Unsupervised Learning

Some slides were adapted/taken from various sources, including Prof. Andrew Ng's Coursera Lectures, Stanford University, Prof. Kilian Q. Weinberger's lectures on Machine Learning, Cornell University, Prof. Sudeshna Sarkar's Lecture on Machine Learning, IIT Kharagpur, Prof. Bing Liu's lecture, University of Illinois at Chicago (UIC), CS231n: Convolutional Neural Networks for Visual Recognition lectures, Stanford University, Prof. Alexander Ihler and many more. We thankfully acknowledge them. Students are requested to use this material for their study only and **NOT** to distribute it.

Road map

- **Basic concepts**
- **K-means algorithm**
- **Representation of clusters**
- **Hierarchical clustering**
- **Distance functions**
- **Data standardization**
- **Handling mixed attributes**
- **Which clustering algorithm to use?**
- **Cluster evaluation**
- **Discovering holes and data regions**
- **Summary**

Supervised learning vs. unsupervised learning

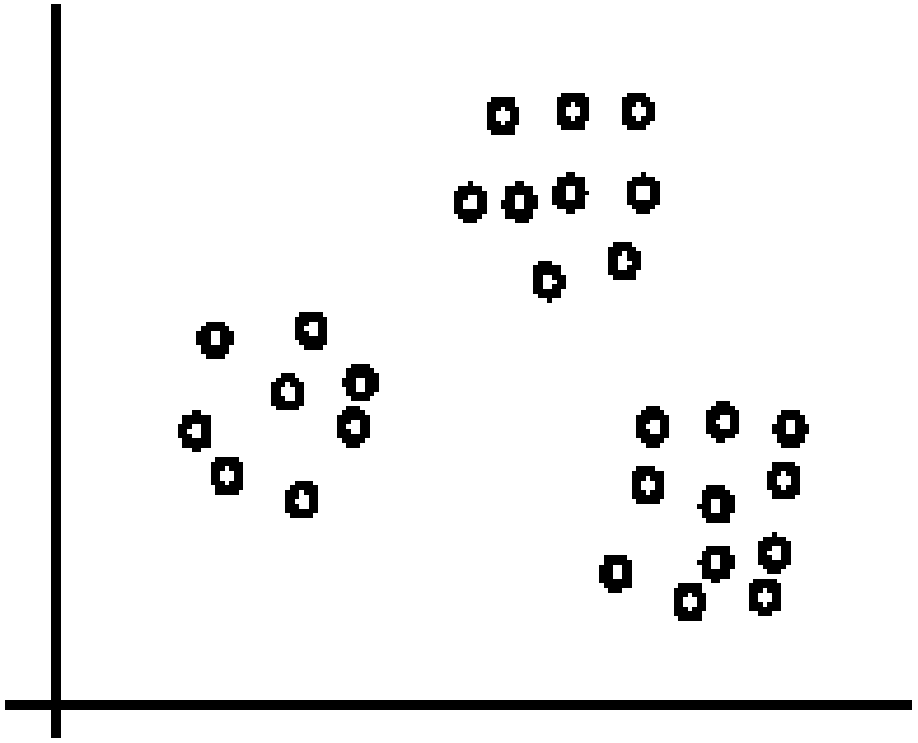
- Supervised learning: discover patterns in the data that relate data attributes with a target (class) attribute.
  - These patterns are then utilized to predict the values of the target attribute in future data instances.
- Unsupervised learning: The data have no target attribute.
  - We want to explore the data to find some intrinsic structures in them.

Clustering

- Clustering is a technique for finding similarity groups in data, called **clusters**. I.e.,
  - it groups data instances that are similar to (near) each other in one cluster and data instances that are very different (far away) from each other into different clusters.
- Clustering is often called an **unsupervised learning** task as no class values denoting an *a priori* grouping of the data instances are given, which is the case in supervised learning.
- Due to historical reasons, clustering is often considered synonymous with unsupervised learning.
  - In fact, association rule mining is also unsupervised
- This chapter focuses on clustering.

An illustration

- The data set has three natural groups of data points, i.e., 3 natural clusters.



What is clustering for?

- Let us see some real-life examples
- Example 1: groups people of similar sizes together to make “small”, “medium” and “large” T-Shirts.
  - Tailor-made for each person: too expensive
  - One-size-fits-all: does not fit all.
- Example 2: In marketing, segment customers according to their similarities
  - To do targeted marketing.

What is clustering for? (cont…)

- Example 3: Given a collection of text documents, we want to organize them according to their content similarities,
  - To produce a topic hierarchy
- In fact, clustering is one of the most utilized data mining techniques.
  - It has a long history, and used in almost every field, e.g., medicine, psychology, botany, sociology, biology, archeology, marketing, insurance, libraries, etc.
  - In recent years, due to the rapid increase of online documents, text clustering becomes important.

Aspects of clustering

- A clustering algorithm
  - Partitional clustering
  - Hierarchical clustering
  - …
- A distance (similarity, or dissimilarity) function
- Clustering quality
  - Inter-clusters distance $\Rightarrow$ maximized
  - Intra-clusters distance $\Rightarrow$ minimized
- The quality of a clustering result depends on the algorithm, the distance function, and the application.

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K-means clustering

- K-means is a partitional clustering algorithm
- Let the set of data points (or instances) D be

  $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$,

  where $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{ir})$ is a vector in a real-valued space $X \subseteq R^r$, and r is the number of attributes (dimensions) in the data.
- The *k*-means algorithm partitions the given data into *k* clusters S = $\{S_1, S_2, \ldots, S_k\}$.
  - Each cluster has a cluster **center**, called **centroid** $(\boldsymbol{\mu_i})$. *k* is specified by the user

Optimization criterion

- WCSS (within cluster sum of square)

$$\sum_{i=1}^{k} \sum_{x \in S_i} ||x_i - \mu_i||^2$$

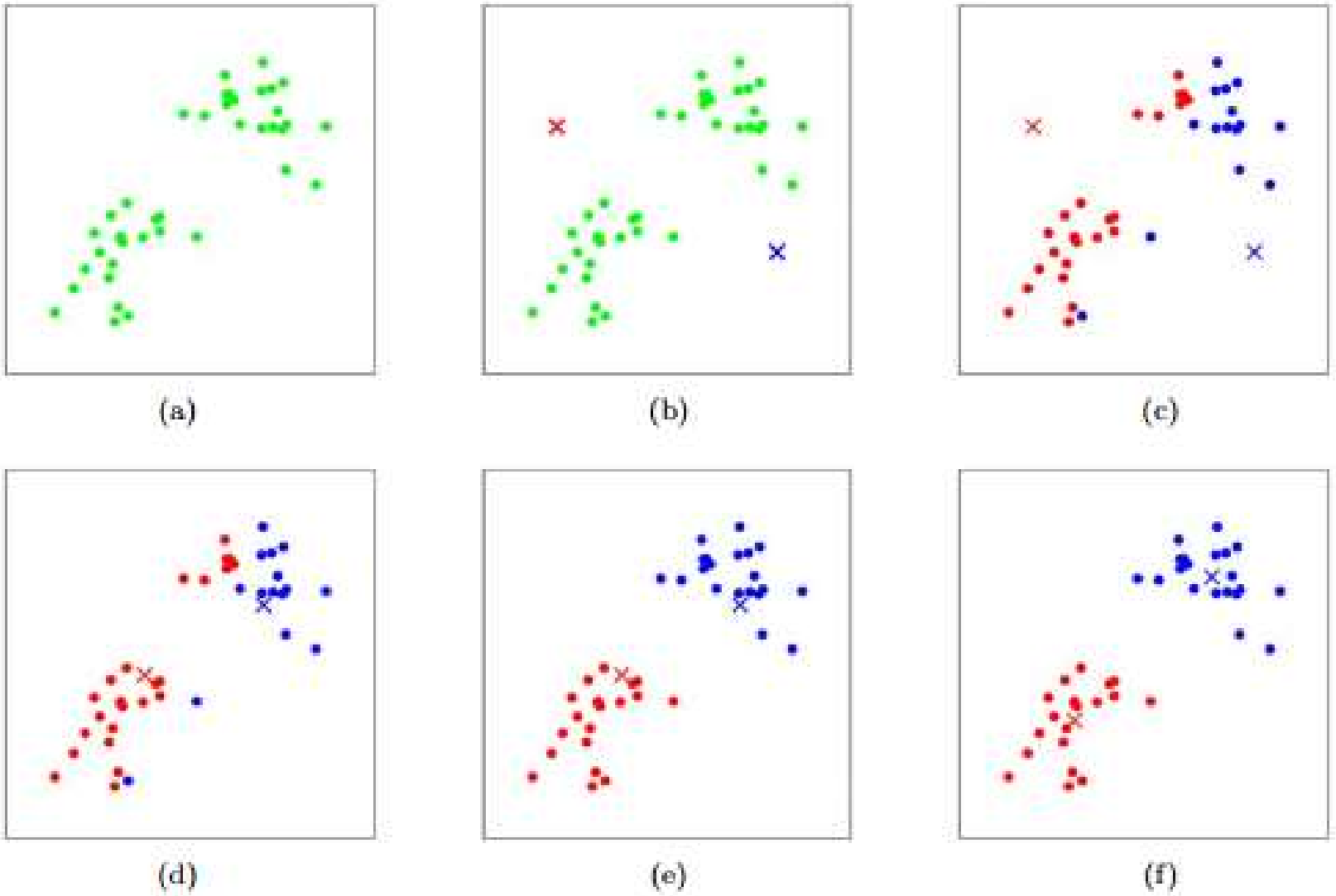
- Find out that set of clusters where WCSS is minimum i.e. optimization criteria is

$$\underset{S}{argmin} \sum_{i=1}^{k} \sum_{x \in S_i} ||x_i - \mu_i||^2$$

K-means algorithm

Macqueen, 1967

- Given *k*, the *k-means (heuristic based)* algorithm works as follows:
  1) Randomly choose *k* data points (seeds) to be the initial centroids, cluster centers
  2) Assign each data point to the closest centroid
  3) Re-compute the centroids using the current cluster memberships.
  4) If a convergence criterion is not met, goto step 2.


(a)
(b)
(c)
(d)
(e)
(f)

K-means algorithm – (cont …)

Algorithm *k*-means(*k*, *D*)

1 Choose *k* data points as the initial centroids (cluster centers)
2 **repeat**
3 **for** each data point $\mathbf{x} \in D$ do
4 compute the distance from **x** to each centroid;
5 assign **x** to the closest centroid // a centroid represents a cluster
6 **endfor**
7 re-compute the centroids using the current cluster memberships
8 **until** the stopping criterion is met

Stopping/convergence criterion

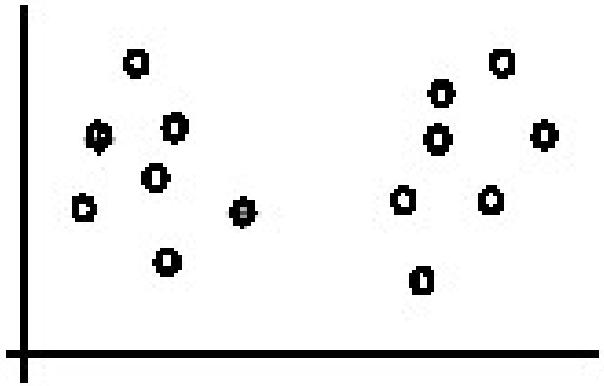
1. no (or minimum) re-assignments of data points to different clusters,
2. no (or minimum) change of centroids, or
3. minimum decrease in the **sum of squared error** (SSE),

$$SSE = \sum_{i=1}^{k} \sum_{x \in S_i} ||x_i - \mu_i||^2 \qquad (1)$$

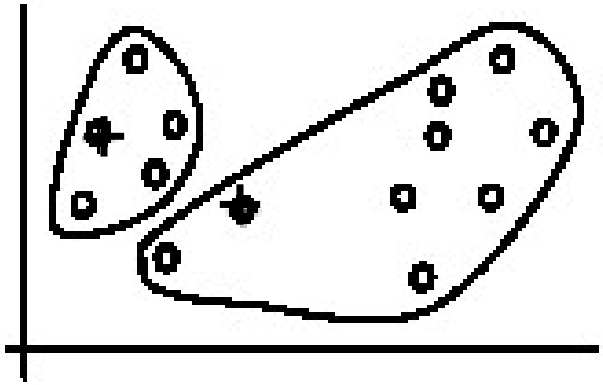
where S_i is the *i*th cluster, μ_i is the centroid of cluster S_i (the mean vector of all the data points in S_i), and *dist*$(x_i, \mu_i) = ||x_i - \mu_i||^2$ is the distance between data point **x** and centroid S_i.

- The **sum of squared error** (SSE) is keep on decreasing in subsequent iterations.
- The process is bound to converge.
- It will converge to local minima of within cluster sum of square distance which may or may not meet the global minima.

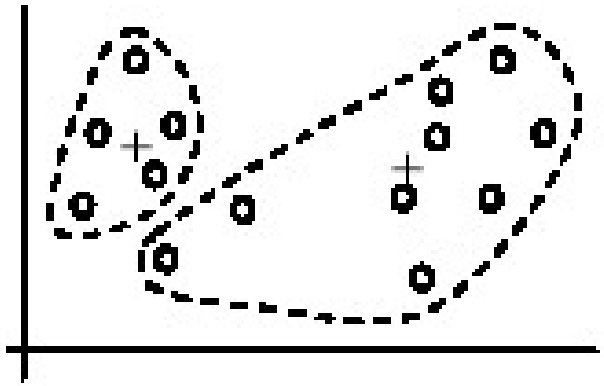
An example



(A). Random selection of k centers

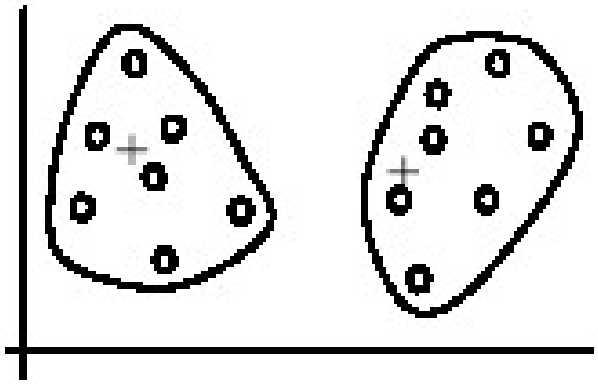


Iteration 1: (B). Cluster assignment

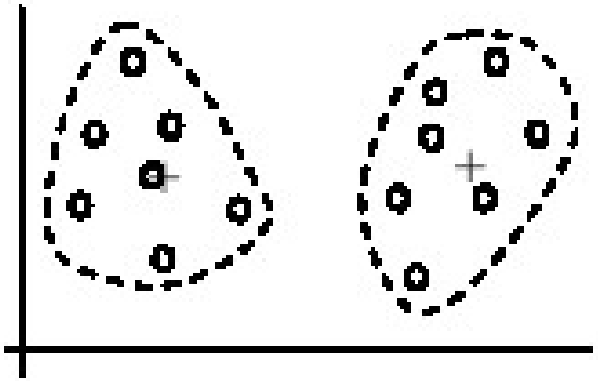


(C). Re-compute centroids

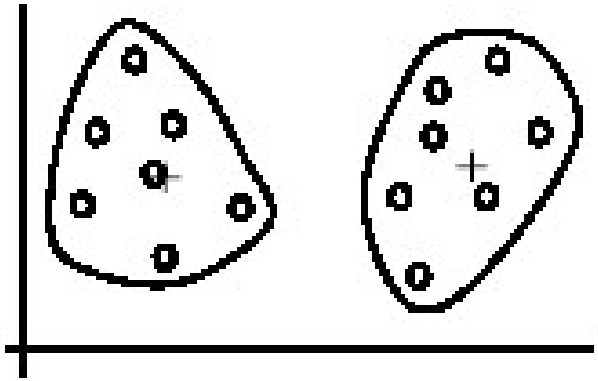
An example (cont …)



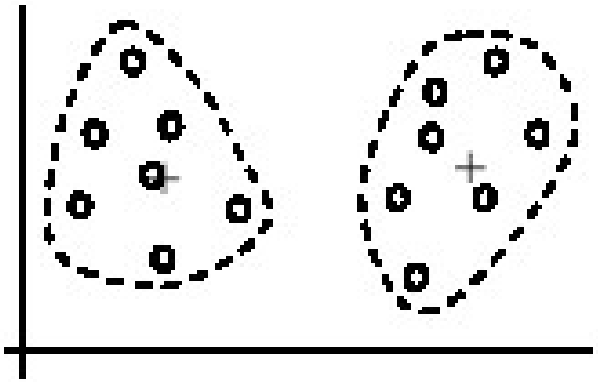
Iteration 2: (D). Cluster assignment



(E). Re-compute centroids



Iteration 3: (F). Cluster assignment



(G). Re-compute centroids

An example distance function

- Minkowski Distance:

$$d(x_i, x_j) = \left(\sum_{s=1}^{n} |x_{is} - x_{js}|^p\right)^{\frac{1}{p}}$$

- Euclidean Distance (p=2):

$$\sqrt{\sum_{s=1}^{n} |x_{is} - x_{js}|^2}$$

- Manhattan (City-Block) Distance (p=1):

$$\sum_{S=1}^{n} |x_{is} - x_{js}|$$

An example distance function

- Mahalanobis Distance: Dissimilarity measure between two random vectors $x_i \; and \; x_j$ of the same distribution with the covariance matrix $\sum$

$$d(x_i, x_i) = \sqrt{(x_i - x_j)\Sigma^{-1}(x_i - x_j)}$$

- Pearson correlation:

$$r(x_i, x_j) = \frac{Cov(x_i, x_j)}{\sigma_{x_i}\sigma_{x_j}}$$

Computational Complexity

- Computing distance between two items is $O(n)$ where n is the dimensionality of the vectors.
- Reassigning clusters: $O(km)$ distance computations, or $O(kmn)$
- Computing centroids:Each item gets added once to some centroid: $O(mn)$
- Assume these two steps are each done once for each t iterations: $O(tknm)$

Strengths of k-means

- Strengths:
  - Simple: easy to understand and to implement
  - Efficient: Time complexity: $O(tkn)$,

    where n is the number of data points,

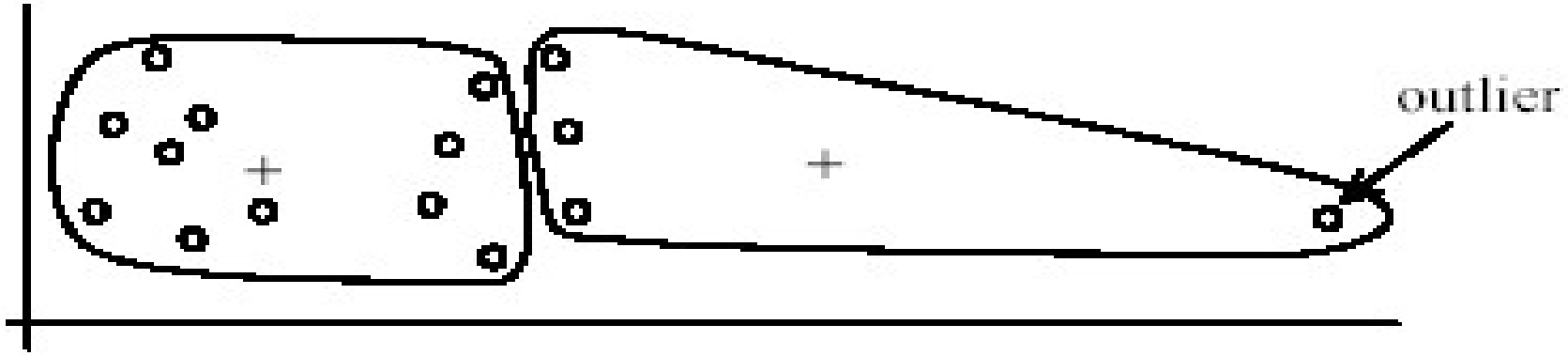
    k is the number of clusters, and

    t is the number of iterations.
  - Since both k and t are small. k-means is considered a linear algorithm.
- K-means is the most popular clustering algorithm.
- Note that: it terminates at a local optimum if SSE is used. The global optimum is hard to find due to complexity.

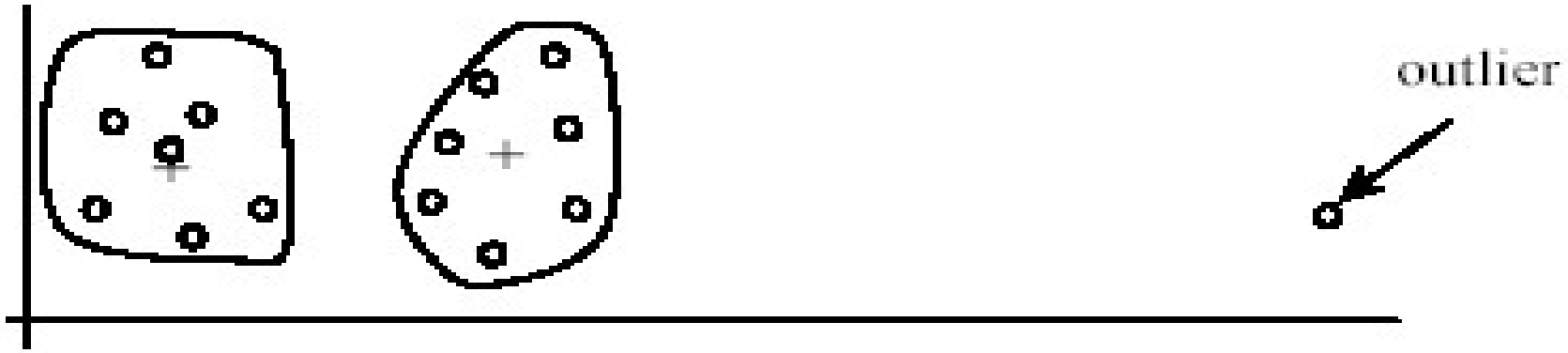
Weaknesses of k-means

- The algorithm is only applicable if the mean is defined.
  - For categorical data, *k*-mode - the centroid is represented by most frequent values.
- The user needs to specify *k*.
- The algorithm is sensitive to **outliers**
  - Outliers are data points that are very far away from other data points.
  - Outliers could be errors in the data recording or some special data points with very different values.

Weaknesses of k-means: Problems with outliers



(A): Undesirable clusters



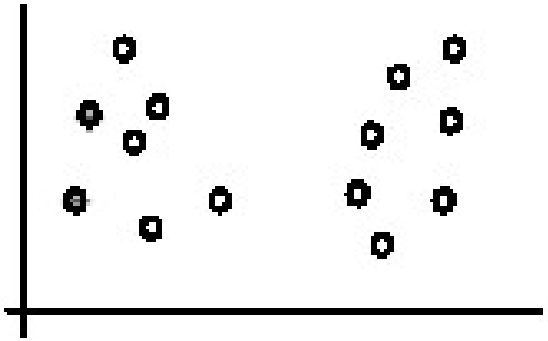
(B): Ideal clusters

Weaknesses of k-means: To deal with outliers

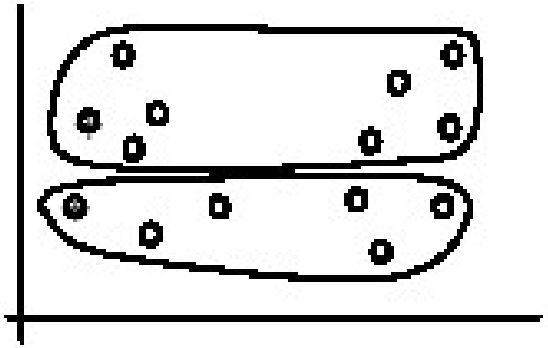
- One method is to remove some data points in the clustering process that are much further away from the centroids than other data points.
  - To be safe, we may want to monitor these possible outliers over a few iterations and then decide to remove them.
- Another method is to perform random sampling. Since in sampling we only choose a small subset of the data points, the chance of selecting an outlier is very small.
  - Assign the rest of the data points to the clusters by distance or similarity comparison, or classification

Weaknesses of k-means (cont …)

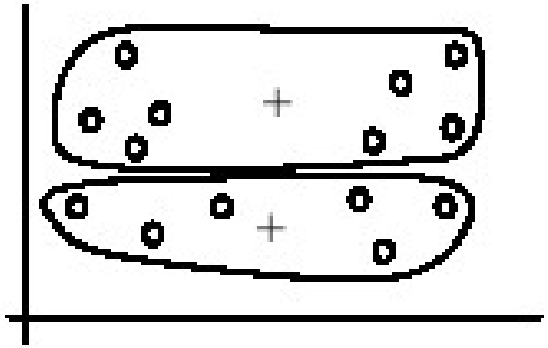
- The algorithm is sensitive to initial seeds.



(A). Random selection of seeds (centroids)



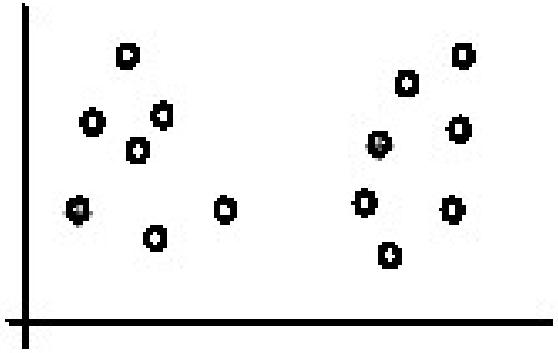
(B). Iteration 1



(C). Iteration 2

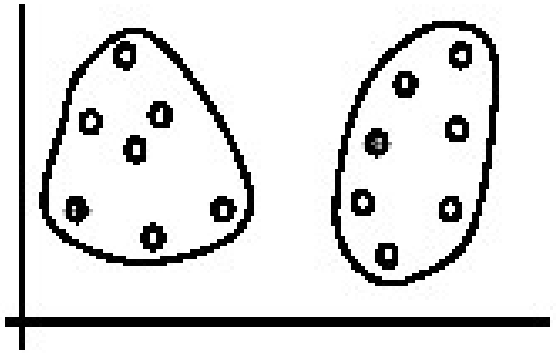
Weaknesses of k-means (cont …)

- If we use different seeds: good results

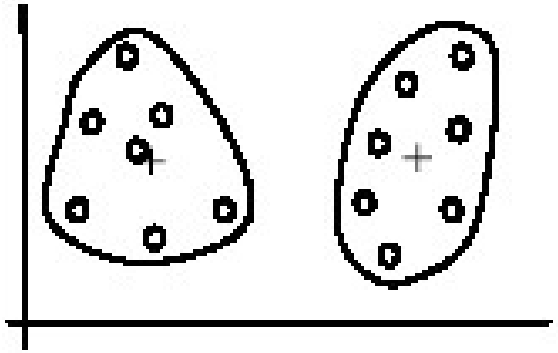


(A). Random selection of k seeds (centroids)

- There are some methods to help choose good seeds



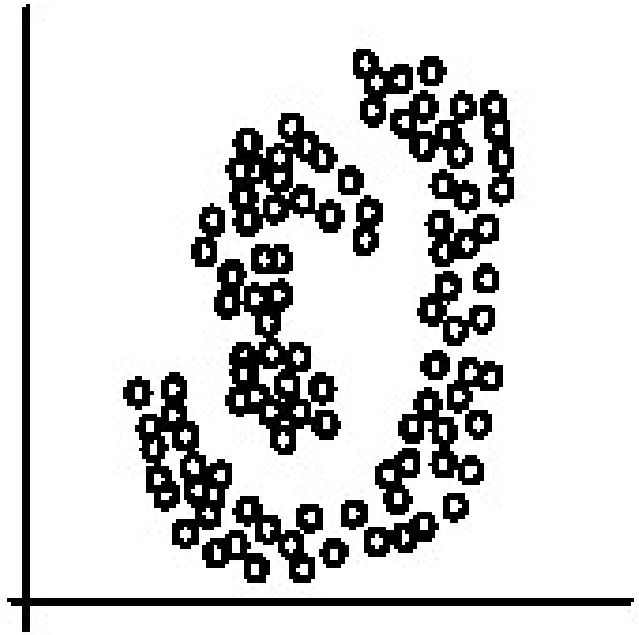
(B). Iteration 1



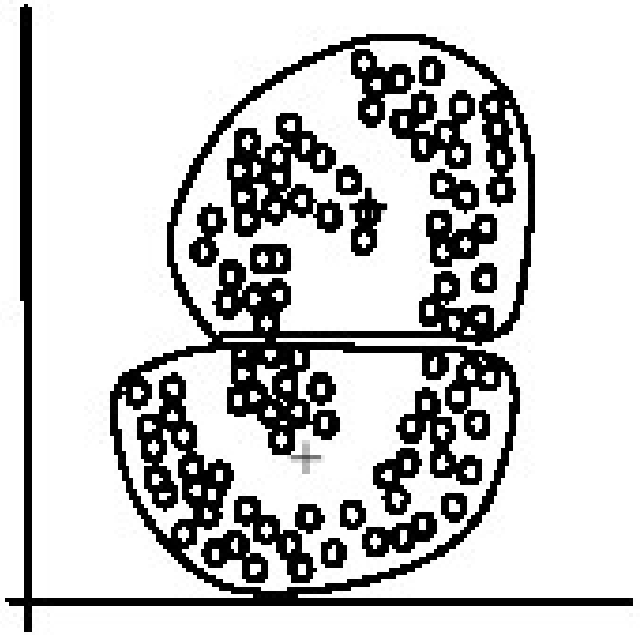
(C). Iteration 2

Weaknesses of k-means (cont …)

- The *k*-means algorithm is not suitable for discovering clusters that are not hyper-ellipsoids (or hyper-spheres).



(A): Two natural clusters



(B): *k*-means clusters

K-means summary

- Despite weaknesses, *k*-means is still the most popular algorithm due to its simplicity, efficiency and
  - other clustering algorithms have their own lists of weaknesses.
- No clear evidence that any other clustering algorithm performs better in general
  - although they may be more suitable for some specific types of data or applications.
- Comparing different clustering algorithms is a difficult task. No one knows the correct clusters!

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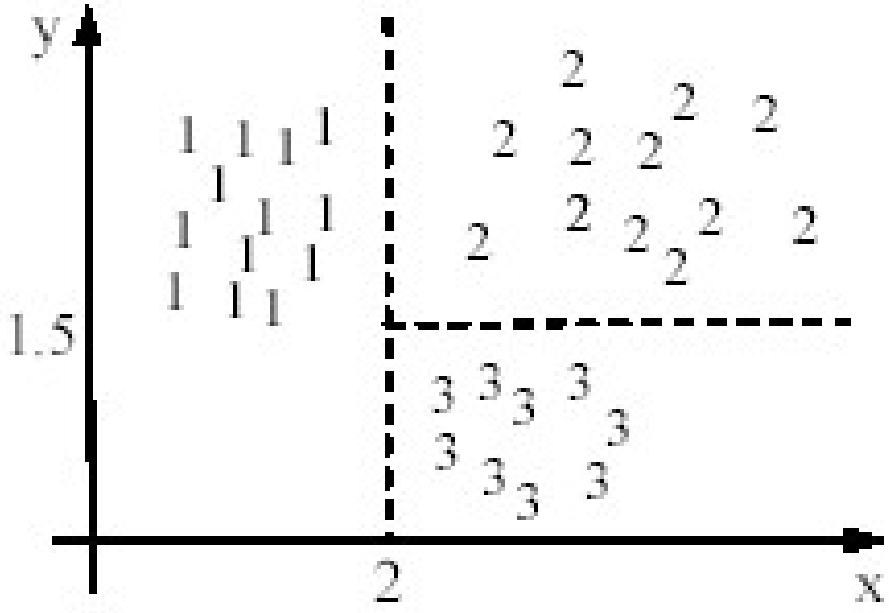
Common ways to represent clusters

- Use the centroid of each cluster to represent the cluster.
  - compute the radius and
  - standard deviation of the cluster to determine its spread in each dimension

  - The centroid representation alone works well if the clusters are of the hyper-spherical shape.
  - If clusters are elongated or are of other shapes, centroids are not sufficient

Using classification model

- All the data points in a cluster are regarded to have the same class label, e.g., the cluster ID.
  - run a supervised learning algorithm on the data to find a classification model.



$x \leq 2 \rightarrow$ cluster 1

$x > 2, y > 1.5 \rightarrow$ cluster 2

$x > 2, y \leq 1.5 \rightarrow$ cluster 3

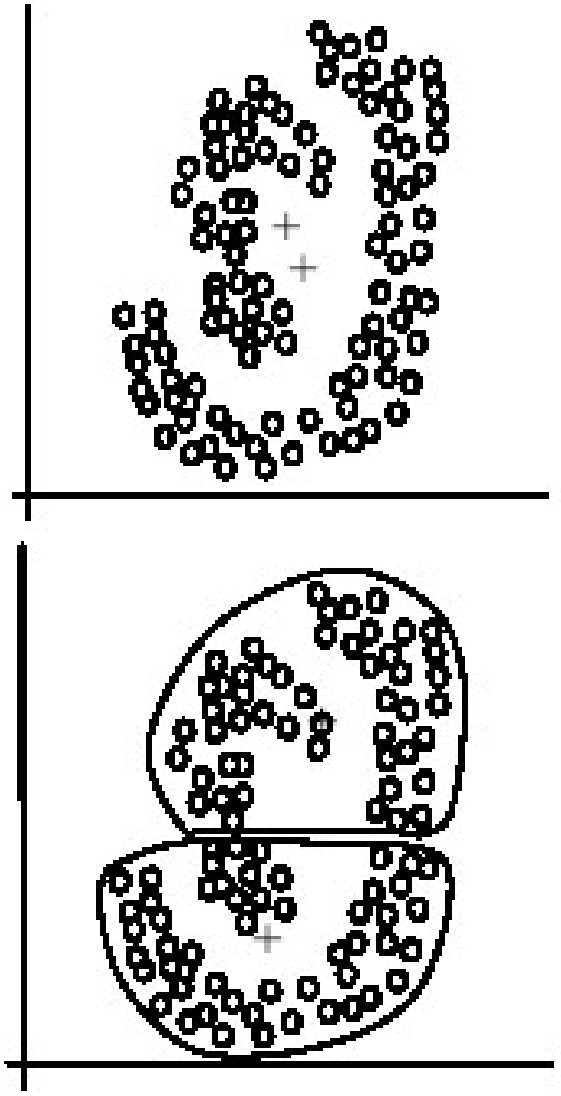
Use frequent values to represent cluster

- This method is mainly for clustering of categorical data (e.g., *k*-modes clustering).

- Main method used in text clustering, where a small set of frequent words in each cluster is selected to represent the cluster.

Clusters of arbitrary shapes

- Hyper-elliptical and hyper-spherical clusters are usually easy to represent, using their centroid together with spreads.
- Irregular shape clusters are hard to represent. They may not be useful in some applications.
  - Using centroids are not suitable (upper figure) in general
  - K-means clusters may be more useful (lower figure), e.g., for making 2 size T-shirts.



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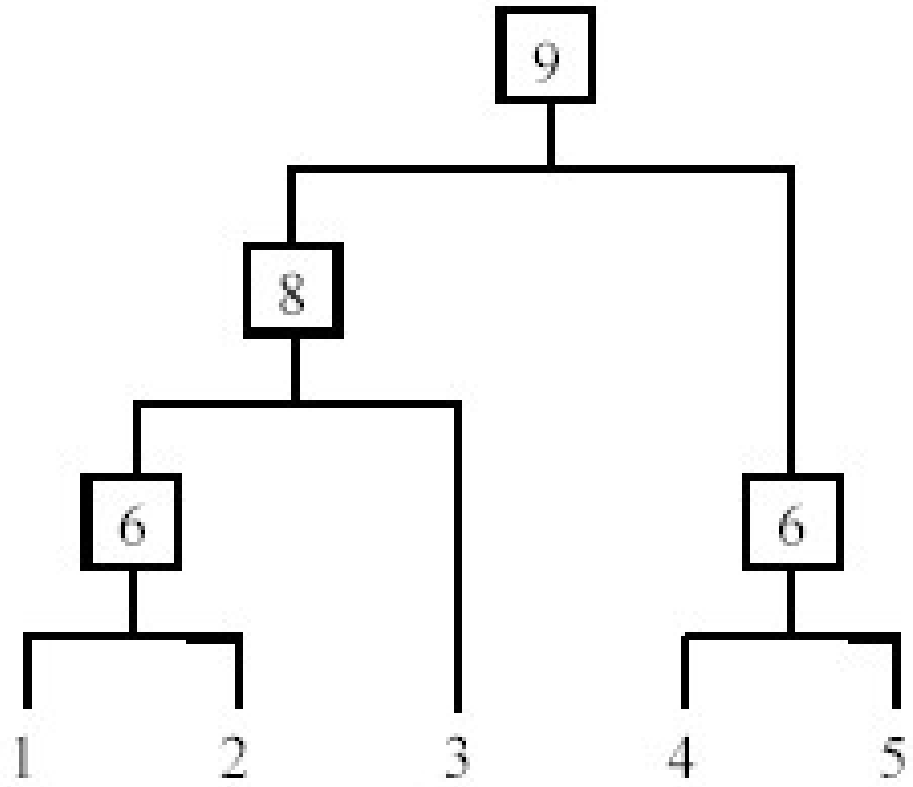
Hierarchical Clustering

- Produce a nested sequence of clusters, a tree, also called Dendrogram.



Types of hierarchical clustering

- Agglomerative (bottom up) clustering: It builds the dendrogram (tree) from the bottom level, and
  - merges the most similar (or nearest) pair of clusters
  - stops when all the data points are merged into a single cluster (i.e., the root cluster).
- Divisive (top down) clustering: It starts with all data points in one cluster, the root.
  - Splits the root into a set of child clusters. Each child cluster is recursively divided further
  - stops when only singleton clusters of individual data points remain, i.e., each cluster with only a single point

Agglomerative clustering

It is more popular then divisive methods.

- At the beginning, each data point forms a cluster (also called a node).
- Merge nodes/clusters that have the least distance.
- Go on merging
- Eventually all nodes belong to one cluster

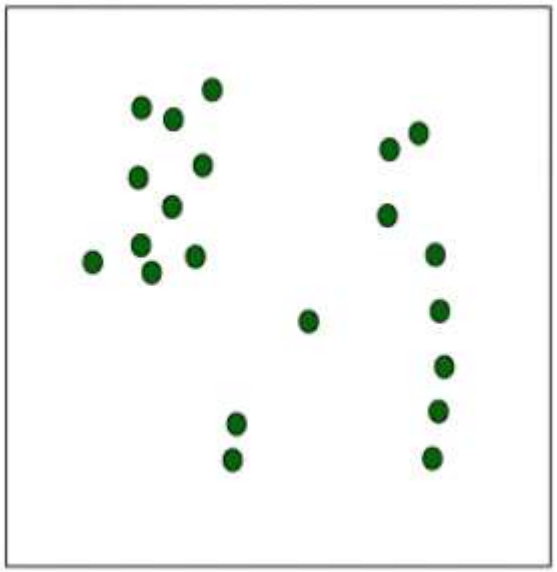
Agglomerative clustering algorithm

Algorithm Agglomerative(D)

1 Make each data point in the data set D a cluster,
2 Compute all pair-wise distances of $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n \in D$;
2 **repeat**
3 find two clusters that are nearest to each other;
4 merge the two clusters form a new cluster c;
5 compute the distance from c to all other clusters;
12 **until** there is only one cluster left

Visualization

Data:

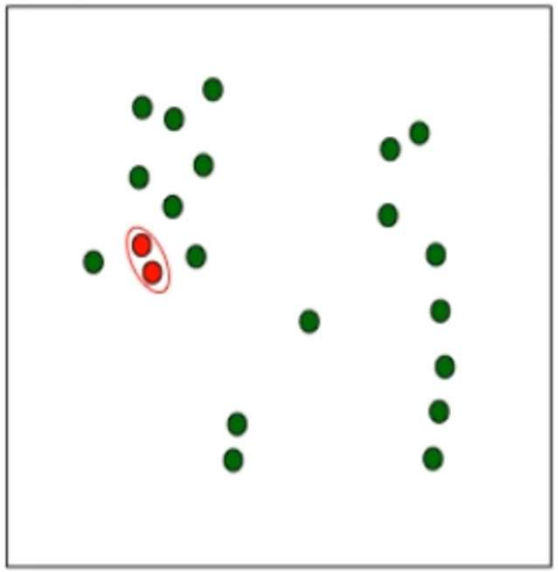


Initially every datum is a cluster.

- A simple algorithm.
- Define a distance (or dissimilarity) between clusters.
- Initialize: every sample is a cluster.
- Iterate:
  - Compute distance between all clusters. Complexity **$O(m^2 \log m)$**
  - Merge two closest clusters.
- Save both clustering and sequence of cluster operations
- A data structure called "**Dendrogram**" is used.

Visualization

Iteration 1



Buildup a sequence of clusters.

Compute distance between all clusters. Find the clusters with smallest distance.

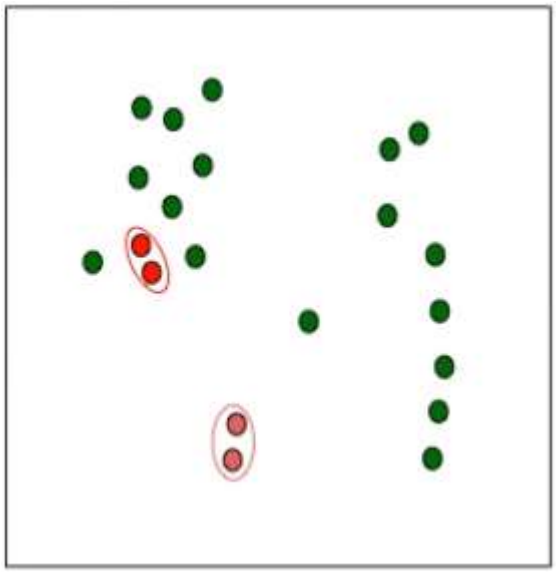
Dendrogram:

Height of the join indicates dissimilarity

Complexity **$O(m^2 \log m) + O(m \log m)$**

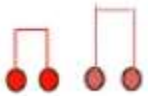
Visualization

Iteration 2



Again, compute distance between all clusters pair including newly formed cluster. Find the cluster pair with smallest distance.

Dendrogram:

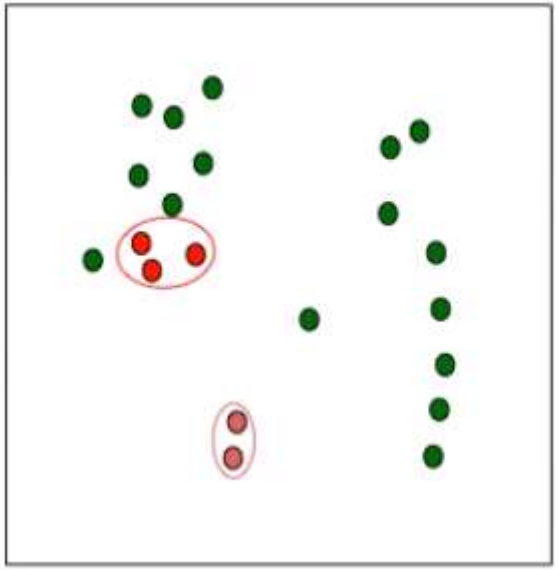


Height of the join indicates dissimilarity

Complexity **$O(m^2 \log m) + 2*O(m \log m)$**

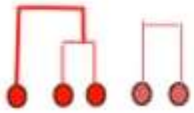
Visualization

Iteration 3



Repeat the same steps to find closest cluster pair.

Dendrogram:

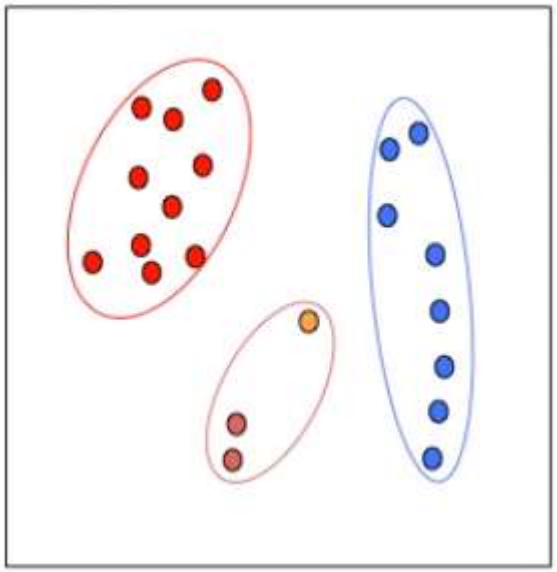


Height of the join indicates dissimilarity

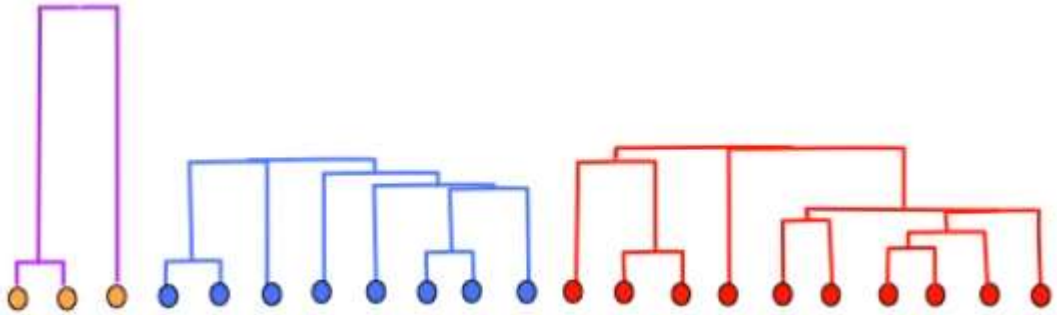
Complexity **$O(m^2 \log m) + 3*O(m \log m)$**

Visualization

Iteration m-3



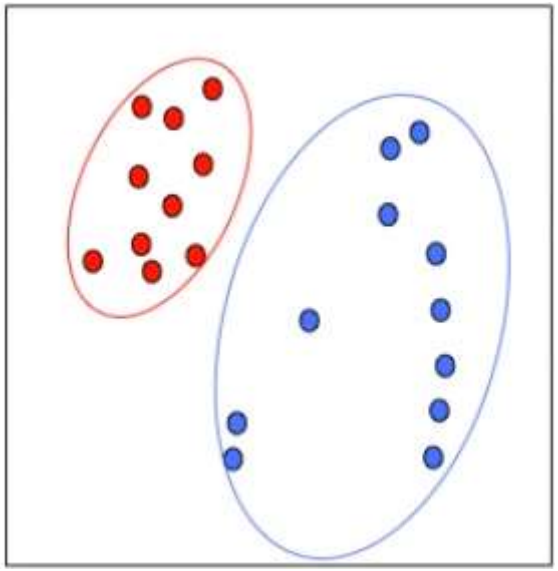
Dendrogram

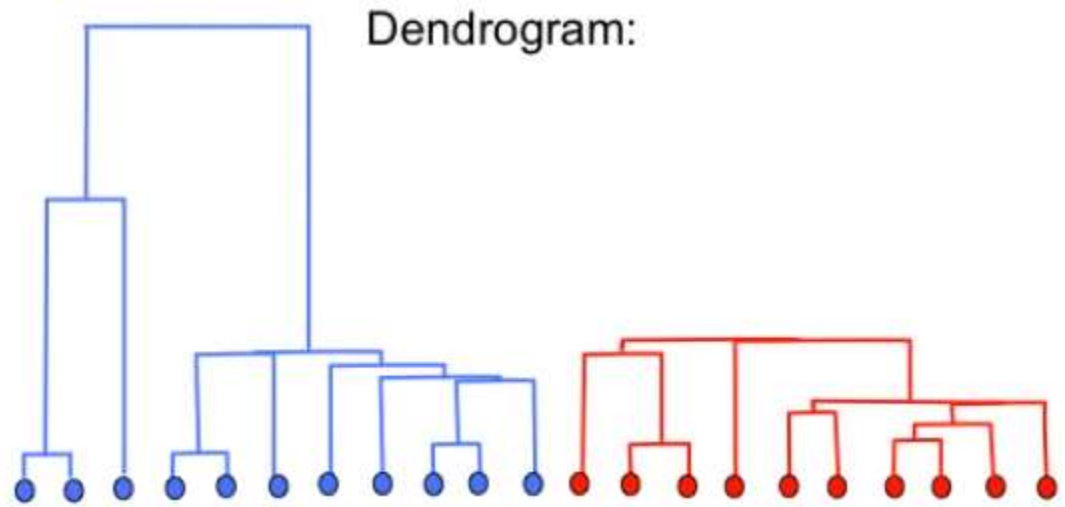


Complexity $\mathbf{O(m^2 \log m) + (m-3)*O(m \log m)}$

Visualization

Iteration m-2

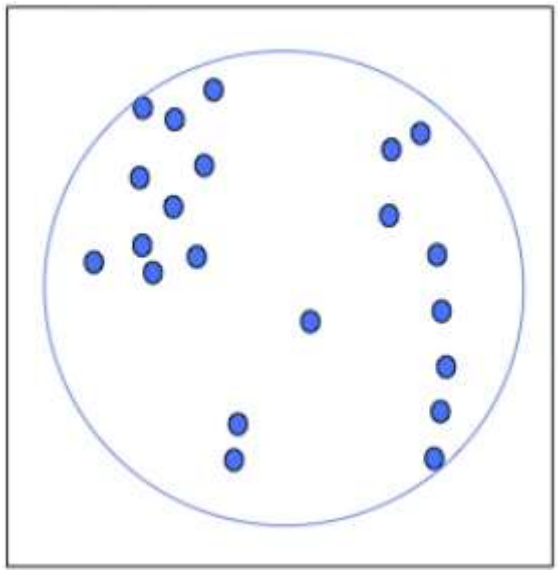


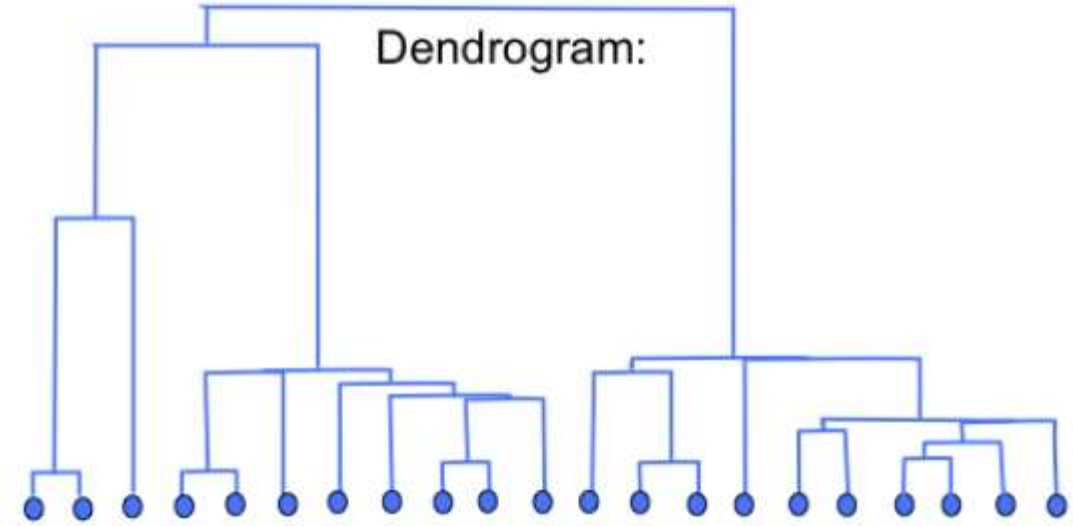


Complexity **$O(m^2 \log m) + (m-2)*O(m \log m)$**

Visualization

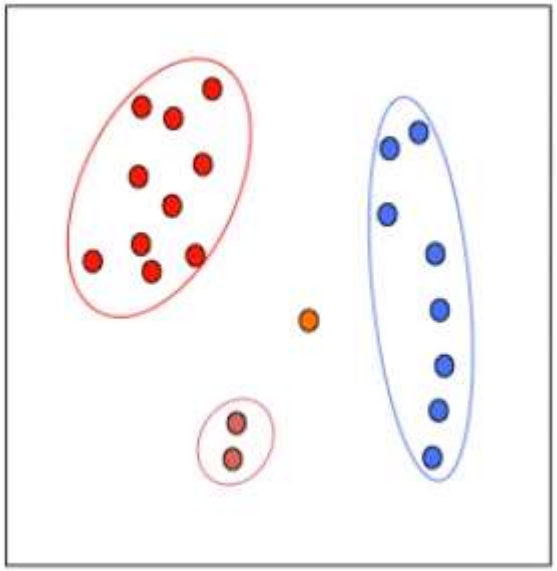
Iteration m-1

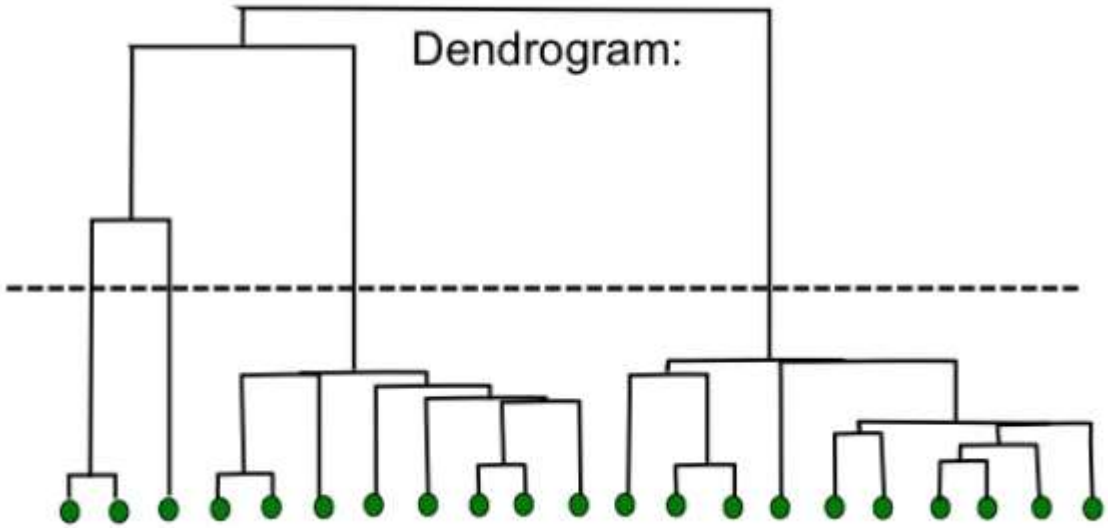




Complexity $\mathbf{O(m^2 \log m) + (m-1)*O(m \log m) = O(m^2 \log m)}$

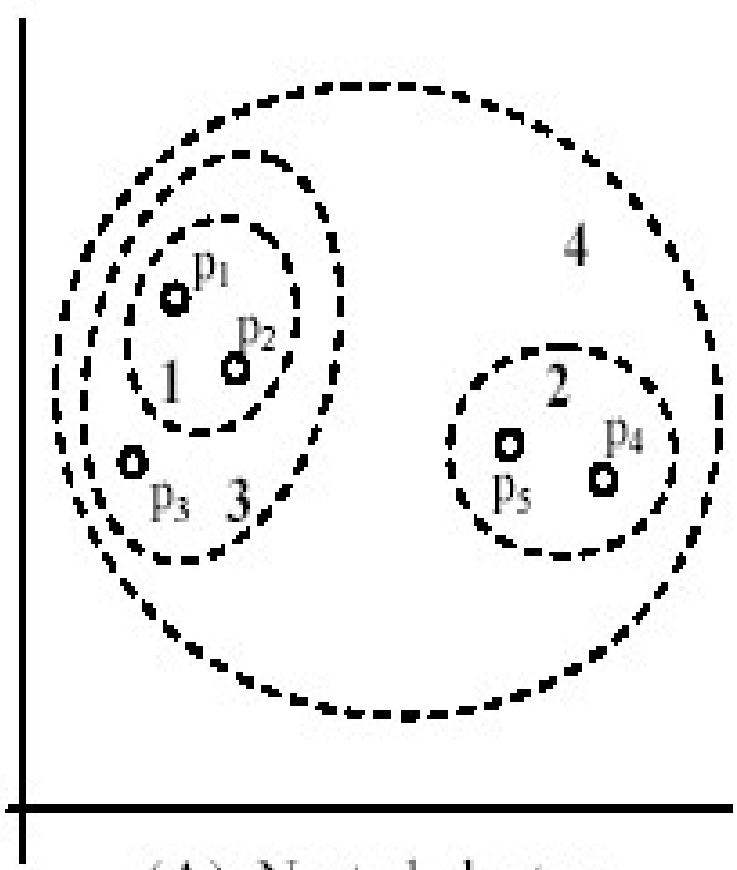
Visualization



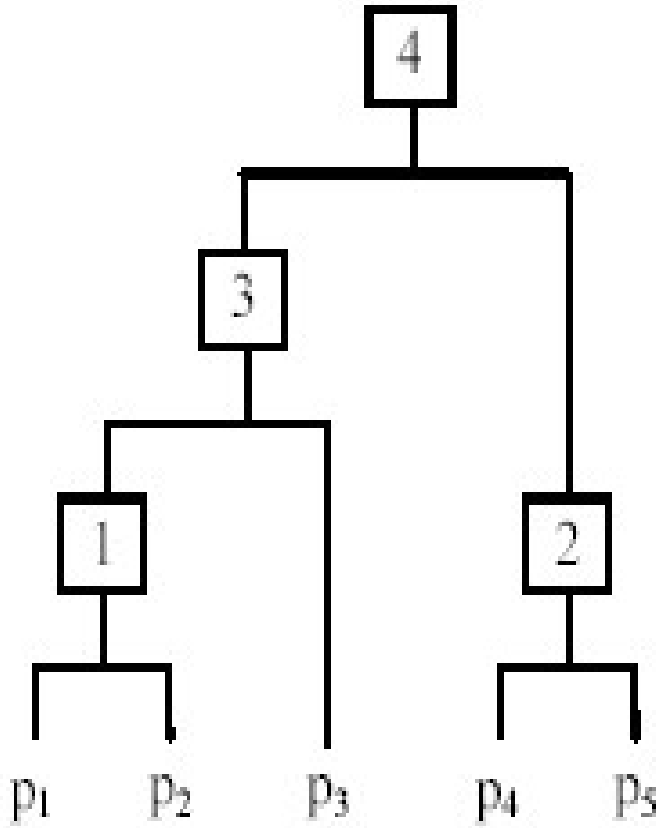


Given the sequence, can select a number of clusters or a dissimilarity threshold

An example: working of the algorithm



(A). Nested clusters



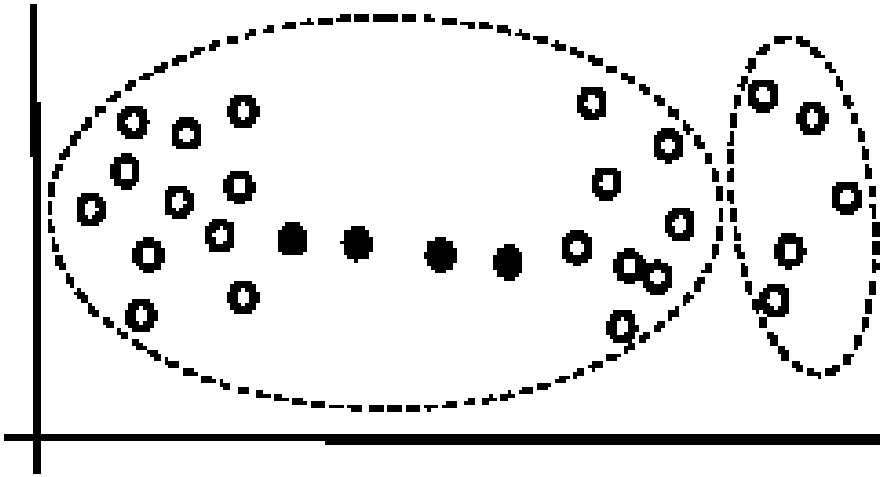
(B) Dendrogram

Measuring the distance of two clusters

- A few ways to measure distances of two clusters.
- Results in different variations of the algorithm.
  - Single link
  - Complete link
  - Average link
  - Centroids
  - …

Single link method

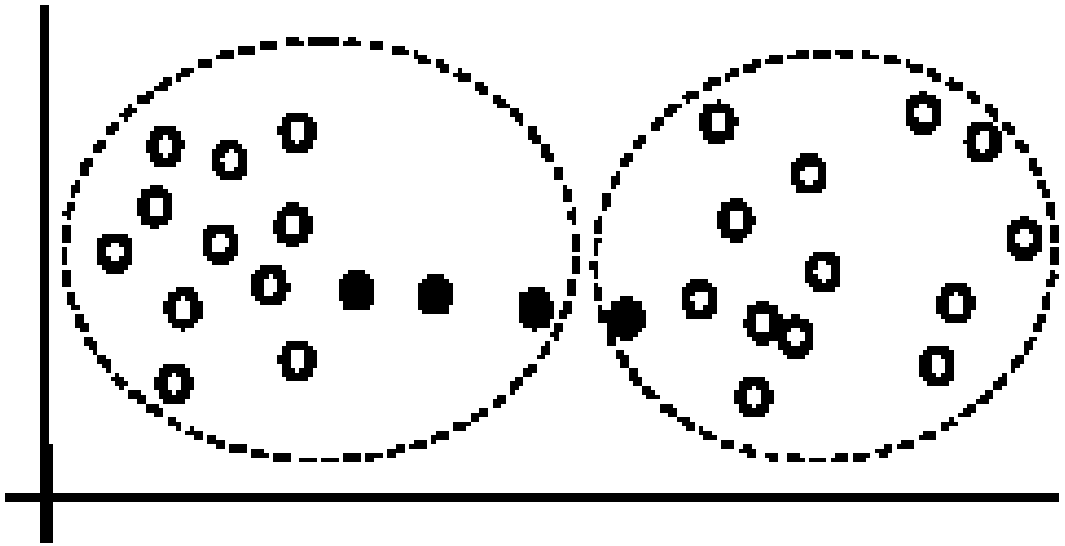
- The distance between two clusters is the distance between two closest data points in the two clusters, one data point from each cluster.
- It can find arbitrarily shaped clusters, but
  - It may cause the undesirable "chain effect" by noisy points



Two natural clusters are split into two

Complete link method

- The distance between two clusters is the distance of two furthest data points in the two clusters.
- It is sensitive to outliers because they are far away

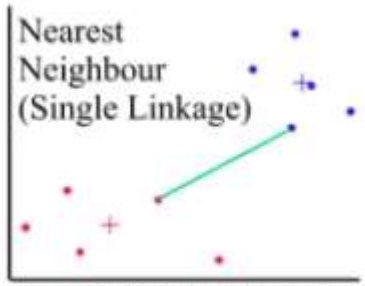


Average link and centroid methods

- Average link: A compromise between
  - the sensitivity of complete-link clustering to outliers and
  - the tendency of single-link clustering to form long chains that do not correspond to the intuitive notion of clusters as compact, spherical objects.
  - In this method, the distance between two clusters is the average distance of all pair-wise distances between the data points in two clusters.
- Centroid method: In this method, the distance between two clusters is the distance between their centroids

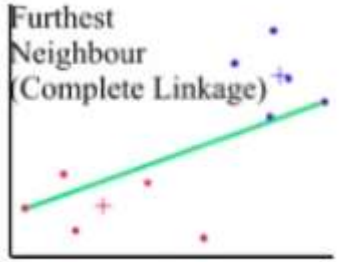
Cluster Distances

$$D_{\min}(C_i, C_j) = \min_{x \in C_i,\ y \in C_j} \|x - y\|^2$$



produces minimal spanning tree.

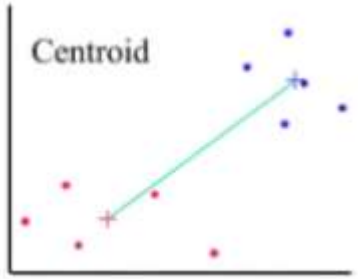
$$D_{\max}(C_i, C_j) = \max_{x \in C_i,\ y \in C_j} \|x - y\|^2$$



avoids elongated clusters.

$$D_{\text{avg}}(C_i, C_j) = \frac{1}{|C_i||C_j|} \sum_{x \in C_i,\ y \in C_j} \|x - y\|^2$$

$$D_{\text{means}}(C_i, C_j) = \|\mu_i - \mu_j\|^2$$



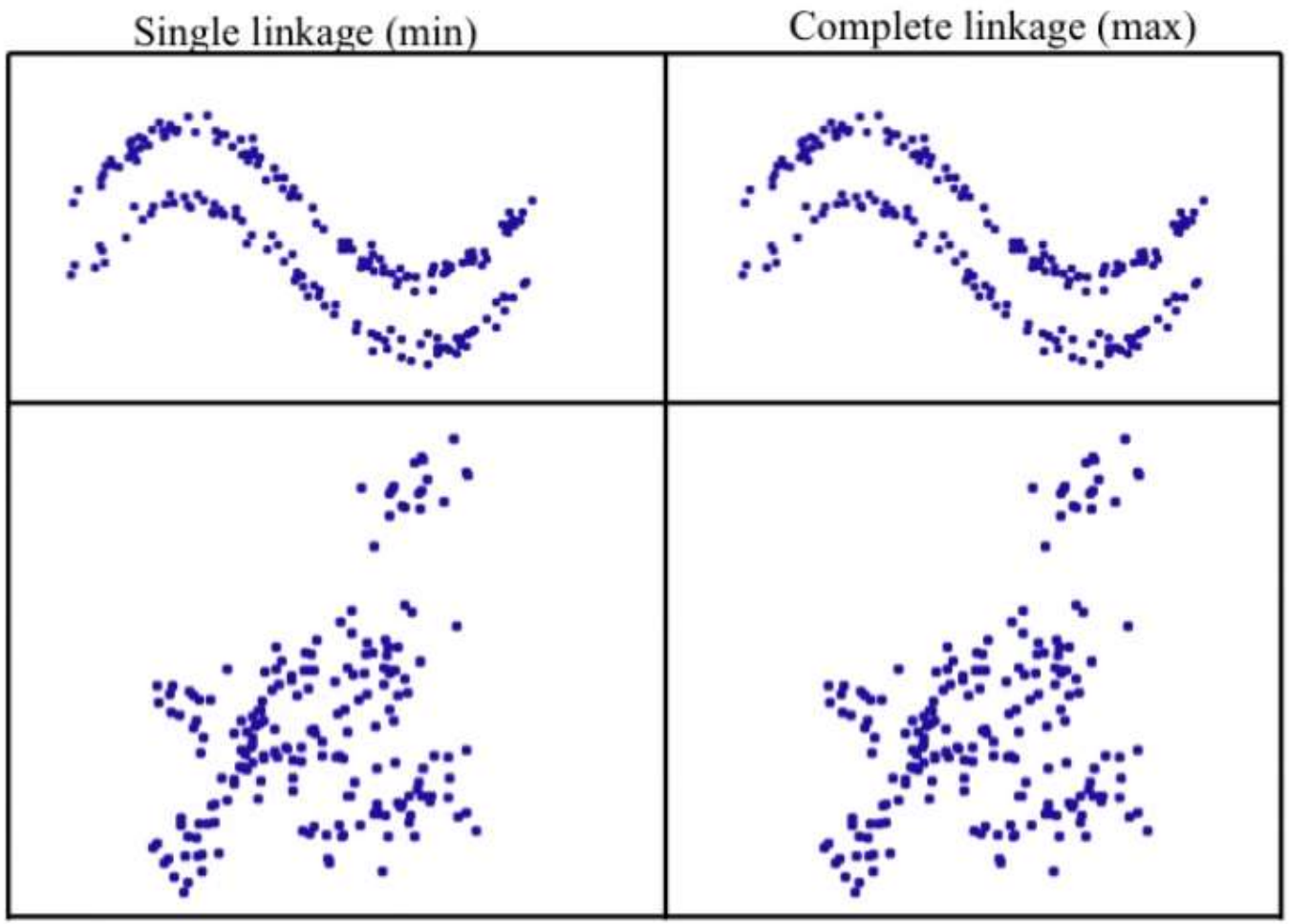
Need:

D(A,C) → D(A+B,C)

D(B,C) →

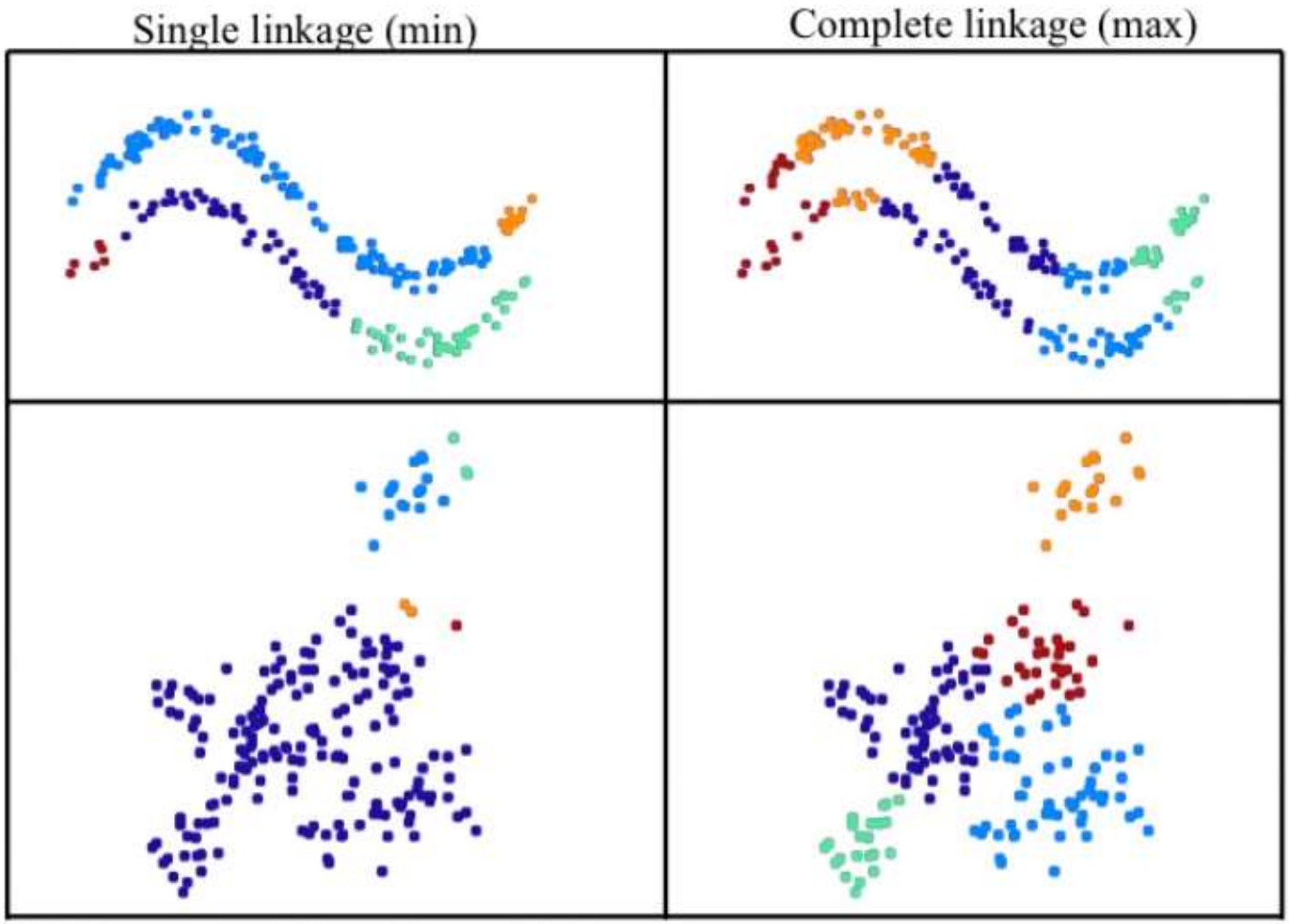
Cluster Distance

Dissimilarity choice will affect the clusters created



Cluster Distance

Dissimilarity choice will affect the clusters created



The complexity

- All the algorithms are at least $O(n^2)$. n is the number of data points.
- Single link can be done in $O(n^2)$.
- Complete and average links can be done in $O(n^2 \log n)$.
- Due the complexity, hard to use for large data sets.
  - Sampling
  - Scale-up methods (e.g., BIRCH).

Road map

- Basic concepts
- K-means algorithm
- Representation of clusters
- Hierarchical clustering
- Probability Density Estimation
- Distance functions
- Data standardization
- Handling mixed attributes
- Which clustering algorithm to use?
- Cluster evaluation
- Discovering holes and data regions
- Summary

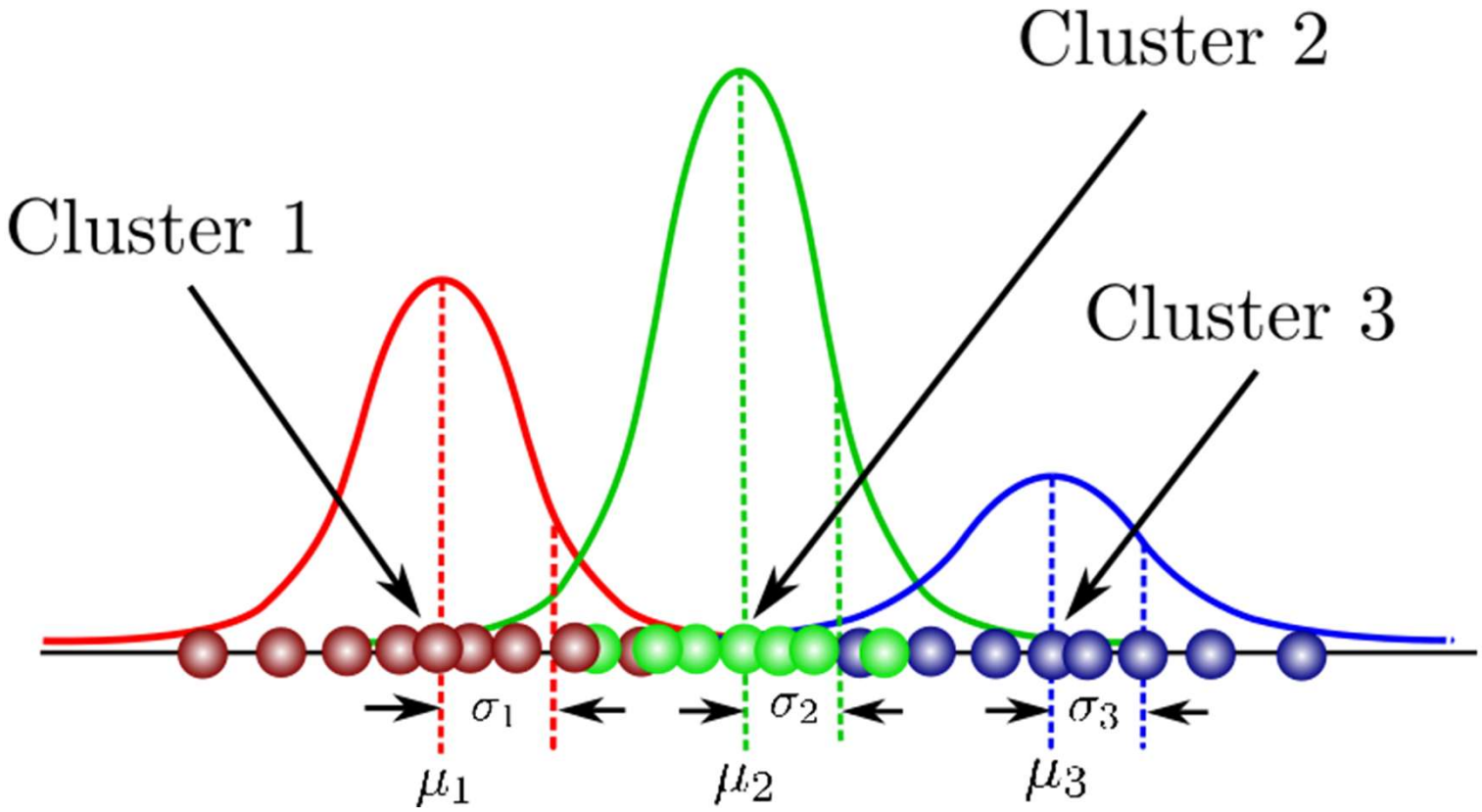
Probability Density Estimation

- Gaussian Mixture Model
- Expectation Maximization

Why Mixture of Gaussian

- Gaussian is in general more closer to the natural distributions and mathematically is more easy to handle (series of differentiations etc.).
- In most cases, specially Mahalanobis Distance, Covariance matrix etc., it has been assumed that the underline data distribution is Gaussian in nature. But, in practical scenario, it may not always necessarily true.
- Sometimes, a dataset with complicated data distribution can be approximated by a weighted summation of multiple Gaussian distributions (popularly called mixture of Gaussian).
- We can cluster the data in several components/parts and assume that each of such components follows Gaussian distribution.

Gaussian Mixture Model



Univariate Gaussian Distribution

- Gaussian or normal distribution, 1D

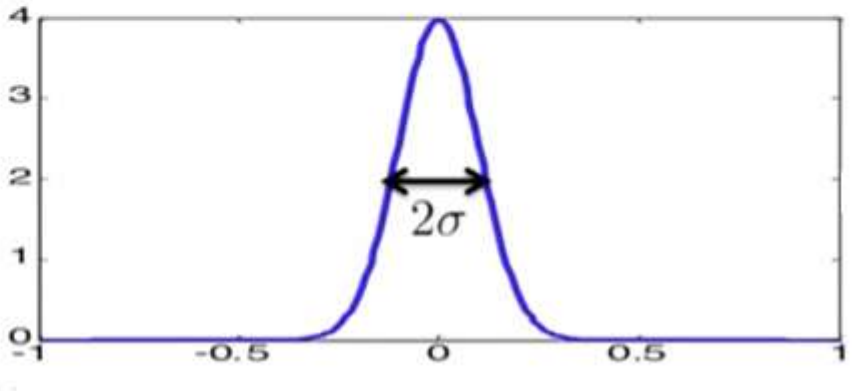
$$\mathcal{N}(x\ ;\ \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2}(x-\mu)^2/\sigma^2\right]$$

  - Parameters: mean μ, variance σ^2
    (standard deviation σ)

Maximum Likelihood estimates

$$\hat{\mu} = \frac{1}{N}\sum_i x^{(i)}$$

$$\hat{\sigma}^2 = \frac{1}{N}\sum_i (x^{(i)} - \hat{\mu})^2$$

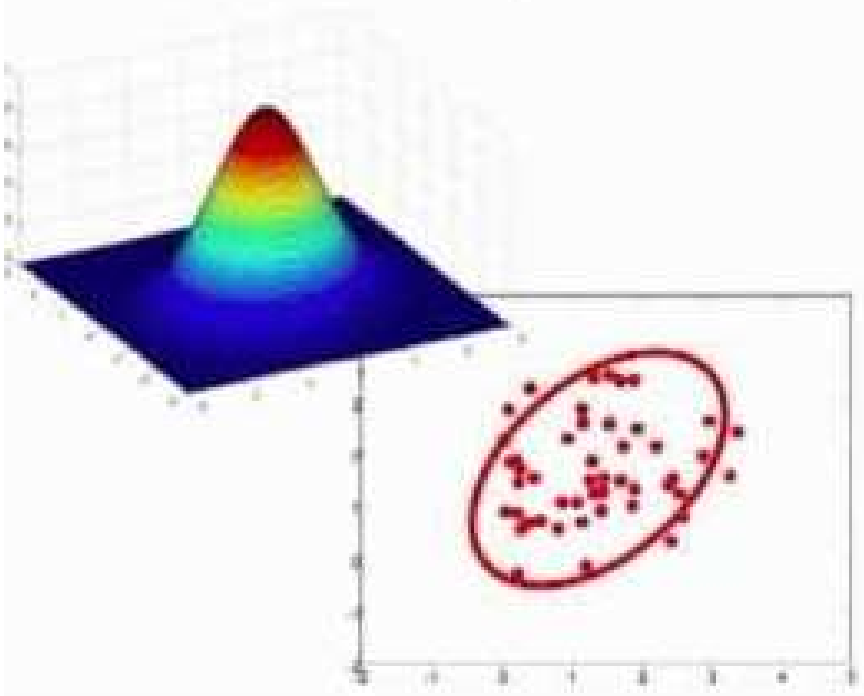


Slide Credit: Alexander Ihler

Multivariate Gaussian Distribution

- Similar to univariate case

$$\mathcal{N}(\underline{x}; \underline{\mu}, \Sigma) = \frac{1}{(2\pi)^{d/2}} |\Sigma|^{-1/2} \exp\left\{ -\frac{1}{2} (\underline{x} - \underline{\mu}) \Sigma^{-1} (\underline{x} - \underline{\mu})^T \right\}$$



μ = length-d row vector
Σ = d x d matrix

$|\Sigma|$ = matrix determinant

Maximum likelihood estimate:

$$\hat{\mu} = \frac{1}{m} \sum_j \underline{x}^{(j)}$$

$$\hat{\Sigma} = \frac{1}{m} \sum_j (\underline{x}^{(j)} - \hat{\mu})^T (\underline{x}^{(j)} - \hat{\mu})$$

(average of dxd matrices)

Slide Credit: Alexander Ihler

Goal:

- We want to estimate μ and Σ of a distribution.
- Method: Maximum Likelihood Estimation (MLE)

ML method for estimating parameters

- Consider the log of Gaussian distribution

$$\ln p(x \mid \mu, \Sigma) = -\frac{1}{2}\ln(2\pi) - \frac{1}{2}\ln|\Sigma| - \frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)$$

- Take the derivatives and equate them to zero

$$\frac{\partial \ln p(x \mid \mu, \Sigma)}{\partial \mu} = 0$$

$$\frac{\partial \ln p(x \mid \mu, \Sigma)}{\partial \Sigma} = 0$$

$$\mu_{ML} = \frac{1}{N}\sum_{n=1}^{N} x_n$$

$$\Sigma_{ML} = \frac{1}{N}\sum_{n=1}^{N} (x_n - \mu_{ML})(x_n - \mu_{ML})^T$$

where N is no. of data samples

Gaussian Mixture

- Linear superposition of Gaussian

$$p(x) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x \mid \mu_k, \Sigma_k)$$

Number of Gaussians

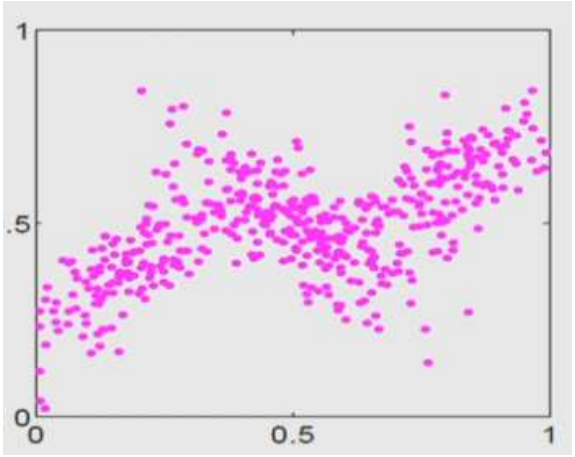
Mixing coefficient: weightage for each Gaussian dist.

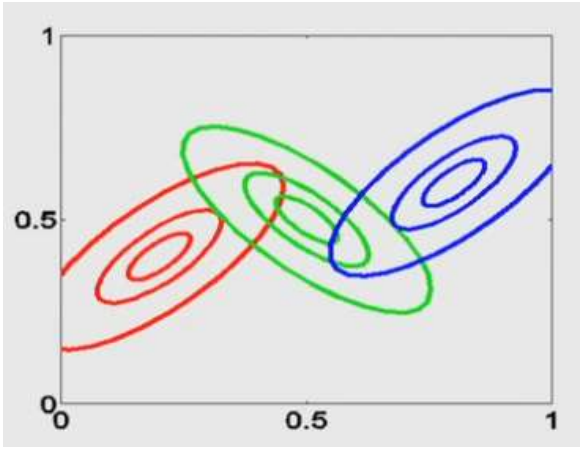
where $0 \le \pi_k \le 1, \quad \sum_{k=1}^{K} \pi_k = 1$

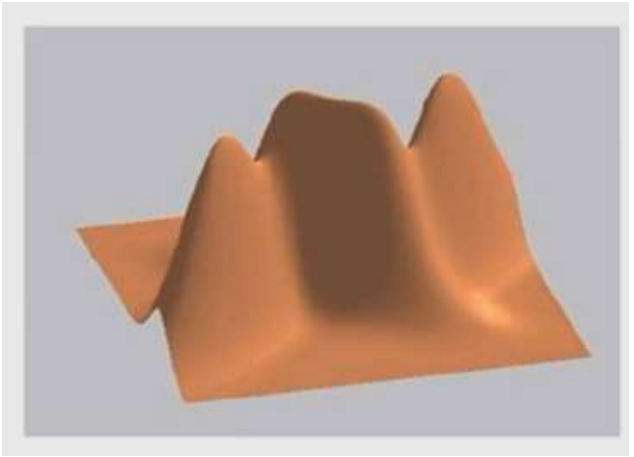
- Log likelihood of the overall function: $\ln p(X|\mu, \Sigma, \pi) =$

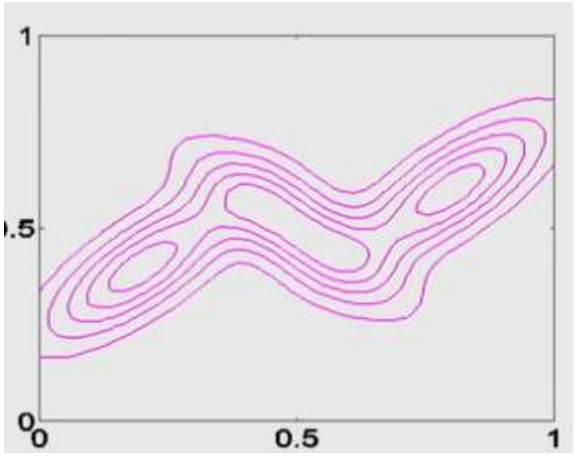
$$\sum_{n=1}^{N} \ln p(x_n) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n \mid \mu_k, \Sigma_k) \right\}$$

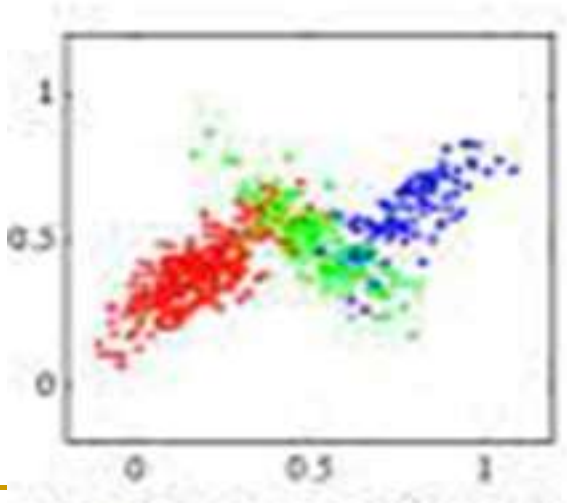
Example: GMM











Problem

- ML is not suitable here as it does not provide any closed form solution.

- Parameters can be calculated using
  - Expectation Maximization (EM) technique

to continue...

Distance functions

- Key to clustering. “similarity” and “dissimilarity” can also commonly used terms.
- There are numerous distance functions for
  - Different types of data
    - Numeric data
    - Nominal data
  - Different specific applications

Distance functions for numeric attributes

- Most commonly used functions are
  - Euclidean distance and
  - Manhattan (city block) distance
- We denote distance with: *dist*($\mathbf{x}_i$, $\mathbf{x}_j$), where $\mathbf{x}_i$ and $\mathbf{x}_j$ are data points (vectors)
- They are special cases of Minkowski distance. h is positive integer.

$$dist(\mathbf{x}_i, \mathbf{x}_j) = ((x_{i1} - x_{j1})^h + (x_{i2} - x_{j2})^h + ... + (x_{ir} - x_{jr})^h)^{\frac{1}{h}}$$

Euclidean distance and Manhattan distance

- If *h* = 2, it is the Euclidean distance

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{(x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \ldots + (x_{ir} - x_{jr})^2}$$

- If *h* = 1, it is the Manhattan distance

$$dist(\mathbf{x}_i, \mathbf{x}_j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + \ldots + |x_{ir} - x_{jr}|$$

- Weighted Euclidean distance

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{w_1(x_{i1} - x_{j1})^2 + w_2(x_{i2} - x_{j2})^2 + \ldots + w_r(x_{ir} - x_{jr})^2}$$

Squared distance and Chebychev distance

- Squared Euclidean distance: to place progressively greater weight on data points that are further apart.

$$dist(\mathbf{x}_i, \mathbf{x}_j) = (x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \ldots + (x_{ir} - x_{jr})^2$$

- Chebychev distance: one wants to define two data points as "different" if they are different on any one of the attributes.

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \max(|x_{i1} - x_{j1}|, |x_{i2} - x_{j2}|, \ldots, |x_{ir} - x_{jr}|)$$

Distance functions for binary and nominal attributes

- Binary attribute: has two values or states but no ordering relationships, e.g.,
  - Gender: male and female.
- We use a confusion matrix to introduce the distance functions/measures.
- Let the *i*th and *j*th data points be $\mathbf{x}_i$ and $\mathbf{x}_j$ (vectors)

Confusion matrix

Data point i \ Data point j	1	0	
1	a	b	$a+b$
0	c	d	$c+d$
	$a+c$	$b+d$	$a+b+c+d$

(10)

a: the number of attributes with the value of 1 for both data points.

b: the number of attributes for which $x_{if} = 1$ and $x_{jf} = 0$, where x_{if} (x_{jf}) is the value of the fth attribute of the data point $\mathbf{x}_i$ ($\mathbf{x}_j$).

c: the number of attributes for which $x_{if} = 0$ and $x_{jf} = 1$.

d: the number of attributes with the value of 0 for both data points.

Symmetric binary attributes

- A binary attribute is **symmetric** if both of its states (0 and 1) have equal importance, and carry the same weights, e.g., male and female of the attribute Gender
- Distance function: Simple Matching Coefficient, proportion of mismatches of their values

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \frac{b + c}{a + b + c + d}$$

Symmetric binary attributes: example

$\mathbf{x}_1$	1	1	1	0	1	0	0
$\mathbf{x}_2$	0	1	1	0	0	1	0

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \frac{2+1}{2+2+1+2} = \frac{3}{7} = 0.429$$

Asymmetric binary attributes

- Asymmetric: if one of the states is more important or more valuable than the other.
  - By convention, state 1 represents the more important state, which is typically the rare or infrequent state.
  - Jaccard coefficient is a popular measure

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \frac{b + c}{a + b + c}$$

  - We can have some variations, adding weights

Nominal attributes

- Nominal attributes: with more than two states or values.
  - the commonly used distance measure is also based on the simple matching method.
  - Given two data points $\mathbf{x}_i$ and $\mathbf{x}_j$, let the number of attributes be r, and the number of values that match in $\mathbf{x}_i$ and $\mathbf{x}_j$ be q.

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \frac{r - q}{r}$$

Distance function for text documents

- A text document consists of a sequence of sentences and each sentence consists of a sequence of words.
- To simplify: a document is usually considered a "bag" of words in document clustering.
  - Sequence and position of words are ignored.
- A document is represented with a vector just like a normal data point.
- It is common to use similarity to compare two documents rather than distance.
  - The most commonly used similarity function is the **cosine similarity**. We will study this later.

Road map

- Basic concepts
- K-means algorithm
- Representation of clusters
- Hierarchical clustering
- Distance functions
- Data standardization
- Handling mixed attributes
- Which clustering algorithm to use?
- Cluster evaluation
- Discovering holes and data regions
- Summary

Data standardization

- In the Euclidean space, standardization of attributes is recommended so that all attributes can have equal impact on the computation of distances.
- Consider the following pair of data points
  - $\mathbf{x}_i$: (0.1, 20) and $\mathbf{x}_j$: (0.9, 720).

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{(0.9 - 0.1)^2 + (720 - 20)^2} = 700.000457,$$

- The distance is almost completely dominated by (720-20) = 700.
- Standardize attributes: to force the attributes to have a common value range

Interval-scaled attributes

- Their values are real numbers following a linear scale.
  - The difference in Age between 10 and 20 is the same as that between 40 and 50.
  - The key idea is that intervals keep the same importance through out the scale
- Two main approaches to standardize interval scaled attributes, **range** and **z-score**. *f* is an attribute

$$range(x_{if}) = \frac{x_{if} - \min(f)}{\max(f) - \min(f)},$$

Interval-scaled attributes (cont …)

- Z-score: transforms the attribute values so that they have a mean of zero and a **mean absolute deviation** of 1. The mean absolute deviation of attribute *f*, denoted by s_f, is computed as follows

$$s_f = \frac{1}{n}\left(| x_{1f} - m_f | + | x_{2f} - m_f | + ... + | x_{nf} - m_f | \right),$$

$$m_f = \frac{1}{n}\left(x_{1f} + x_{2f} + ... + x_{nf} \right),$$

Z-score: $$z(x_{if}) = \frac{x_{if} - m_f}{s_f}.$$

Ratio-scaled attributes

- Numeric attributes, but unlike interval-scaled attributes, their scales are exponential,
- For example, the total amount of microorganisms that evolve in a time *t* is approximately given by

  $$Ae^{Bt},$$

  - where *A* and *B* are some positive constants.
- Do log transform: $\log(x_{if})$
  - Then treat it as an interval-scaled attribuete

Nominal attributes

- Sometime, we need to transform nominal attributes to numeric attributes.
- Transform nominal attributes to binary attributes.
  - The number of values of a nominal attribute is *v*.
  - Create *v* binary attributes to represent them.
  - If a data instance for the nominal attribute takes a particular value, the value of its binary attribute is set to 1, otherwise it is set to 0.
- The resulting binary attributes can be used as numeric attributes, with two values, 0 and 1.

Nominal attributes: an example

- Nominal attribute *fruit*: has three values,
  - Apple, Orange, and Pear
- We create three binary attributes called, Apple, Orange, and Pear in the new data.
- If a particular data instance in the original data has Apple as the value for *fruit*,
  - then in the transformed data, we set the value of the attribute Apple to 1, and
  - the values of attributes Orange and Pear to 0

Ordinal attributes

- Ordinal attribute: an ordinal attribute is like a nominal attribute, but its values have a numerical ordering. E.g.,
  - Age attribute with values: Young, MiddleAge and Old. They are ordered.
  - Common approach to standardization: treat is as an interval-scaled attribute.

Road map

- Basic concepts
- K-means algorithm
- Representation of clusters
- Hierarchical clustering
- Distance functions
- Data standardization
- Handling mixed attributes
- Which clustering algorithm to use?
- Cluster evaluation
- Discovering holes and data regions
- Summary

Mixed attributes

- Our distance functions given are for data with all numeric attributes, or all nominal attributes, etc.
- Practical data has different types:
  - Any subset of the 6 types of attributes,
    - **interval-scaled**,
    - **symmetric binary**,
    - **asymmetric binary**,
    - **ratio-scaled**,
    - **ordinal** and
    - **nominal**

Convert to a single type

- One common way of dealing with mixed attributes is to
  - Decide the dominant attribute type, and
  - Convert the other types to this type.
- E.g, if most attributes in a data set are interval-scaled,
  - we convert ordinal attributes and ratio-scaled attributes to interval-scaled attributes.
  - It is also appropriate to treat symmetric binary attributes as interval-scaled attributes.

Convert to a single type (cont …)

- It does not make much sense to convert a nominal attribute or an asymmetric binary attribute to an interval-scaled attribute,
  - but it is still frequently done in practice by assigning some numbers to them according to some hidden ordering, e.g., prices of the fruits
- Alternatively, a nominal attribute can be converted to a set of (symmetric) binary attributes, which are then treated as numeric attributes.

Combining individual distances

- This approach computes individual attribute distances and then combine them.

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \frac{\sum_{f=1}^{r} \delta_{ij}^f d_{ij}^f}{\sum_{f=1}^{r} \delta_{ij}^f}$$

This distance value is between 0 and 1. r is the number of attributes in the data set. The indicator δ_{ij}^f is 1 when both values x_{if} and x_{jf} for attribute f are non-missing, and it is set to 0 otherwise. It is also set to 0 if attribute f is asymmetric and the match is 0-0. Equation (25) cannot be computed if all δ_{ij}^f's are 0. In such a case, some default value may be used or one of the data points is removed.

d_{ij}^f is the distance contributed by attribute f, and it is in the 0-1 range.

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How to choose a clustering algorithm

- Clustering research has a long history. A vast collection of algorithms are available.
  - We only introduced several main algorithms.
- Choosing the "best" algorithm is a challenge.
  - Every algorithm has limitations and works well with certain data distributions.
  - It is very hard, if not impossible, to know what distribution the application data follow. The data may not fully follow any "ideal" structure or distribution required by the algorithms.
  - One also needs to decide how to standardize the data, to choose a suitable distance function and to select other parameter values.

Choose a clustering algorithm (cont …)

- Due to these complexities, the common practice is to
  - run several algorithms using different distance functions and parameter settings, and
  - then carefully analyze and compare the results.
- The interpretation of the results must be based on insight into the meaning of the original data together with knowledge of the algorithms used.
- Clustering is highly application dependent and to certain extent subjective (personal preferences).

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Cluster Evaluation: hard problem

- The quality of a clustering is very hard to evaluate because
  - We do not know the correct clusters
- Some methods are used:
  - User inspection
    - Study centroids, and spreads
    - Rules from a decision tree.
    - For text documents, one can read some documents in clusters.

Cluster evaluation: ground truth

- We use some labeled data (for classification)
- Assumption: Each class is a cluster.
- After clustering, a confusion matrix is constructed. From the matrix, we compute various measurements, entropy, purity, precision, recall and F-score.
  - Let the classes in the data D be $C = (c_1, c_2, \ldots, c_k)$. The clustering method produces k clusters, which divides D into k disjoint subsets, $D_1, D_2, \ldots, D_k$.

Evaluation measures: Entropy

Entropy: For each cluster, we can measure its entropy as follows:

$$entropy(D_i) = -\sum_{j=1}^{k} \Pr_i(c_j) \log_2 \Pr_i(c_j), \qquad (29)$$

where $\Pr_i(c_j)$ is the proportion of class c_j data points in cluster i or D_i. The total entropy of the whole clustering (which considers all clusters) is

$$entropy_{total}(D) = \sum_{i=1}^{k} \frac{|D_i|}{|D|} \times entropy(D_i) \qquad (30)$$

Evaluation measures: purity

Purity: This again measures the extent that a cluster contains only one class of data. The purity of each cluster is computed with

$$purity(D_i) = \max_j(\Pr_i(c_j)) \tag{31}$$

The total purity of the whole clustering (considering all clusters) is

$$purity_{total}(D) = \sum_{i=1}^{k} \frac{|D_i|}{|D|} \times purity(D_i) \tag{32}$$

An example

Example 14: Assume we have a text collection D of 900 documents from three topics (or three classes), Science, Sports, and Politics. Each class has 300 documents. Each document in D is labeled with one of the topics (classes). We use this collection to perform clustering to find three clusters. Note that class/topic labels are not used in clustering. After clustering, we want to measure the effectiveness of the clustering algorithm.

Cluster	Science	Sports	Politics		Entropy	Purity
1	250	20	10		0.589	0.893
2	20	180	80		1.198	0.643
3	30	100	210		1.257	0.617
Total	300	300	300		1.031	0.711

A remark about ground truth evaluation

- Commonly used to compare different clustering algorithms.
- A real-life data set for clustering has no class labels.
  - Thus although an algorithm may perform very well on some labeled data sets, no guarantee that it will perform well on the actual application data at hand.
- The fact that it performs well on some label data sets does give us some confidence of the quality of the algorithm.
- This evaluation method is said to be based on **external data** or information.

Evaluation based on internal information

- **Intra-cluster cohesion** (compactness):
  - Cohesion measures how near the data points in a cluster are to the cluster centroid.
  - Sum of squared error (SSE) is a commonly used measure.
- **Inter-cluster separation** (isolation):
  - Separation means that different cluster centroids should be far away from one another.
- In most applications, expert judgments are still the key.

Indirect evaluation

- In some applications, clustering is not the primary task, but used to help perform another task.
- We can use the performance on the primary task to compare clustering methods.
- For instance, in an application, the primary task is to provide recommendations on book purchasing to online shoppers.
  - If we can cluster books according to their features, we might be able to provide better recommendations.
  - We can evaluate different clustering algorithms based on how well they help with the recommendation task.
  - Here, we assume that the recommendation can be reliably evaluated.

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Holes in data space

- All the clustering algorithms only group data.
- Clusters only represent one aspect of the knowledge in the data.
- Another aspect that we have not studied is the **holes**.
  - A hole is a region in the data space that contains no or few data points. Reasons:
    - insufficient data in certain areas, and/or
    - certain attribute-value combinations are not possible or seldom occur.

Holes are useful too

- Although clusters are important, holes in the space can be quite useful too.
- For example, in a disease database
  - we may find that certain symptoms and/or test values do not occur together, or
  - when a certain medicine is used, some test values never go beyond certain ranges.
- Discovery of such information can be important in medical domains because
  - it could mean the discovery of a cure to a disease or some biological laws.

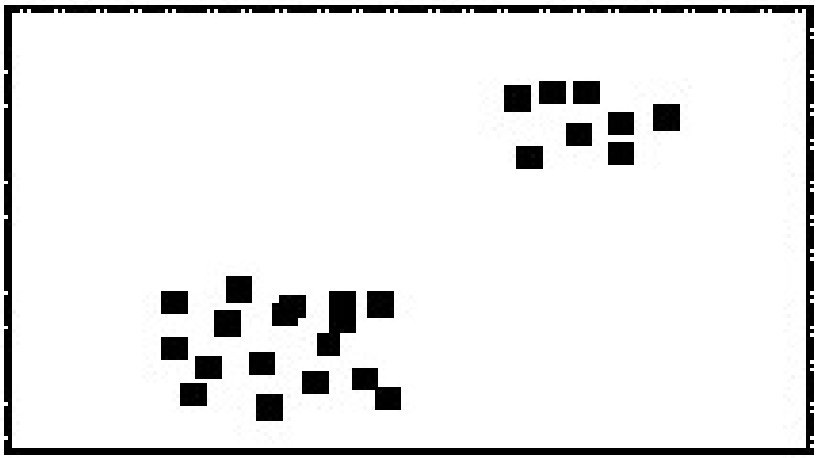
Data regions and empty regions

- Given a data space, separate
  - data regions (clusters) and
  - empty regions (holes, with few or no data points).
- Use a supervised learning technique, i.e., decision tree induction, to separate the two types of regions.
- Due to the use of a supervised learning method for an unsupervised learning task,
  - an interesting connection is made between the two types of learning paradigms.

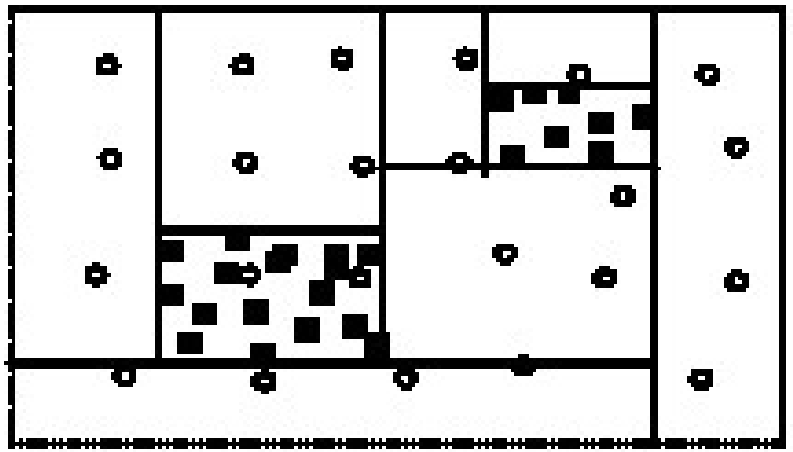
Supervised learning for unsupervised learning

- Decision tree algorithm is not directly applicable.
  - it needs at least two classes of data.
  - A clustering data set has no class label for each data point.
- The problem can be dealt with by a simple idea.
  - Regard each point in the data set to have a class label *Y*.
  - Assume that the data space is uniformly distributed with another type of points, called **non-existing points**. We give them the class, *N*.
- With the *N* points added, the problem of partitioning the data space into data and empty regions becomes a supervised classification problem.

An example



(A): The original data space



(B). Partitioning with added N points

- A decision tree method is used for partitioning in (B).

Can it done without adding N points?

- Yes.
- Physically adding N points increases the size of the data and thus the running time.
- More importantly: it is unlikely that we can have points truly uniformly distributed in a high dimensional space as we would need an exponential number of points.
- Fortunately, no need to physically add any N points.
  - We can compute them when needed

Characteristics of the approach

- It provides representations of the resulting data and empty regions in terms of hyper-rectangles, or rules.
- It detects outliers automatically. Outliers are data points in an empty region.
- It may not use all attributes in the data just as in a normal decision tree for supervised learning.
  - It can automatically determine what attributes are useful. Subspace clustering …
- Drawback: data regions of irregular shapes are hard to handle since decision tree learning only generates hyper-rectangles (formed by axis-parallel hyper-planes), which are rules.

Building the Tree

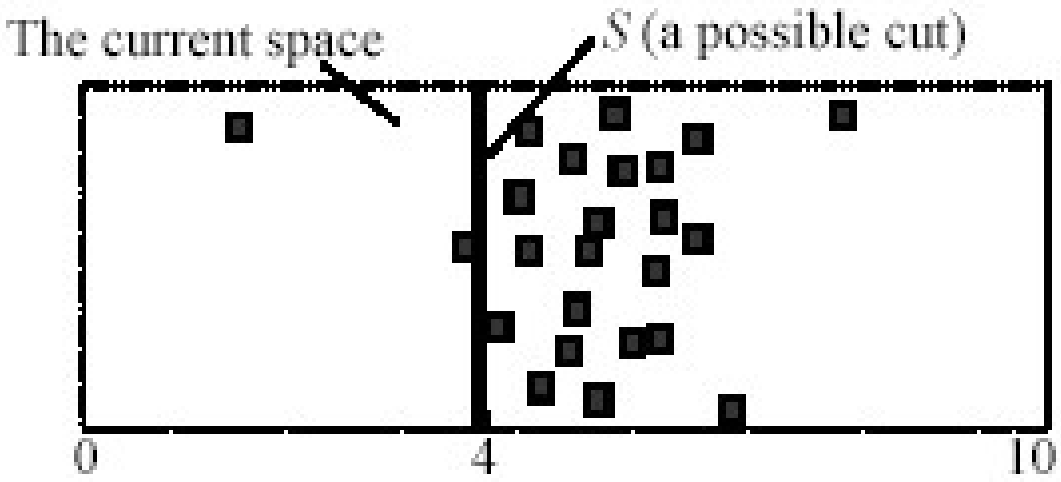
- The main computation in decision tree building is to evaluate entropy (for information gain):

$$entropy(D) = -\sum_{j=1}^{|C|} \Pr(c_j) \log_2 \Pr(c_j)$$

- Can it be evaluated without adding *N* points? Yes.
- Pr(c_j) is the probability of class c_j in data set *D*, and |*C*| is the number of classes, *Y* and *N* (2 classes).
  - To compute Pr(c_j), we only need the number of *Y* (data) points and the number of *N* (non-existing) points.
  - We already have *Y* (or data) points, and we can compute the number of *N* points on the fly. Simple: as we assume that the *N* points are uniformly distributed in the space.

An example

- The space has 25 data (*Y*) points and 25 *N* points. Assume the system is evaluating a possible cut *S*.
  - # *N* points on the left of *S* is 25 * 4/10 = 10. The number of *Y* points is 3.
  - Likewise, # *N* points on the right of *S* is 15 (= 25 - 10).The number of *Y* points is 22.
- With these numbers, entropy can be computed.



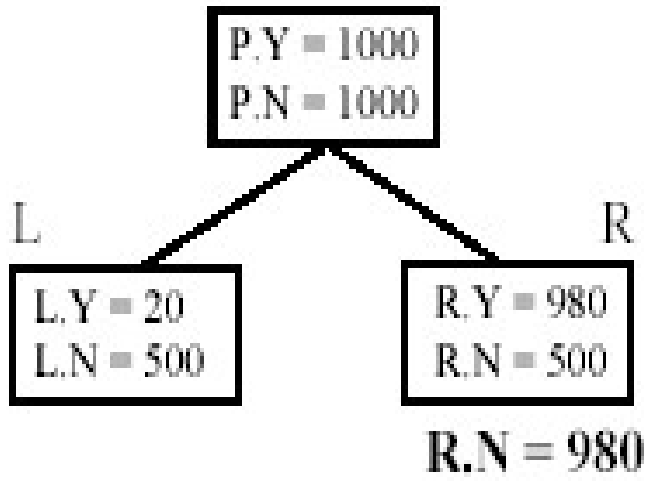
How many *N* points to add?

- We add a different number of *N* points at each different node.
  - The number of *N* points for the current node *E* is determined by the following rule (note that at the root node, the number of inherited *N* points is 0):

1 **If** the number of N points inherited from the parent node of E is less than the number of Y points in E **then**
2 the number of N points for E is increased to the number of Y points in E
3 **else** the number of inherited N points is used for E

An example

Example 17: Fig. 20 gives an example. The (parent) node P has two children nodes L and R. Assume P has 1000 Y points and thus 1000 N points, stored in $P.Y$ and $P.N$ respectively. Assume after splitting, L has 20 Y points and 500 N points, and R has 980 Y points and 500 N points. According to the above rule, for subsequent partitioning, we increase the number of N points at R to 980. The number of N points at L is unchanged.



How many *N* points to add? (cont…)

- Basically, for a *Y* node (which has more data points), we increase *N* points so that

  #Y = #N

- The number of *N* points is not reduced if the current node is an *N* node (an *N* node has more *N* points than *Y* points).
  - A reduction may cause outlier *Y* points to form *Y* nodes (a *Y* node has an equal number of *Y* points as *N* points or more).
  - Then data regions and empty regions may not be separated well.

Building the decision tree

- Using the above ideas, a decision tree can be built to separate data regions and empty regions.
- The actual method is more sophisticated as a few other tricky issues need to be handled in
  - tree building and
  - tree pruning.

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Summary

- Clustering is has along history and still active
  - There are a huge number of clustering algorithms
  - More are still coming every year.
- We only introduced several main algorithms. There are many others, e.g.,
  - density based algorithm, sub-space clustering, scale-up methods, neural networks based methods, fuzzy clustering, co-clustering, etc.
- Clustering is hard to evaluate, but very useful in practice. This partially explains why there are still a large number of clustering algorithms being devised every year.
- Clustering is highly application dependent and to some extent subjective.