BABEŞ-BOLYAI UNIVERSITY
Faculty of Computer Science and Mathematics

ARTIFICIAL INTELLIGENCE

Intelligent systems

Machine learning

Support Vector Machines

K-means

Useful information

- Chapter 15 of *C. Groşan, A. Abraham, Intelligent Systems: A Modern Approach, Springer, 2011*

- Chapter 9 of *T. M. Mitchell, Machine Learning, McGraw-Hill Science, 1997*

- Documents from *svm* folder

Intelligent systems – Machine Learning

- Typology
  - Experience criteria:
    - Supervised learning
    - Unsupervised learning
    - Active learning
    - Reinforcement learning
  - Algorithm criteria
    - Decision trees
    - Artificial Neural Networks
    - Evolutionary Algorithms
    - **Support Vector Machines**
    - Hidden Markov Models
    - K-means

Intelligent Systems – Support Vector Machines

- Support Vector Machines (SVMs)
  - Definition
  - Solved problems
  - Advantages
  - Difficulties
  - Tools

Intelligent Systems – Support Vector Machines

- Definition
  - Developed by Vapnik in 1970
  - Popularised after 1992
  - Linear classifiers that identify the hyper-plane that separates the positive and negative classes
  - Have a theoretical foundation
  - Work very well for large data (text mining, image analysis)

  - **Remember**
    - Supervised learning problem – a data set:
      - (x^d, t^d), with:
      - $x^d \in \mathbf{R}^m \rightarrow x^d=(x^d_1, x^d_2, \ldots, x^d_m)$
      - $t^d \in \mathbf{R} \rightarrow t^d \in \{1, -1\}$, 1 $\rightarrow$ positive class, -1 $\rightarrow$ negative class
      - where $d = 1,2,\ldots,n,n+1,n+2,\ldots,N$
    - First n data (x^d and t^d are known) are used as training data
    - Last N-n data (x^d is known, t^d is unknown) are used as testing data

Intelligent Systems – Support Vector Machines

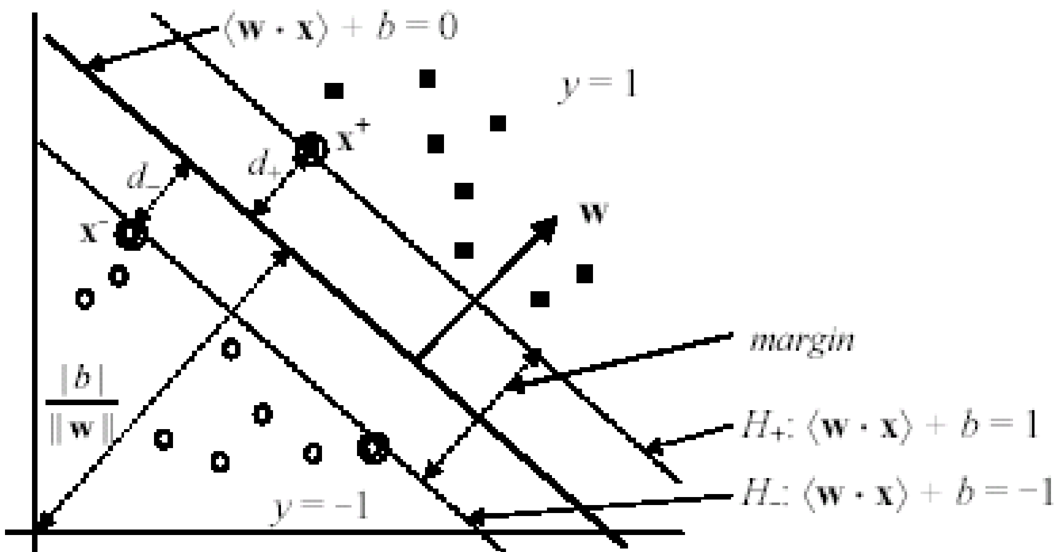
- Definition
  - SVM finds a linear function *f*(**x**) = ⟨**w** · **x**⟩ + *b*, (**w** –weight vector) such as

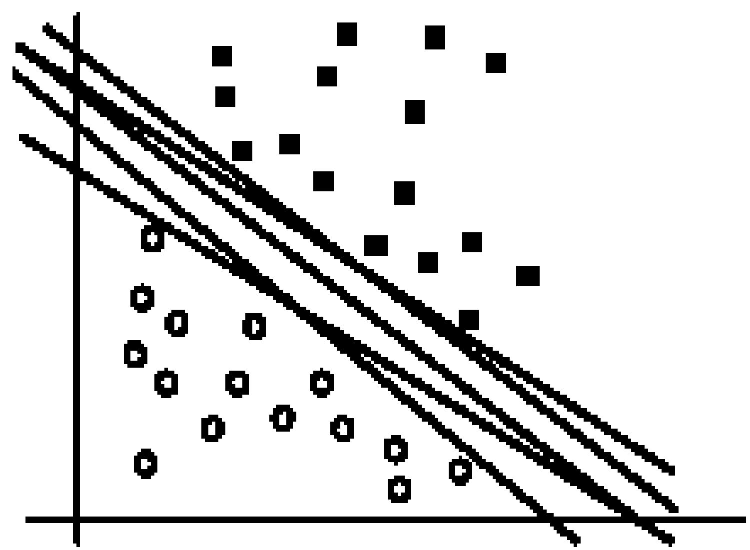
$$y_i = \begin{cases} 1 & \text{if } \langle w \cdot x_i \rangle + b \geq 0 \\ -1 & \text{if } \langle w \cdot x_i \rangle + b < 0 \end{cases}$$

  - ⟨**w** · **x**⟩ + *b* = 0 → decision hyper-plane that separates the two classes

Intelligent Systems – Support Vector Machines

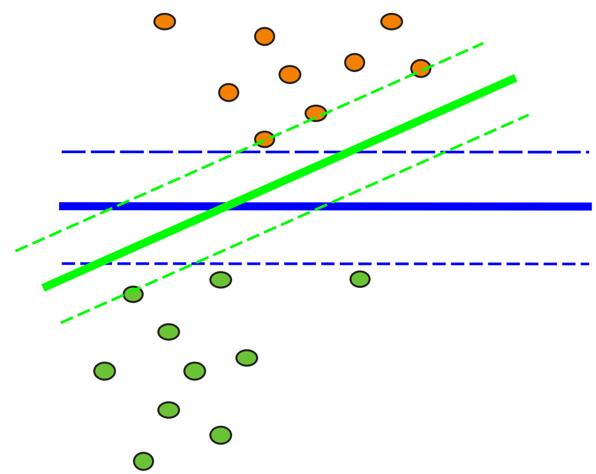
- Definition
  - There are more hyper-planes
    - Which is the best hyper-plane?
  - SVM searches the hyper-plane with the largest margin (that minimises the generalisation error)
    - SMO (*Sequential minimal optimization*) algorithm



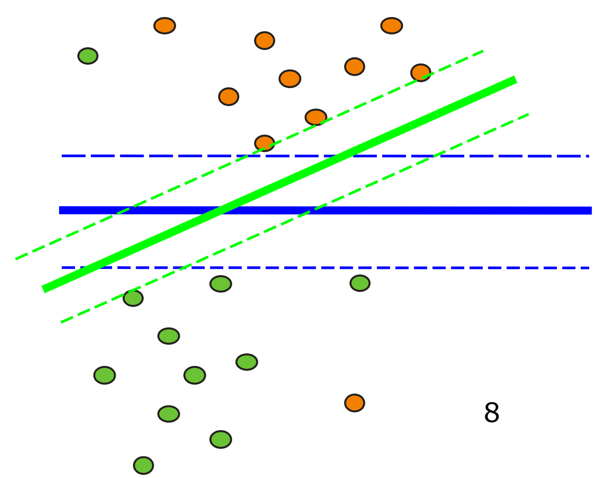


Intelligent Systems – Support Vector Machines

- Solved problems
  - Classification problems → more cases (based on the data type):
    - Linear separable

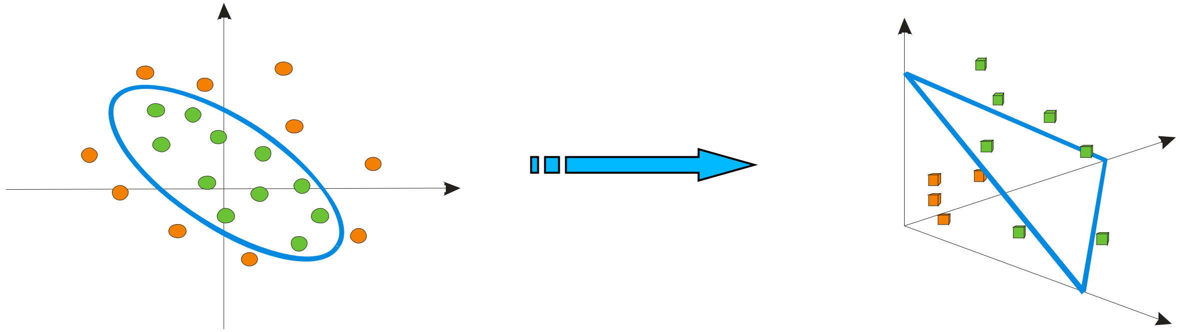


      - Separable
        - Error = 0
      - Non-separable
        - Constrains are relaxed → some error are allowed
        - C – penalisation coefficient



Intelligent Systems – Support Vector Machines

- Solved problems → classification problems → data cases:
  - Non-linear separable
    - Input space is transformed (mapped) into a space of more dimensions (feature space) by using kernel function – in this new space the data becomes linear separable
    - In SVMs the kernel function computes the distance among 2 points
      - → kernel ~ similarity function



Intelligent Systems – Support Vector Machines

- Solved problems → classification problems → data cases:
  - Non-linear separable → possible kernels
    - Classic kernels
      - Polynomial kernel: $K(\mathbf{x}^{d1}, \mathbf{x}^{d2}) = (\mathbf{x}^{d1}, \mathbf{x}^{d2} + 1)^p$
      - RBF kernel: $K(\mathbf{x}^{d1}, \mathbf{x}^{d2}) = exp(- ||\mathbf{x}^{d1} - \mathbf{x}^{d2}||^2/2\sigma^2)$
    - Multiple Kernels
      - Linear : $K(\mathbf{x}^{d1}, \mathbf{x}^{d2}) = \sum w_i K_i (\mathbf{x}^{d1}, \mathbf{x}^{d2})$
      - Non-linear
        - Without coefficients: $K(\mathbf{x}^{d1}, \mathbf{x}^{d2}) = K_1(\mathbf{x}^{d1}, \mathbf{x}^{d2}) + K_2(\mathbf{x}^{d1}, \mathbf{x}^{d2}) * exp(K_3(\mathbf{x}^{d1}, \mathbf{x}^{d2}))$
        - With coefficients: $K(\mathbf{x}^{d1}, \mathbf{x}^{d2}) = K_1 (\mathbf{x}^{d1}, \mathbf{x}^{d2}) + c_1 * K_2 *(\mathbf{x}^{d1}, \mathbf{x}^{d2}) exp(c_2 + K_3(\mathbf{x}^{d1}, \mathbf{x}^{d2}))$
    - Kernels for strings
    - Kernels for images
    - Kernels for graphs

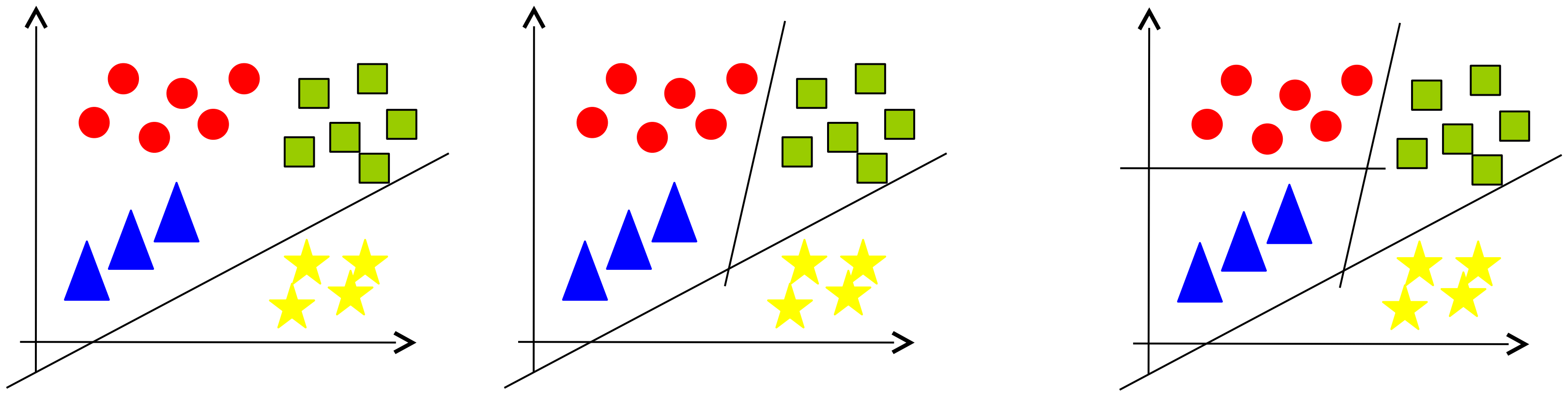
Intelligent Systems – Support Vector Machines

- SVM setting
  - SVM's parameters
    - Penalisation coefficient C
      - C- small → slowly convergence
      - C – large → fast convergence

    - Kernel parameters (what kernel and what parameters)
      - If m (# of attributes) is larger than n (# of data)
        - SVM by a linear kernel (SVM without kernel) → $K(\boldsymbol{x}^{d1}, \boldsymbol{x}^{d2}) = \boldsymbol{x}^{d1} \cdot \boldsymbol{x}^{d2}$
      - If m (# of attributes) is large and n (# of data) is medium
        - SVM with Gaussian kernel $K(\boldsymbol{x}^{d1}, \boldsymbol{x}^{d2}) = \exp(-||\boldsymbol{x}^{d1} - \boldsymbol{x}^{d2}||^2/2\sigma^2)$
        - σ – dispersion of training data
        - Attributes must be normalised (scalled to (0,1))
      - If m (# of attributes) is small and n (# of data) is large
        - Ad new attributes and than SVM with linear kernel

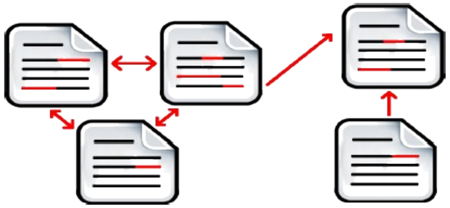
Intelligent Systems – Support Vector Machines

- SVM for multi-class classification problems (more than 2 classes)
  - one *vs.* all

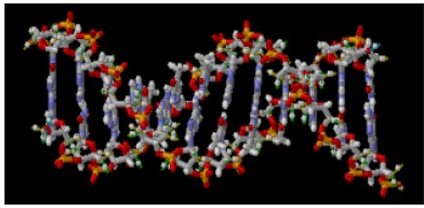


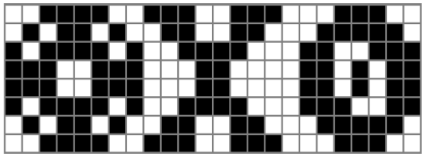
Intelligent Systems – Support Vector Machines

- Structured SVMs
  - Machine Learning
    - Simple SVM f:$X \rightarrow$ R
      - Any type of inputs
      - Numerical outputs (natural numbers, integers, real numbers)
    - Structured SVM:$X \rightarrow y$
      - Any type of inputs
      - Any type of outputs (numerical or structured outputs)



  - Structured information
    - Texts and hyper-texts
    - Molecules and molecular structures
    - Images





Intelligent Systems – Support Vector Machines

- Structured SVMs
  - Applications
    - Natural Language Processing
      - Automatic translation (outputs → sentences)
      - Syntactic and/or morphologic analysis of sentences (outputs → syntactic and/or morphologic tree)
    - Bioinformatic
      - Prediction of secondary structures (outputs → bi=partite graphs)
      - Prediction of enzyme function (outputs → paths in trees)
    - Speech processing
      - Automatic transcriptions (outputs → sentences)
      - Transformation of texts in voice (outputs → audio signal)
    - Robotics
      - Planning (outputs → sequences of actions)

Intelligent Systems – Support Vector Machines

- Advantages
  - Can work with any type of data (linear or non-linear separable, uniform distributed or not, with known or unknown distribution)
    - Kernel function that creates new attributes (features) → hidden layers of an ANN
  - If the problem is convex SVM finds a unique solution → global optima
    - ANNs can associates more solutions → local optima
  - Automatic selection of the learnt model (by support vectors)
    - In ANNs hidden layers have to be configured a priori
  - Avoid over fitting
    - ANNs have over fitting problems even the cross-validation is involved

- Difficulties
  - Real attributes only
  - Binary classification problems only
  - Difficult mathematical background

- Tools
  - LibSVM → http://www.csie.ntu.edu.tw/~cjlin/libsvm/
  - Weka → SMO
  - SVMLight → http://svmlight.joachims.org/
  - SVMTorch → http://www.torch.ch/
  - http://www.support-vector-machines.org/

Intelligent systems – Machine Learning

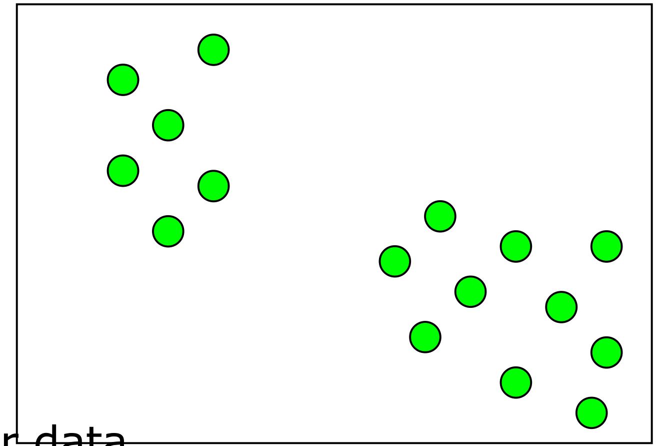
- Typology

  - Experience criteria:
    - Supervised learning
    - Unsupervised learning
    - Active learning
    - Reinforcement learning

  - Algorithm criteria
    - Decision trees
    - Artificial Neural Networks
    - Evolutionary Algorithms
    - Support Vector Machines
    - Hidden Markov Models
    - **K-means**

Unsupervised learning

- Aim
  - Finds a model or a structure of data
- Solved problems
  - Identification of groups (clusters)
    - Analysis of genes
    - Image processing
    - Analysis of social networks
    - Market segmentation
    - Analysis of astronomic data
    - Clusters of computers
  - Dimension reduction
  - Identification of causes (explanations) for data
  - Modelling the data densities



- Specific
  - Data are not annotated (labelled)

Unsupervised learning – definition

Separates the un- labeled examples in disjoint sub-sets (clusters) such as:

- Examples of the same cluster are similar
- Examples of different clusters are different

Definition

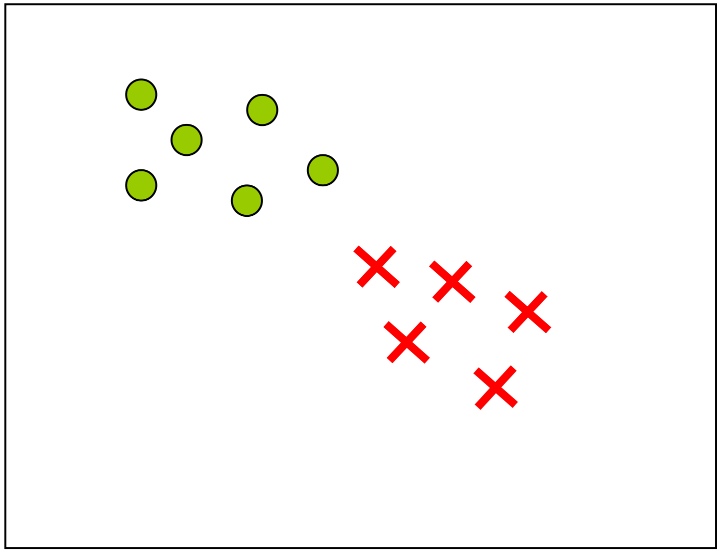
- Given
  - A set of data (examples, instances, cases)
    - Training data
      - As ***atribute_data**$_i$*, where
        - $i = 1, N$ (N = # of training data
        - ***atribute_data**$_i$*= (atr_{i1}, atr_{i2}, ..., atr_{im}), m – # of attributes (characteristics, properties) of data
    - Testing data
      - As (***atribute_data**$_i$*), $i = 1, n$ (n = # of testing data)
- Determine
  - An unknown function that groups the training data in more classes
    - # of classes can be pre-defined (k) or un-known
    - Data of the same class are similar
  - The class of a new testing data by using the learnt grouping (on training data)

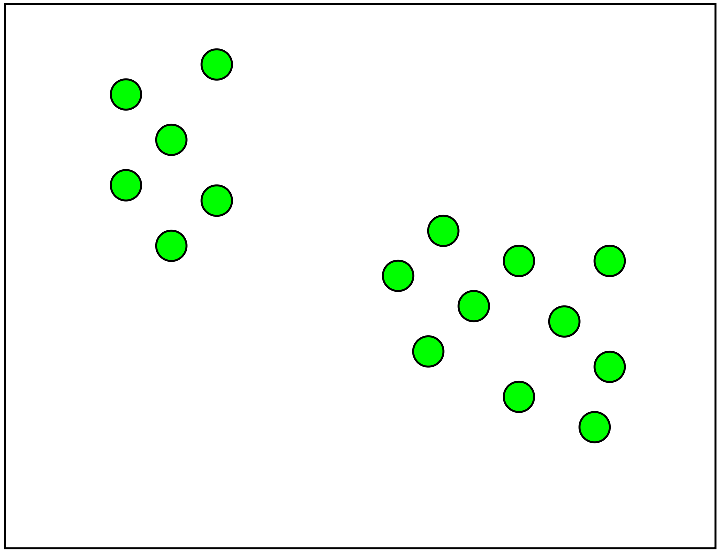
Other names

- Clustering

Unsupervised learning – definition

- Supervised *vs.* un-supervised





Unsupervised learning – definition

- Distance between 2 elements ***p*** and ***q*** $\epsilon\ R^m$
  - Euclid distance
    - $d(\mathbf{p},\mathbf{q})=sqrt(\Sigma_{j=1,2,\ldots,m}(p_j-q_j)^2)$
  - Manhattan distance
    - $d(\mathbf{p},\mathbf{q})=\Sigma_{j=1,2,\ldots,m}|p_j-q_j|$
  - Mahalanobis distance
    - $d(\mathbf{p},\mathbf{q})=sqrt(\mathbf{p}-\mathbf{q})S^{-1}(\mathbf{p}-\mathbf{q}))$,
      - Where S is the covariance matrix ($S= E[(\mathbf{p}-E[\mathbf{p}])(\mathbf{q}-E[\mathbf{q}])]$)
  - Internal product
    - $d(\mathbf{p},\mathbf{q})=\Sigma_{j=1,2,\ldots,m}p_jq_j$
  - Cosine distance
    - $d(\mathbf{p},\mathbf{q})=\Sigma_{j=1,2,\ldots,m}p_jq_j / (sqrt(\Sigma_{j=1,2,\ldots,m}p_j^2) * sqrt(\Sigma_{j=1,2,\ldots,m}q_j^2))$
  - Hamming distance
    - # of differences between ***p*** and ***q***
  - Levenshtein distance
    - Minimal # of operations required for transforming ***p*** in ***q***

- Distance *vs.* similarity
  - Distance → minimisation
  - Similarity → maximisation

Unsupervised learning – definition

Application

- Gene clustering
- Market segmentation (for client clustering)
- news.google.com

Unsupervised learning – process

Process

- 2 steps:
  - Learning
    - Determine (learn), by using an algorithm, the existing clusters
  - Testing
    - Include a new data in one of the identified (during training) clusters

Learning quality (clustering validation)

- Internal criteria
  - Large similarity inside the cluster and reduce similarity between clusters
- External criteria
  - Using benchmarks composed of *apriori* grouped data

Unsupervised learning – evaluation

Performance measures

- Internal criteria
  - Distance inside the cluster
  - Distance between clusters
  - Davies-Bouldin index
  - Dunn index

- External criteria
  - Comparison with known data – impossible in real-world applications
  - Precision
  - Recall
  - F-measure

Unsupervised learning – typology

- How the clusters are forming
  - Hierarchic clustering
  - Non-hierarchic (partitioned) clustering
  - Clustering based on data density
  - Clustering based on a grid

Unsupervised learning – typology

- How the clusters are forming
  - Hierarchic clustering
    - Creates a dendogram (taxonomic tree)
      - Creates the clusters (recursively)
      - k (# of clusters) is un-known
    - Aglomerativ clustering (bottom-up) → small clusters to large clusters
    - Divisiv clustering (top-down) → large clusters to small clusters
    - Eg.
      - Clustering ierarhic aglomerativ

Unsupervised learning – typology

- How the clusters are formed
  - Non-hierarchic
    - Partition → determine a data separation → all the clusters in the same time
    - Optimises an objective function defined
      - Locally – by using some features only
      - Globally – by using all attributes

      that can be:

      - squared error – sum of squared distances between data and the cluster's centroid → min
        - Ex. *K-means*
      - Graph-based
        - Ex. Clustering based in minimum spanning tree
      - Based on probabilistic models
        - Ex. Identify the data distribution → expectation maximisation
      - Based on the nearest neighbour
    - Required to fix k apriori → fix the initial clusters
      - Algorithm is run more times with different parameters and the most efficient version is selected
    - Ex. *K-means, ACO*

Unsupervised learning – typology

- How the clusters are forming
  - Based on data densities
    - Data density and data connectivity
      - Cluster formation is based on data density from a given region
      - Cluster formation is based on data connectivity from a given region
    - Function of data density
      - Tries to model the data distribution
    - Advantage:
      - Modeling of clusters of any shape

Unsupervised learning – typology

- How the cluster are forming
  - Based on a grid
    - Is not a distinct approach
      - Can be hierarchic, partitional or density-based
    - Involves data space segmentation in regular areas
    - Objects are placed on a multi-dimensional grid
    - Eg. ACO

Unsupervised learning – typology

- How the algorithms work
  - Agglomerative clustering
    1. Initially, each instance form a cluster
    2. Compute the distance between any 2 clusters
    3. Reunion the closest 2 clusters
    4. Repeat steps 3 and 4 until a single cluster is obtained or other stop criterion is satisfied
  - Divisive clustering
    1. Establish the number of clusters (k)
    2. Initialise the centre of each cluster
    3. Determine a data separation
    4. Re-compute the center of each cluster
    5. Repeat steps 3 and 4 until the partition is unchanged (algorithm converges)

- How the algorithm takes into account the attributes (features)
  - Monotonic – attributes are taken into account one-by-one
  - Poly-tonic – attributes are simultaneous taken into

Unsupervised learning – typology

- How the data belong to clusters
  - Exact clustering (hard clustering)
    - Each instance x_i has associated a label (class) c_j
  - Fuzzy clustering
    - Each instance has associated a membership degree (probability) f_{ij} to a given class c_j → an instance xi can belongs to more clusters
    - Asociază fiecarei intrări $\boldsymbol{x_i}$ un grad (probabilitate) de apartenență f_{ij} la o anumită clasă c_j ➔ o instanță $\boldsymbol{x_i}$ poate aparține mai multor clusteri

Unsupervised learning – algorithms

- Agglomerative hierarchical clustering
- K-means
- AMA
- Probabilistic models
- Nearest neighbor
- Fuzzy
- Artificial Neural Network
- Evolutionary algorithms
- ACO

Unsupervised learning – algorithms

Agglomerate hierarchical clustering

- Consider a distance between 2 instances $d(x_{i1}, x_{i2})$
- Form N clusters, each of them containing an instance
- Repeat
  - Determine the closest 2 clusters
  - Reunion the 2 clusters → a cluster
- Until a single cluster is obtained (that contains all the instances)

Unsupervised learning – algorithms

Agglomerate hierarchical clustering

- Distance between 2 clusters c_i and c_j:
  - Simple link → minimal distance between the objects of 2 clusters
    - $d(c_i, c_j) = max_{\ xi1\epsilon ci,\ xi2\epsilon cj}\ sim(\mathbf{x}_{i1}, \mathbf{x}_{i2})$
  - Complete link → maximal distance between the objects of 2 clusters
    - $d(c_i, c_j) = min_{\ xi1\epsilon ci,\ xi2\epsilon cj}\ sim(\mathbf{x}_{i1}, \mathbf{x}_{i2})$
  - Average link → mean of distances between the objects of 2 clusters
    - $d(c_i, c_j) = 1 / (n_i * n_j) \sum_{xi1\epsilon ci} \sum_{xi2\epsilon cj} d(\mathbf{x}_{i1}, \mathbf{x}_{i2})$
  - Average link over group → distance between the means (centroids) of 2 clusters
    - $d(c_i, c_j) = \rho(\boldsymbol{\mu}_i, \boldsymbol{\mu}_j)$, ρ – distance, $\boldsymbol{\mu}_j = 1/n_j \sum_{xi\epsilon cj} \mathbf{x}_i$

Unsupervised learning – algorithms

K-means (Lloyd algorithm / Voronoi iteration)

- Suppose that k clusters will form

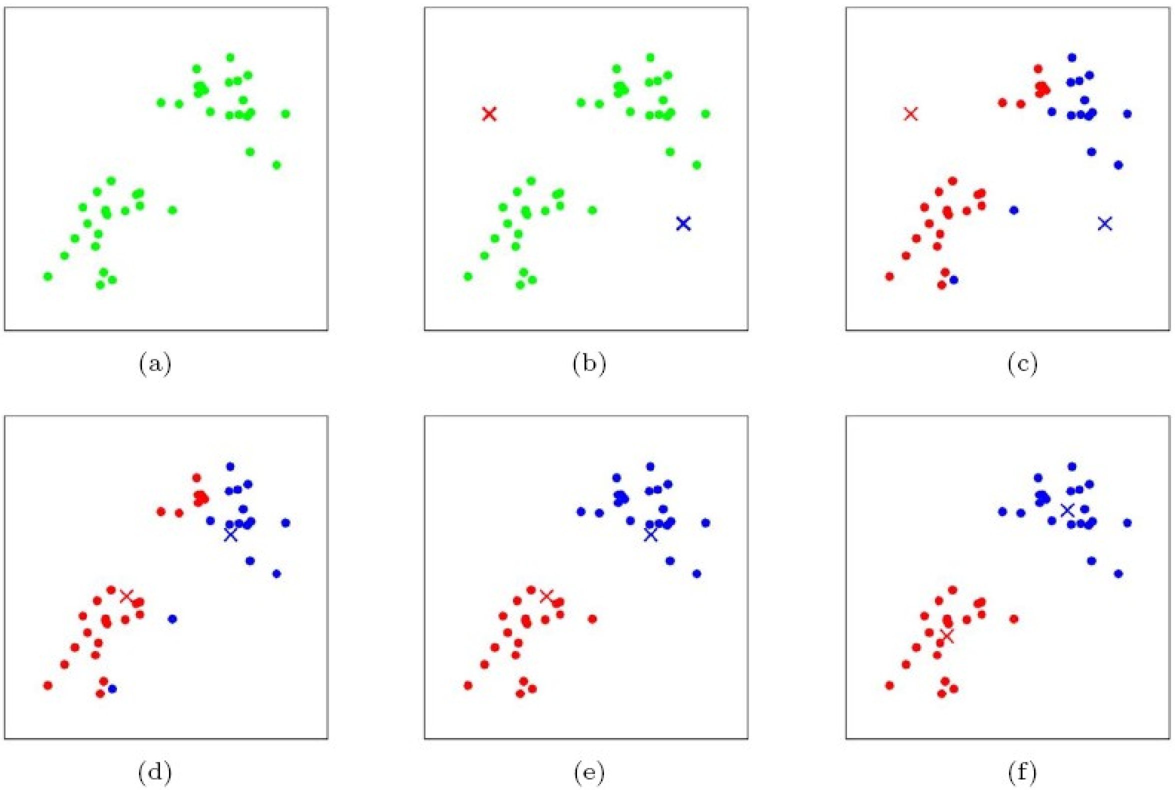
- Initialize k centroids $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_k$
  - A centroid $\boldsymbol{\mu}_j$ ($i=1,2, \ldots, k$) is a vector of m values (m - # of features)

- Repeat until convergence
  - Associated to each instance the nearest centroid → for each instance $\boldsymbol{x}_i$, $i = 1, 2, \ldots, N$
    - $c_i = arg\ min_{j = 1, 2, \ldots, k} ||\boldsymbol{x}_i - \boldsymbol{\mu}_j||^2$

  - Re-compute the centroids by moving them in the mean of instances associated to it → for each cluster c_j, $j = 1, 2, \ldots, k$
    - $\boldsymbol{\mu}_j = \sum_{i=1,2,\ldots N} 1_{ci=j}\ \boldsymbol{x}_i / \sum_{i=1,2,\ldots N} 1_{ci=j}$

Unsupervised learning – algorithms

- K-means



Unsupervised learning – algorithms

K-means

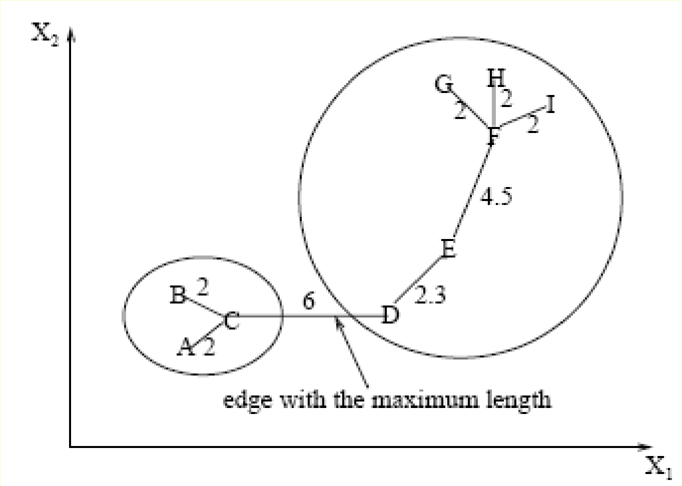
- Initialisation of *k* centroids $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_k$
  - With random values (in the definition domain of the problem)
  - With *k* instances of *N* (randomly selected)

- Does algorithm converge always?
  - Yes, because of distortion function J
    - $J(c, \mu) = \sum_{i=1,2,\ldots,N} ||\boldsymbol{x}_i - \boldsymbol{\mu}_{cj}||^2$

    which is decreasing
  - Converges in a local optima
  - Finding the global optima → NP-difficult problem

Clustering based on minimum spanning tree

- Construct the minimum spanning tree of data
- Eliminate from the tree the longest edges and form clusters



Învăţare ne-supervizată – algoritmi
Modele probabilistice

- http://www.gatsby.ucl.ac.uk/~zoubin/course04/ul.pdf
- http://learning.eng.cam.ac.uk/zoubin/nipstut.pdf