kNN, LVQ, SOM

- Instance Based Learning
- K-Nearest Neighbor Algorithm

- (LVQ) Learning Vector Quantization
- (SOM) Self Organizing Maps

Instance based learning

- Approximating real valued or discrete-valued target functions
- Learning in this algorithm consists of storing the presented training data
- When a new query instance is encountered, a set of similar related instances is retrieved from memory and used to classify the new query instance

- Construct only local approximation to the target function that applies in the neighborhood of the new query instance
- Never construct an approximation designed to perform well over the entire instance space
- Instance-based methods can use vector or symbolic representation
- Appropriate definition of „neighboring“ instances

- Disadvantage of instance-based methods is that the costs of classifying new instances can be high
- Nearly all computation takes place at classification time rather than learning time

K-Nearest Neighbor algorithm

- Most basic instance-based method
- Data are represented in a vector space
- Supervised learning

Feature space

- $\left\{ < \vec{x}^{(1)}, f(\vec{x}^{(1)}) >, < \vec{x}^{(2)} f(\vec{x}^{(2)}) >, \ldots, < \vec{x}^{(n)}, f(\vec{x}^{(n)}) > \right\}$

$$\vec{x} = \begin{cases} x_1 \\ x_2 \\ .. \\ .. \\ x_d \end{cases} \in \Re^d \qquad \|\vec{x} - \vec{y}\| = \sqrt{\sum_{i=1}^{d} (x_i - y_i)^2}$$

- In nearest-neighbor learning the target function may be either discrete-valued or real valued
- Learning a discrete valued function
- $f : \Re^d \to V$, *V* is the finite set *{v_1,......,v_n}*
- For discrete-valued, the *k*-NN returns the most common value among the k training examples nearest to *x_q*.

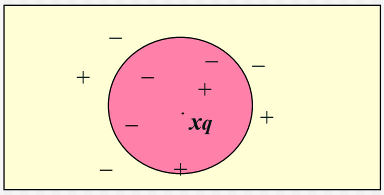
- Training algorithm
  - For each training example <*x,f(x)*> add the example to the list
- Classification algorithm
  - Given a query instance x_q to be classified
    - Let $x_1,..,x_k$ k instances which are nearest to x_q

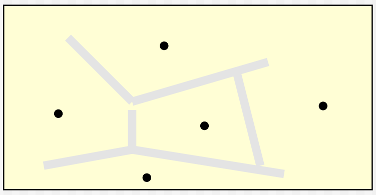
$$\hat{f}(x_q) \leftarrow \underset{v \in V}{\arg\max} \sum_{i=1}^{k} \delta(v, f(x_i))$$

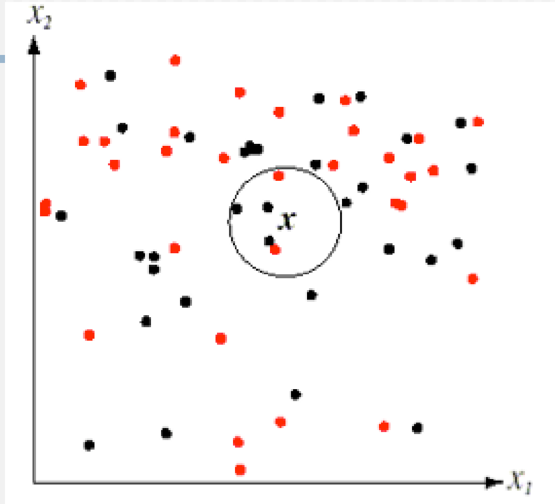
    - Where $\delta(a,b)=1$ if $a=b$, else $\delta(a,b)=0$ (Kronecker function)

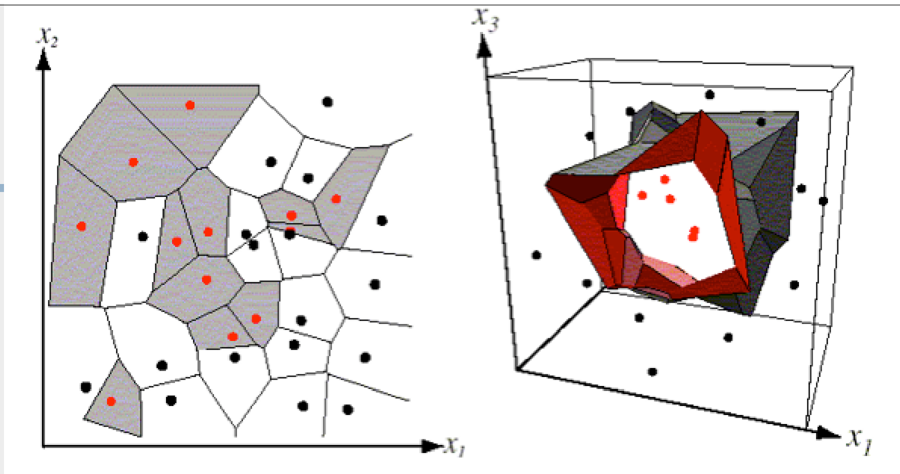
Definition of Voronoi diagram

- the decision surface induced by 1-NN for a typical set of training examples.







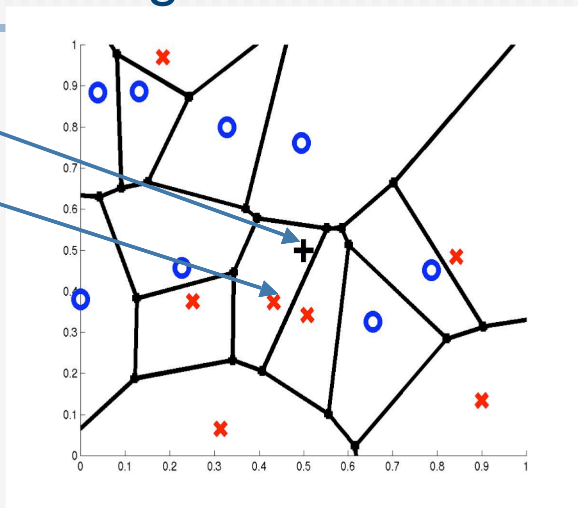


- kNN rule leeds to partition of the space into cells (Vornoi cells) enclosing the training points labelled as belonging to the same class
- The decision boundary in a Vornoi tessellation of the feature space resembles the surface of a crystall

1-Nearest Neighbor

query point q_f

nearest neighbor q_i

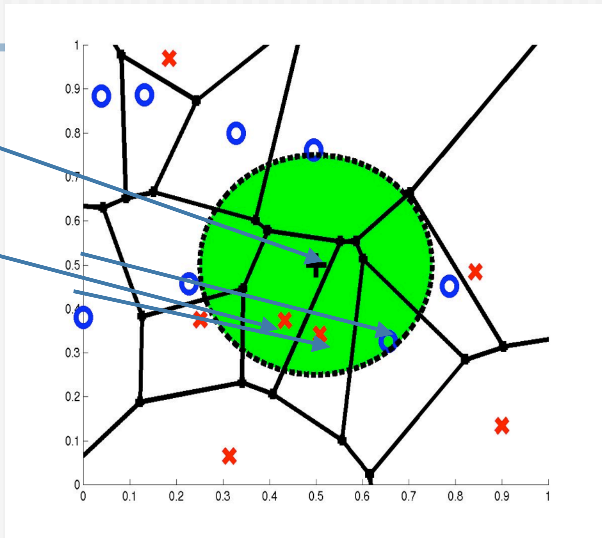


3-Nearest Neighbors

query point q_f

3 nearest neighbors

2x,1o

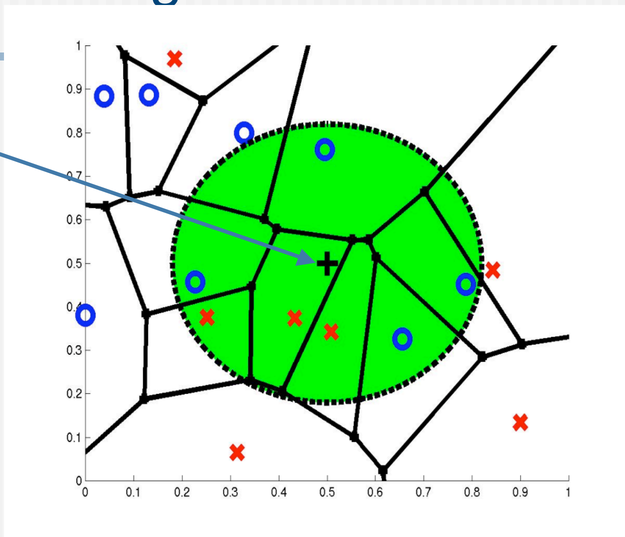


7-Nearest Neighbors

query point q_f

7 nearest neighbors

3x,4o



How to determine the good value for k?

- Determined experimentally
- Start with k=1 and use a test set to validate the error rate of the classifier
- Repeat with k=k+2
- Choose the value of k for which the error rate is minimum

- Note: k should be odd number to avoid ties

Continous-valued target functions

- kNN approximating continous-valued target functions
- Calculate the mean value of the *k* nearest training examples rather than calculate their most common value

$$f : \Re^d \rightarrow \Re \qquad \hat{f}(x_q) \leftarrow \frac{\sum_{i=1}^{k} f(x_i)}{k}$$

Distance Weighted

- Refinement to kNN is to weight the contribution of each *k* neighbor according to the distance to the query point x_q
  - Greater weight to closer neighbors
  - For discrete target functions

$$\hat{f}(x_q) \leftarrow \underset{v \in V}{\arg\max} \sum_{i=1}^{k} w_i \delta(v, f(x_i))$$

$$w_i = \begin{cases} \dfrac{1}{d(x_q, x_i)^2} & if \quad x_q \neq x_i \\ 1 & else \end{cases}$$

Distance Weighted

- For real valued functions

$$\hat{f}(x_q) \leftarrow \frac{\sum_{i=1}^{k} w_i f(x_i)}{\sum_{i=1}^{k} w_i}$$

$$w_i = \begin{cases} \frac{1}{d(x_q, x_i)^2} & if \quad x_q \neq x_i \\ 1 & else \end{cases}$$

Curse of Dimensionality

- Imagine instances described by 20 features (attributes) but only 3 are relevant to target function
- Curse of dimensionality: nearest neighbor is easily misled when instance space is high-dimensional
- Dominated by large number of irrelevant features

Possible solutions

- Stretch j-th axis by weight z_j, where $z_1,\ldots,z_n$ chosen to minimize prediction error (weight different features differently)
- Use cross-validation to automatically choose weights $z_1,\ldots,z_n$
- Note setting z_j to zero eliminates this dimension alltogether (feature subset selection)
- PCA

When to Consider Nearest Neighbors

- Instances map to points in R^d
- Less than 20 features (attributes) per instance, typically normalized
- Lots of training data

Advantages:

- Training is very fast
- Learn complex target functions
- Do not loose information

Disadvantages:

- Slow at query time
  - Presorting and indexing training samples into search trees reduces time
- Easily fooled by irrelevant features (attributes)

LVQ (Learning Vector Quantization)

- A nearest neighbor method, because the smallest distance of the unknown vector from a set of reference vectors is sought
- However not all examples are stored as in kNN, but a a **fixed number** of reference vectors for each class *v* (for discrete function *f*) $\{v_1,......,v_n\}$
- The value of the reference vectors is optimized during learning process

- The supervised learning
  - rewards correct classification
  - puished incorrect classification

- $0 < \alpha(t) < 1$ is a monotonically decreasing scalar function

LVQ Learning (Supervised)

Initialization of reference vectors ***m***; t=0;
do
{
chose $\boldsymbol{x}_i$ from the dataset
$\boldsymbol{m}_c$ nearest reference vector according to d_2
if classified correctly, the class ***v*** of $\boldsymbol{m}_c$ is equal to class of ***v*** of $\boldsymbol{x}_i$

$$m_c(t+1) = m_c(t) + \alpha(t)[x_i(t) - m_c(t)]$$

if classified incorrectly, the class ***v*** of $\boldsymbol{m}_c$ is different to class of ***v*** of $\boldsymbol{x}_i$

$$m_c(t+1) = m_c(t) - \alpha(t)[x_i(t) - m_c(t)]$$

t++;
}
until number of iterations *t max_iterations*

- After learning the space $\mathbf{R}^d$ is partitioned by a Vornoi tessalation corresponding to $\boldsymbol{m}_i$
- The exist extension to the basic LVQ, called LVQ2, LVQ3

LVQ Classification

- Given a query instance $\boldsymbol{x}_q$ to be classified
- Let $\boldsymbol{x}_{answer}$ be the reference vector which is nearest to $\boldsymbol{x}_q$, determine the corresponding $\boldsymbol{v}_{answer}$

Kohonen Self Organizing Maps

- Unsupervised learning
- Labeling, supervised

- Perform a topologically ordered mapping from high dimensional space onto two-dimensional space
- The centroids (units) are arranged in a layer (two dimensional space), units physically near each other in a two-dimensional space respond to similar input

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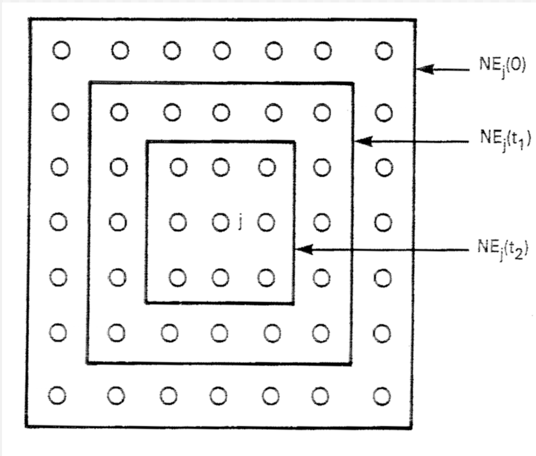
- $0 < \alpha(t) < 1$ is a monotonically decreasing scalar function
- *NE(t)* is a neighborhood function is decreasing with time *t*
- The topology of the map is defined by *NE(t)*
  - The dimension of the map is smaller (equal) then the dimension of the data space
  - Usually the dimension of a map is two
- For tow dimensional map the number of the centroids should have a integer valued square root
  - a good value to start is around 10^2 centroids

Neighborhood on the map



SOM Learning (Unsupervised)

Initialization of center vectors ***m***; t=0;
do
{
chose $\boldsymbol{x}_i$ from the dataset
$\boldsymbol{m}_c$ nearest reference vector according to d_2
For all $\boldsymbol{m}_r$ near $\boldsymbol{m}_c$ on the map

$$m_r(t+1) = m_r(t) + \alpha(t)[x_i(t) - m_r(t)] \qquad for \qquad r \in NE_C(t)$$

t++;
}
until number of iterations *t max_iterations*

Supervised labeling

- The network can be labeled in two ways
- (A) For each known class represented by a vector the closest centroid is searched and labeled accordingly
- (B) For every centroid is is tested to which known class represented by a vector it is closest

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- Example of labeling of 10 classes, 0,..,9
- 10*10 centroids
- 2-dim map

(A)

#	0	#	#	2	#	#	#	#
#	#	#	#	#	#	#	#	8
#	#	#	#	#	#	#	#	#
#	4	#	#	#	#	3	#	#
#	#	#	#	#	#	#	#	#
1	#	#	#	#	#	#	#	#
#	#	#	#	#	#	#	#	6
#	#	#	#	#	#	#	#	#
5	#	#	#	9	#	#	7	#

(B)

0	0	0	2	2	2	8	8	8
0	0	4	2	2	2	8	8	8
4	4	4	4	2	3	8	8	8
4	4	4	4	3	3	3	3	8
4	4	4	4	3	3	3	6	6
1	1	4	4	3	3	3	6	6
1	1	5	9	9	9	6	6	6
5	5	5	9	9	9	7	7	7
5	5	5	9	9	9	7	7	7

Animal example

Table 3.4. Animal names and their attributes

		dove	hen	duck	goose	owl	hawk	eagle	fox	dog	wolf	cat	tiger	lion	horse	zebra	cow
is	small	1	1	1	1	1	1	0	0	0	0	1	0	0	0	0	0
	medium	0	0	0	0	0	0	1	1	1	1	0	0	0	0	0	0
	big	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1
has	2 legs	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0
	4 legs	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1
	hair	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1
	hooves	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1
	mane	0	0	0	0	0	0	0	0	0	1	0	0	1	1	1	0
	feathers	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0
likes to	hunt	0	0	0	0	1	1	1	1	0	1	1	1	1	0	0	0
	run	0	0	0	0	0	0	0	0	1	1	0	1	1	1	1	0
	fly	1	0	1	1	1	1	1	0	0	0	0	0	0	0	0	0
	swim	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0

"birds" occupy the left part of the lattice, "hunters" such as "tiger", "lion" and "cat" are clustered toward the right, and more "peaceful" species such as "zebra", "horse" and "cow" are situated in the upper middle. Within each cluster, a further grouping according to similarity is discernible.

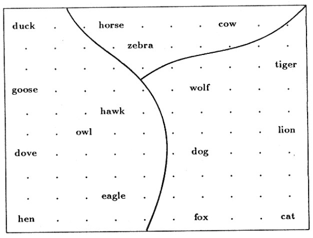
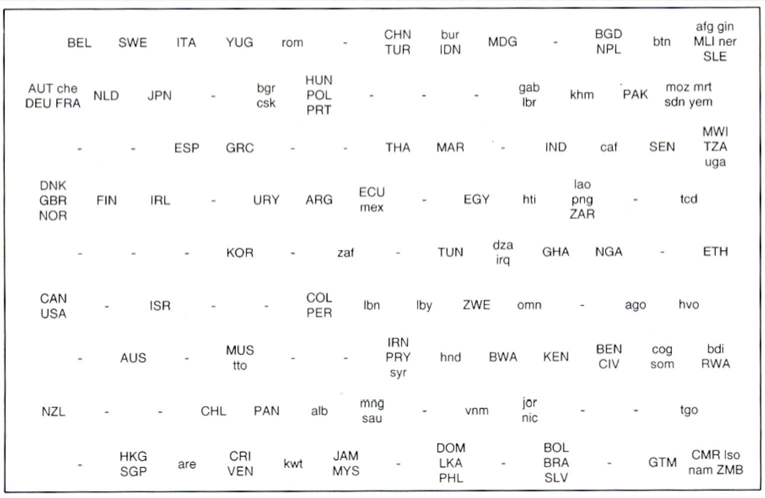


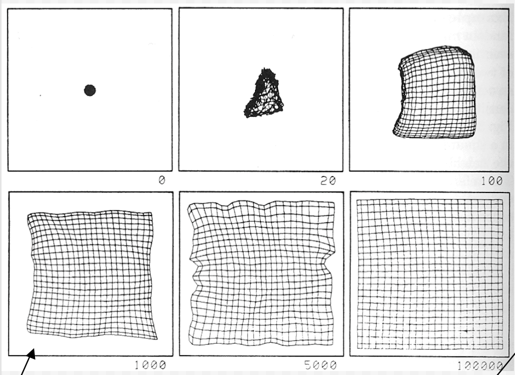
Fig. 3.22. After the network had been trained with inputs describing attribute sets from Table 3.4, the map was calibrated by the columns of Table 3.4 and labeled correspondingly. A grouping according to similarity has emerged

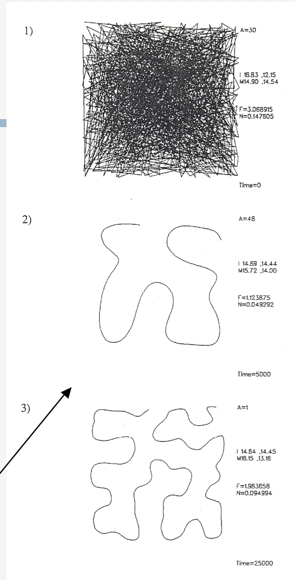
Poverty map of countries



Ordering process of 2 dim data

random 2 dim points





2-dim map

1-dim map

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- K-Nearest Neighbor Algorithm

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- Bayes Classification
- Naive Bayes