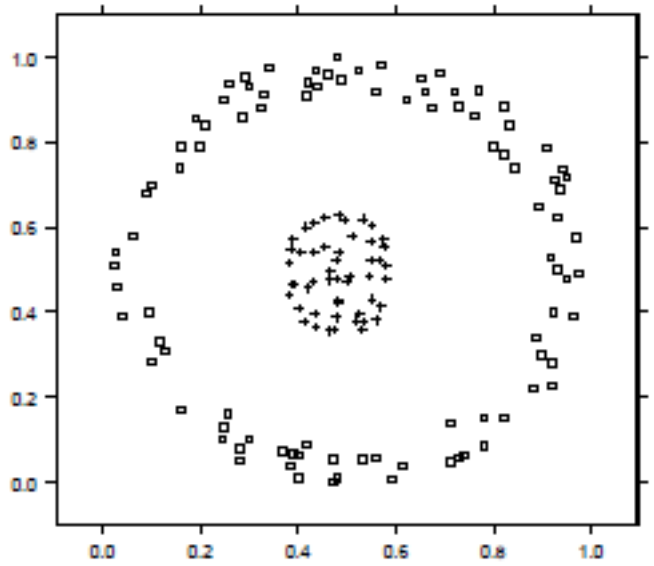
- The update rules are:

$$\mathbf{v}_j^{\Phi\prime} = \mathbf{v}_j^{\Phi} + \varepsilon(t) h(d_{rs}) (\Phi(\mathbf{x}) - \mathbf{v}_j^{\Phi})$$

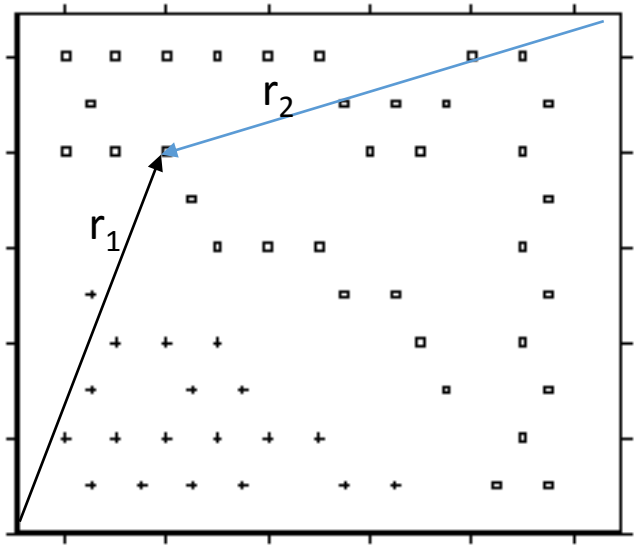
Using (1) we get $\sum_{h=1}^{n} \gamma'_{jh} \Phi(\mathbf{x}_h) = \sum_{h=1}^{n} \gamma_{jh} \Phi(\mathbf{x}_h) + \varepsilon(t) h(d_{rs}) \times \left(\Phi(\mathbf{x}) - \sum_{h=1}^{n} \gamma_{jh} \Phi(\mathbf{x}_h) \right)$

$$\gamma'_{jh} = \begin{cases} (1 - \varepsilon(t) h(d_{rs})) \gamma_{jh} & \text{if } i \neq j, \\ (1 - \varepsilon(t) h(d_{rs})) \gamma_{jh} + \varepsilon(t) h(d_{rs}) & \text{otherwise.} \end{cases}$$

Kernel SOM Example



Input data clustered by Kernel SOM on the right



r_1 - Distance from Neuron 1 in Hilbert Space

r_2 - Distance from Neuron 2 in Hilbert Space

Data clustered by Kernel SOM, using an RBF of 0.1 and 2 clusters

D. Macdonald, C. Fyfe, The kernel self-organising map, in: Fourth International Conference on Knowledge-Based Intelligent Engineering Systems and Allied Technologies 2000, vol. 1, 2000, pp. 317–320.

Neural Gas and Kernel Neural Gas

- Similar to SOM the major difference being a soft adaptation rule in which all neurons are adapted to each individual input.

$$\Delta \mathbf{v}_j = \varepsilon(t) h_\lambda(\rho_j)(\mathbf{x} - \mathbf{v}_j), \varepsilon(t) \in [0, 1] \quad h_\lambda(\rho_j) = \exp(-\rho_j / \lambda)$$

- ρ_j is the rank of closeness of the current code vector *j*, to the input *x*
- λ is the characteristic decay
- For the kernelized version the update rule is:

$$\Delta \mathbf{v}_j^{\Phi} = \varepsilon h_\lambda(\rho_j)(\Phi(\mathbf{x}) - \mathbf{v}_j^{\Phi})$$

Fuzzy C-Means

- Starts by defining a membership matrix, A_{cn} denotes vector space of c x n real matrices; $M_{fc} = \left\{ U \in A_{cn} \;\middle|\; u_{ih} \in [0, 1]\ \forall i, h; \sum_{i=1}^{c} u_{ih} = 1\ \forall h; \quad 0 < \sum_{h=1}^{n} u_{ih} < n\ \forall i \right\}$
- Minimizes functional:

$$J(U, V) = \sum_{h=1}^{n} \sum_{i=1}^{c} (u_{ih})^m \|\mathbf{x}_h - \mathbf{v}_i\|^2$$ with the constraint $$\sum_{i=1}^{c} u_{ih} = 1 \quad \forall i = 1, \ldots, n$$

- *m* controls the fuzziness of the memberships and is usually set close to 2, if *m* tends to 1, the solution tends to the k-means solution
- Lagrangian of the objective is $L_h = \sum_{i=1}^{c} (u_{ih})^m \|\mathbf{x}_h - \mathbf{v}_i\|^2 + \alpha_h \left(\sum_{i=1}^{c} u_{ih} - 1 \right)$
- Taking the derivative with respect to u_{ih} and v_i and setting them to zero yields the iteration scheme: $u_{ih}^{-1} = \sum_{j=1}^{c} \left(\frac{\|\mathbf{x}_h - \mathbf{v}_i\|}{\|\mathbf{x}_h - \mathbf{v}_j\|} \right)^{2/(m-1)}$, $\mathbf{v}_i = \frac{\sum_{h=1}^{n} (u_{ih})^m \mathbf{x}_h}{\sum_{h=1}^{n} (u_{ih})^m}$

Kernel Fuzzy C-Means

- The objective in the kernel space is:

$$J^{\Phi}(U, V) = \sum_{h=1}^{n} \sum_{i=1}^{c} (u_{ih})^m \|\Phi(\mathbf{x}_h) - \Phi(\mathbf{v}_i)\|^2$$

- In case of the Gaussian Kernel the derivative is:

$$\frac{\partial K(\mathbf{x}_h, \mathbf{v}_i)}{\partial \mathbf{v}_i} = \frac{(\mathbf{x}_h - \mathbf{v}_i)}{\sigma^2} K(\mathbf{x}_h, \mathbf{v}_i)$$

- This yields the iteration scheme:

$$u_{ih}^{-1} = \sum_{j=1}^{c} \left(\frac{1 - K(\mathbf{x}_h, \mathbf{v}_i)}{1 - K(\mathbf{x}_h, \mathbf{v}_j)} \right)^{1/(m-1)}, \quad \mathbf{v}_i = \frac{\sum_{h=1}^{n} (u_{ih})^m K(x_h, v_i) \mathbf{x}_h}{\sum_{h=1}^{n} (u_{ih})^m K(x_h, v_i)}$$

Possibilistic C-Means

- Here, the class membership of a data point can be high for more than one class
- Objective that is minimized is:

$$J(U, V) = \sum_{h=1}^{n} \sum_{i=1}^{c} (u_{ih})^m \|\mathbf{x}_h - \mathbf{v}_i\|^2 + \sum_{i=1}^{c} \eta_i \sum_{h=1}^{n} (1 - u_{ih})^m$$

- The iteration scheme is:

$$u_{ih} = \left[1 + \left(\frac{\|\mathbf{x}_h - \mathbf{v}_i\|^2}{\eta_i} \right)^{1/(m-1)} \right]^{-1}, \quad \mathbf{v}_i = \frac{\sum_{h=1}^{n} (u_{ih})^m \mathbf{x}_h}{\sum_{h=1}^{n} (u_{ih})^m}$$

- For the parameter η_i the authors suggest using:

$$\eta_i = \gamma \frac{\sum_{h=1}^{n} (u_{ih})^m \|\mathbf{x}_h - \mathbf{v}_i\|^2}{\sum_{h=1}^{n} (u_{ih})^m}$$

Kernel Possibilistic C-Means

- Kernelization of the metric in the objective yields:

$$J^{\Phi}(U,V)=\sum_{h=1}^{n}\sum_{i=1}^{c}(u_{ih})^{m}\|\Phi(\mathbf{x}_h)-\Phi(\mathbf{v}_i)\|^2+\sum_{i=1}^{c}\eta_i\sum_{h=1}^{n}(1-u_{ih})^{m}$$

- Minimization yields the iteration scheme:

$$u_{ih}^{-1}=1+\left(\frac{\|\Phi(\mathbf{x}_h)-\Phi(\mathbf{v}_i)\|^2}{\eta_i}\right)^{1/(m-1)}$$

$$\mathbf{v}_i=\frac{\sum_{h=1}^{n}(u_{ih})^{m}K(x_h,v_i)\mathbf{x}_h}{\sum_{h=1}^{n}(u_{ih})^{m}K(x_h,v_i)}$$

- For the Gaussian Kernel: $u_{ih}^{-1}=1+2\left(\frac{1-K(\mathbf{x}_h,\mathbf{v}_i)}{\eta_i}\right)^{1/(m-1)}$

One Class Support Vector Machines

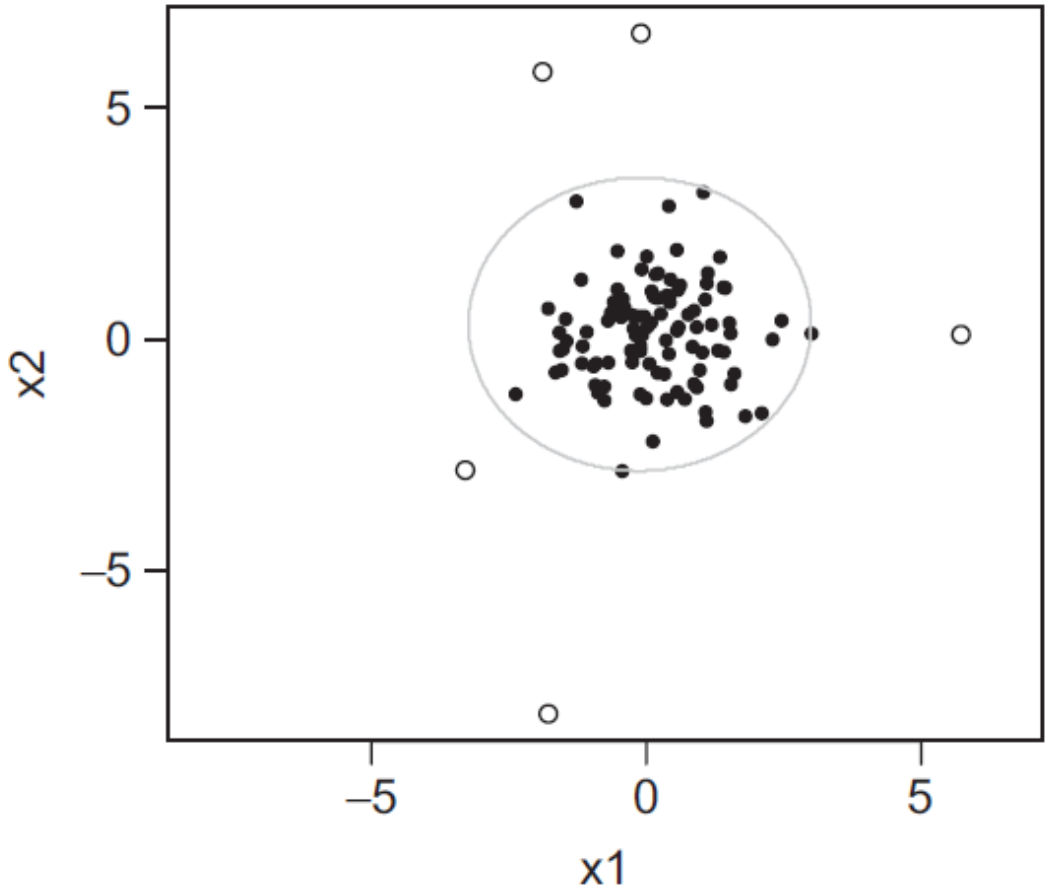
- The idea is to find the smallest enclosing sphere in kernel space of radius *R* centered at *v*: $\|\Phi(\mathbf{x}_j) - \mathbf{v}\|^2 \leqslant R^2 + \xi_j \quad \forall j$,$\xi_i \geq 0$, are the slack variables
- The Lagrangian for the above is:

  $L = R^2 - \sum_j (R^2 + \xi_j - \|\Phi(\mathbf{x}_j) - \mathbf{v}\|^2)\beta_j - \sum_j \xi_j \mu_j + C \sum_j \xi_j$,$\beta_i \geq 0$ and $\mu_i \geq 0$ are Lagrange multipliers, $C \sum_j \xi_j$ is the penalty term with *C* -user defined const.
- Taking the derivative wrt $\xi_j, R,$ v and the KKT complementarity conditions yield the following QP: $\sum_j \beta_j = 1, \quad \mathbf{v} = \sum_j \beta_j \Phi(\mathbf{x}_j), \quad \beta_j = C - \mu_j$

$$\xi_j \mu_j = 0, \quad (R^2 + \xi_j - \|\Phi(\mathbf{x}_j) - \mathbf{v}\|^2)\beta_j = 0$$

- $\xi_i > 0$, for outliers and $\xi_i = 0, 0 < \beta_i < C$ for the support vectors

Example of one class SVMs



One class SVM with a linear kernel applied to a data set with outliers. The gray line shows the projection in input space of the smallest enclosing sphere in feature space

Extension of one class SVMs to Clustering

- Similar to Kernel SVM but here the SVMs are applied to partition the space.
- The Voronoi regions are now spheres:

$$\pi_i^{\Phi}(\rho) = \{\mathbf{x}_j \in \pi_i^{\Phi} \text{ and } \|\Phi(\mathbf{x}_j) - \mathbf{v}_i^{\Phi}\| < \rho\}$$

- Algorithm:
  1. Project the data set *X* into a feature space $\mathcal{F}$, by means of a nonlinear mapping Φ
  2. Initialize the codebook $V^{\Phi} = (\mathbf{v}_1^{\Phi}, \ldots, \mathbf{v}_k^{\Phi})$ with $\mathbf{v}_i^{\Phi} \in \mathcal{F}$
  3. Compute $\pi_i^{\Phi}(\rho)$ for each center $\mathbf{v}_i^{\Phi}$
  4. Apply One Class SVM to each $\pi_i^{\Phi}(\rho)$ and assign the center obtained to $\mathbf{v}_i^{\Phi}$
  5. Go to step 2 until any $\mathbf{v}_i^{\Phi}$ changes.
  6. Return the feature space codebook.