Unsupervised Learning

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Supervised learning

- Learning with labeled data.
  - To learn a mapping from the input to an output
    - labels provided by a supervisor.
- Classification
    - Classify digits from hand written numerals.
- Regression
    - Predict the price of a car given a set of its attributes (brand, year, mileage, engine capacity, etc.).

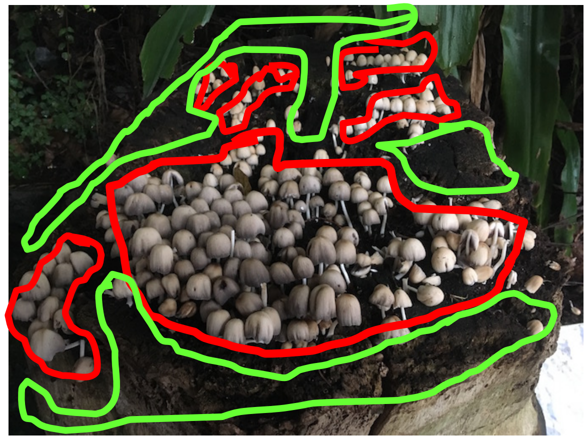
Unsupervised learning

- Learning from only input data.
  - No labels of instances available.
  - no supervisor to provide mapping between input and output.
- The aim is to find the regularities / structures / patterns in the input.
  - Number of clusters?
  - Any hierarchy present among them?
  - How to attribute them with semantics?

Clustering

Clustering: the task of organizing objects into groups whose members are *similar in some way*.

Cluster: a collection of objects *similar to each other*, but dissimilar to the objects belonging to other clusters .



- Regions of homogeneity in an image.
  - Segments.
- Grouping of similar components.

Class and cluster

A class: well studied group of objects identified by their common properties or characteristics.

A cluster: a group with 'loosely' defined similarity among the objects.

- Potential to form a class.

Clustering: Motivation

- finding representatives for homogeneous groups
  - to reduce data.
- discovering natural groups or categories.
  - to describe by their unknown properties.
- finding relevant groups.
  - major groups in the given context.
    - segments of an image.
- detecting unusual data objects
  - outliers.

https://www2.cs.duke.edu/courses/fall03/cps260/notes/lecture18.pdf

K-means clustering

- Given N d-dimensional data points,
  - compute K partitions (clusters) in them
    - so that it minimizes the sum of square of distances between a data point and the center of its respective partition (cluster).

Optimization problem

Minimization of Sum of Squared Errors (SSE)

$$\boxed{E = \sum_{k} \sum_{\forall x \in c_k} \|x - c_k\|^2}$$

where

$$c_k = \frac{1}{|C_k|} \sum_{\forall x \in C_k} x$$

Exhaustive K-Means!

- The number of ways a set of N objects partitioned into K non-empty groups?

$$S(N,K) = \frac{1}{K!}\sum_{i=0}^{K}(-1)^{K-i}\binom{K}{i} i^N$$

Stirling numbers of the second kind.

$$\approx K^N/K!$$

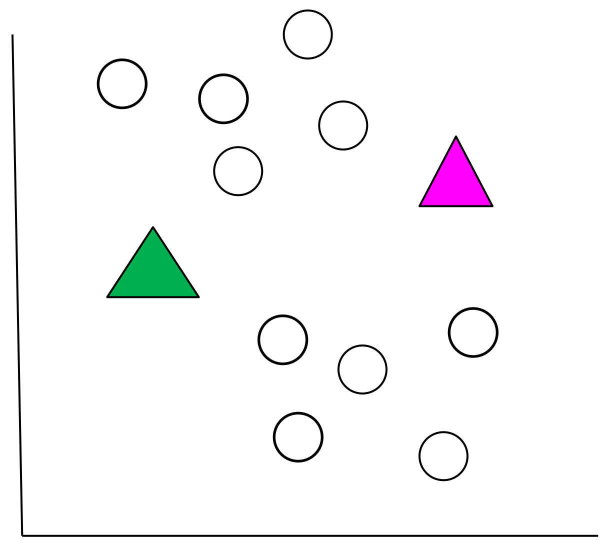
- Checking all possible combinations prohibitive!
  - Of exponential order with input size

An NP-hard problem (K>1).

The Lloyd algorithm (1957) (Batch K-Means)

- Given K initial centers, assign a point to the cluster represented by its center, if it is the closest among them.
- Update the centers.
- Iterate above two steps, till the centers do not change their positions.

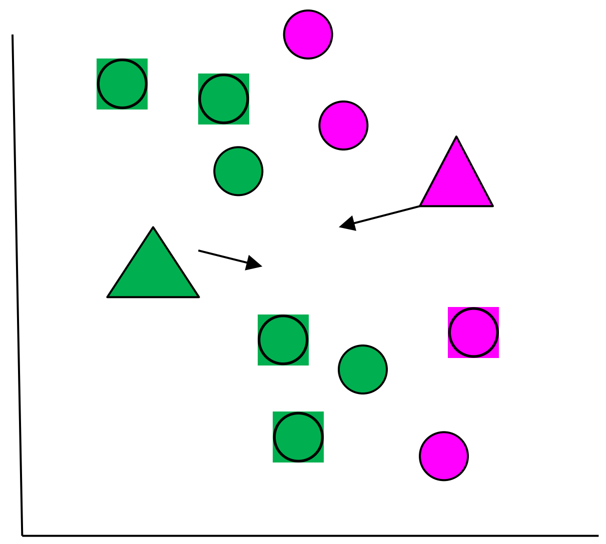
K-means: example (k=2)



Choose initial centers.

Compute partitions.

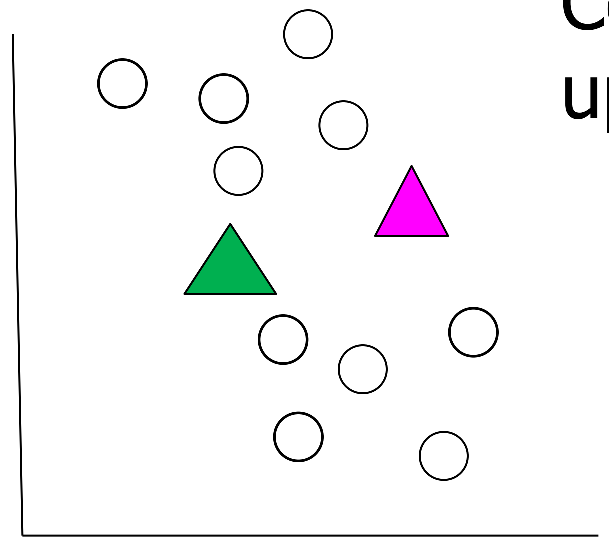
K-means: example (k=2)



Compute partitions.

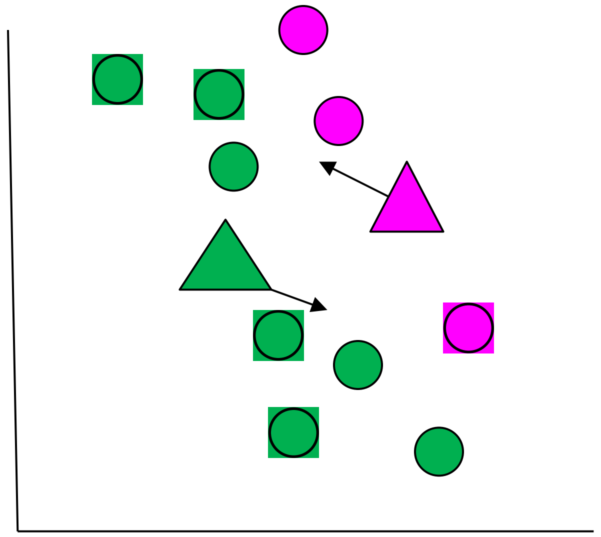
Update centers.

K-means: example (k=2)



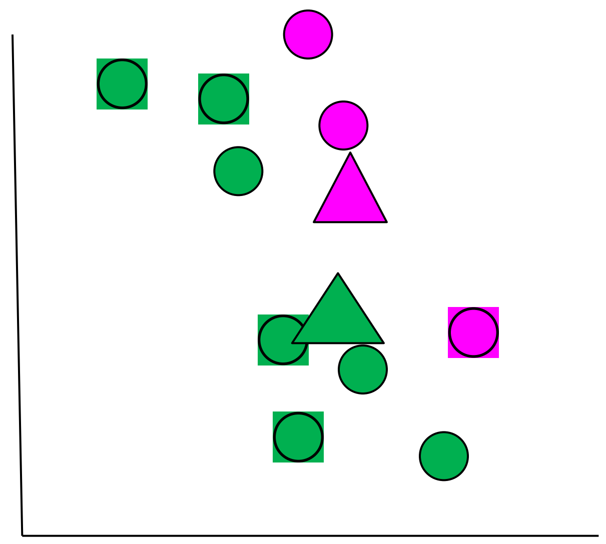
Compute new partitions with updated centers.

K-means: example (k=2)

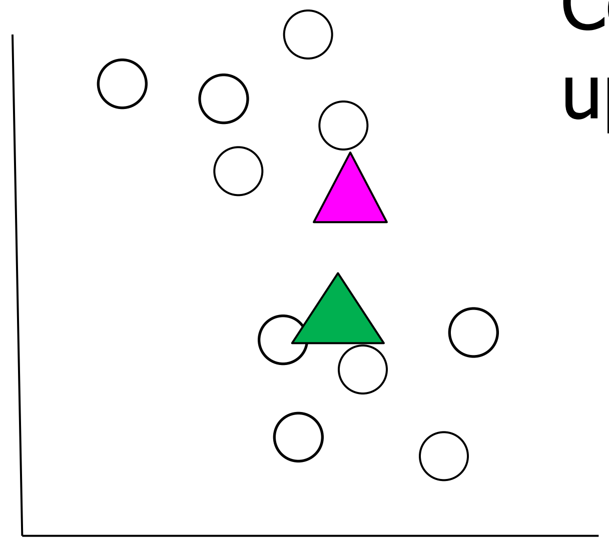


Update centers.

K-means: example (k=2)

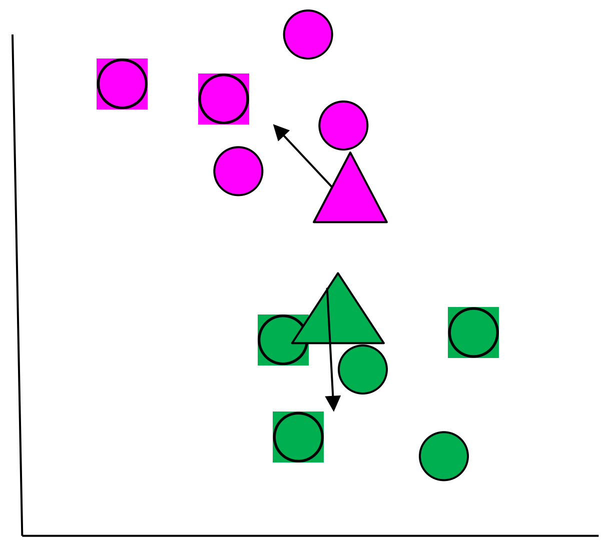


K-means: example (k=2)



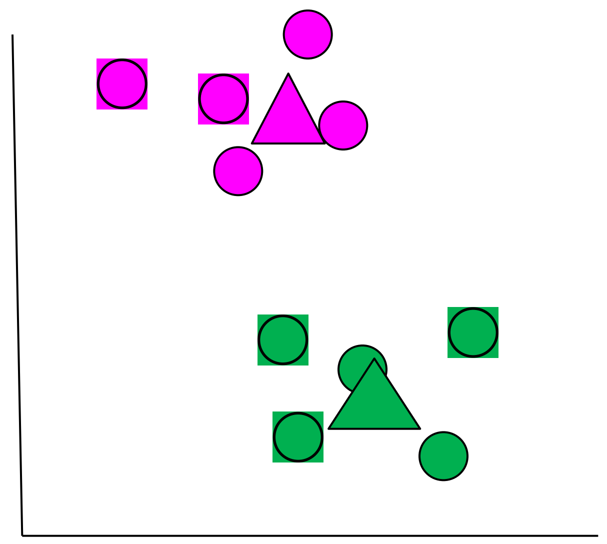
Compute new partitions with updated centers.

K-means: example (k=2)



Update centers.

K-means: example (k=2)



Stop at no change (or a very little change in cluster centers).

A more conservative approach

- Lloyd algorithm fast but not necessarily causing better convergence.
- A more conservative approach to move one data point at a time provided overall cost gets reduced.
- A greedy approach by choosing the transfer of a data point from a class (say, i) to another class (say, j), which causes the best (maximal) cost reduction at that step.

Strength

- Trying to minimize the energy function SSE defined by the sum of divergences of each cluster from its center.

$$E = \sum_{k} \sum_{\forall x \in c_k} \|x - c_k\|^2$$

- Convergence guaranteed at a quadratic rate.
- Linear time complexity in N, d and K.
- Versatile, simple , and invariant to data ordering.

Weakness

- Only detects well separated, compact, hyperspherical clusters.
  - Value of K?
- Sensitive to noise and outlier points
  - Due to squared Euclidean distance.
- May get stuck at local minima.
  - Highly sensitive to the selection of the initial centers
- Improper initialization
  - empty clusters,
  - slower convergence, and
  - a higher chance of getting stuck in bad local minima

Use of an adaptive initialization method!

Various Initialization Approaches

- Each point randomly to one of the clusters (Forgy 1965)
- First K points as the centers. (McQueen 1967)
  - Sensitive to data ordering
  - Choose them randomly
    - Outliers still may get selected.
- Repeated K-means. (Bradley & Fayyad, ICML'98)
  - K-means on J random subsets.
  - Merge all centers and run K-means repeatedly on them
  - Choose the best set of centers minimizing the error, and use them for iterative convergence.

K-means++

- The first center c_1 chosen randomly.
- The i-th ($i=2,3,..,K$) center c_i chosen as x' with a probability proportional to square of the minimum distance from the selected i-1 centers.

$$p(x') = \frac{\min_{j=1,2,..,i-1} \|x' - c_j\|^2}{\sum_x \min_{j=1,2,..,i-1} \|x - c_j\|^2}$$

How do you determine K?

- Use of cluster validity index.
  - Maximize or minimize depending upon the nature of metric.
- Check for stable clustering results with random initialization.
  - Use of different measures of stability.

Cluster validity indices

- External indices using a reference partitioning information, e.g. class labels.
  NMI=2I(Y;C)/(H(Y)+H(C))
  - Normalized Mutual Information (NMI)
  - Fraction of same pairs in same clusters (FM index)
  - Set matching measures
    - Finding matching partition pairs and maximal common coverage

  Y: Cluster Label
  C: Class Label
  I(Y;C)=H(Y)-H(Y|C)

- Internal indices by Looking at variance distribution, structure of clusters
  s(x)=(a(x)-b(x))/max(a(x),b(x)) Avg. of s(x)'s.
  a(x): Avg. dist. of points within the cluster from x
  b(x)=Min. avg. dist. of points of other clusters from x.
  - Silhouette index
    - Higher better in [-1,1]
  - Calinski-Harabasz(CH) Index
    - Higher better.

$$CH(K) = \frac{(J(1) - J(K))/(K-1)}{J(K)/(n-K)}$$

J(i): SSE with K=i

Stability check based clustering

- Repeated clustering should have similar partitioning
  - for an appropriate K.
- Wang's method of cross-validation (2010)
  - Permute the input data c times.
  - Each time divide into three parts,
    - S_1,S_2,and S_3, such that $|S_1|=|S_2|=m$
  - Perform k-means on S_1 and S_2.
    - Test on S_3 both cases to find the cluster numbers.
  - Compute the number of disagreement
    - a pair being in the same or different clusters.
  - Take the average over c observations

Choose K minimizing avg. number of disagreements.

Generalizing K-Means: Mixture densities

Number of components

Component density

$$P(\boldsymbol{x}) = \sum_{i=1}^{K} P(\boldsymbol{x}|G_i)P(G_i)$$

Component proportion

- G_i defines the ith group or cluster.
- K is a hyper-parameter and should be known.
- For multivariate Gaussian distribution:
  - $P(\boldsymbol{x}|G_i) \sim$ N($\boldsymbol{\mu}_i$, Σ_i)
- To estimate $\boldsymbol{\mu}_i$, Σ_i, and $P(G_i)$ for all i. from the set of *iid*. input samples: $X=\{\boldsymbol{x}^t\}$, t=1,2,…,N

Mixture of Gaussians

- Each cluster center is augmented by a covariance matrix, whose values are re-estimated from corresponding samples.
  - Mahalanobis distance function:

$$d(x, \mu_k; \Sigma_k) = (x - \mu_k)^T \Sigma_k^{-1} (x - \mu_k)$$

Covariance matrix

Cluster center

Technique could be refined by computing probabilities of belongingness to a cluster.

Parametric PDF: $p(x|\{\pi_k, \mu_k, \Sigma_k\}) = \sum_k \pi_k N(x|\mu_k, \Sigma_k)$

Mixing coefficients

Expectation Maximization (EM) Algorithm

$$z_{ik} = \frac{1}{Z_i} \pi_k N(x_i | \mu_k, \Sigma_k)$$

Normalizing factor

$$Z_i = \sum_k \pi_k N(x_i \mid \mu_k, \Sigma_k)$$

- Start with initial set : $\{\pi_k, \mu_k, \Sigma_k\}$.
- E-Step (Expectation stage)
  - Compute probability (z_{ik}) of x belonging to kth Gaussian cluster.
  - Assign x to the mth cluster whose probability is maximum.

Optional step. Decision to be taken at the end.

- M-Step (Maximization Stage)
  - Re-estimate parameters ($\{\pi_k, \mu_k, \Sigma_k\}$) from class distribution
- Iterate above two steps till it converges.

Parameter re-estimation

$$z_{ik} = \frac{1}{Z_i} \pi_k N(x | \mu_k, \Sigma_k)$$

Normalizing factor

$$N_k = \sum_i z_{ik}$$

Expected number of pixels in class k.

$$\mu_k = \frac{1}{N_k} \sum_i z_{ik} \, x_i$$

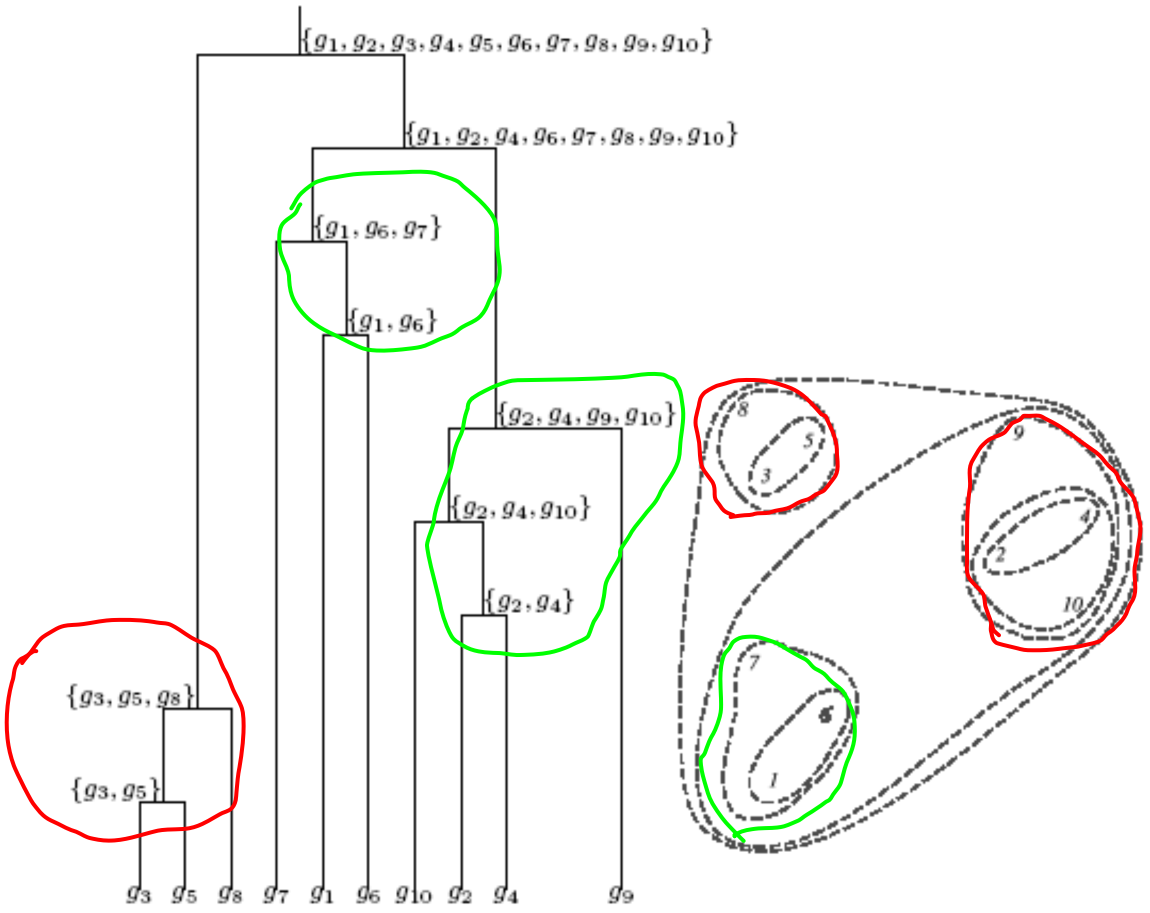
$$\Sigma_k = \frac{1}{N_k} \sum_i z_{ik} \, (x_i - \mu_k)(x_i - \mu_k)^T$$

$$\pi_k = \frac{N_k}{N}$$

Hierarchical clustering

- Builds hierarchy of groups.
  - Usually a bottom-up approach.
- Uses a distance matrix among the samples.
- Explicit feature representation may not be required.
- A non-probabilistic approach.

Hierarchical Clustering: An example



$\{g_1, g_2, g_3, g_4, g_5, g_6, g_7, g_8, g_9, g_{10}\}$
$\{g_1, g_2, g_4, g_6, g_7, g_8, g_9, g_{10}\}$
$\{g_1, g_6, g_7\}$
$\{g_1, g_6\}$
$\{g_2, g_4, g_9, g_{10}\}$
$\{g_2, g_4, g_{10}\}$
$\{g_2, g_4\}$
$\{g_3, g_5, g_8\}$
$\{g_3, g_5\}$
g_3 g_5 g_8 g_7 g_1 g_6 g_{10} g_2 g_4 g_9
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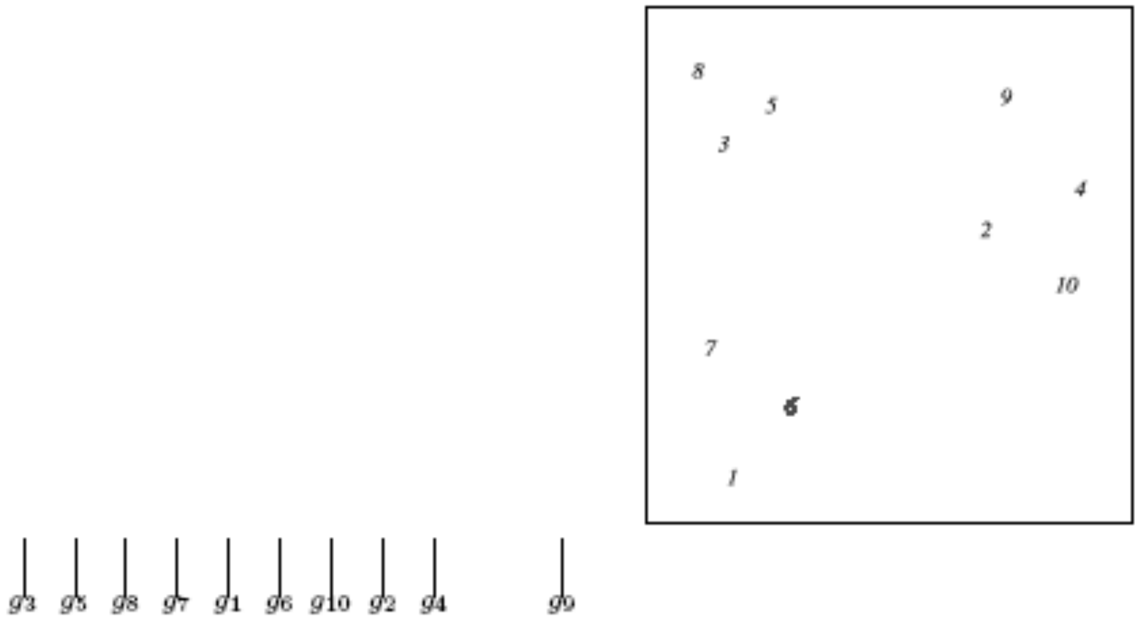
1

Courtesy: www.bioalgorithms.info (Pavel Pevzner)

Hierarchical Clustering: An Example



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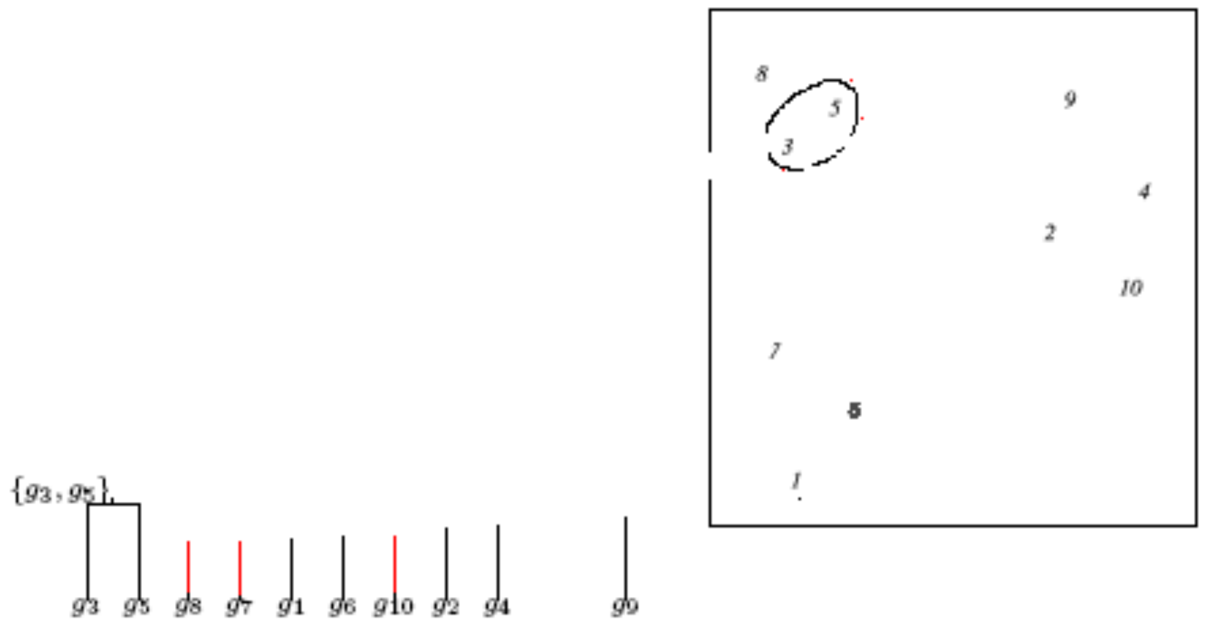
Hierarchical Clustering: Example



$\{g_3, g_5\}$
g_3 g_5 g_8 g_7 g_1 g_6 g_{10} g_2 g_4 g_9
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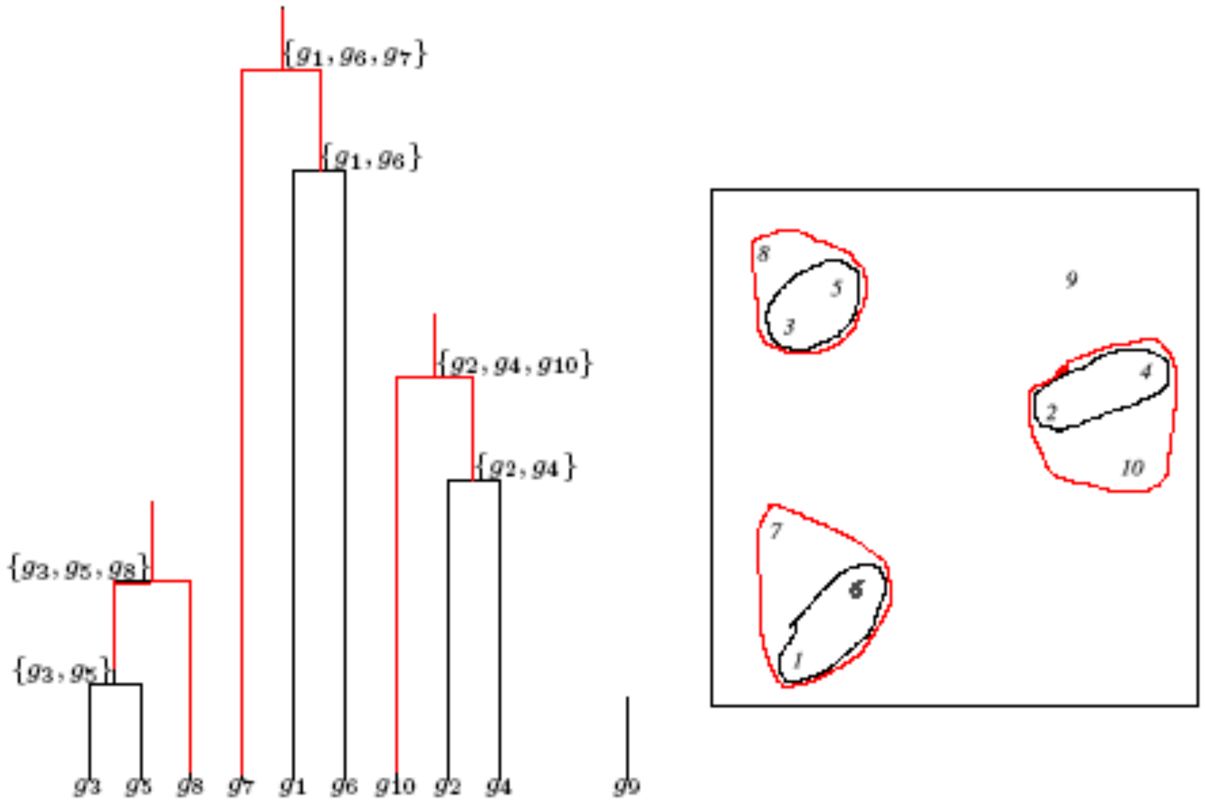
Hierarchical Clustering: Example



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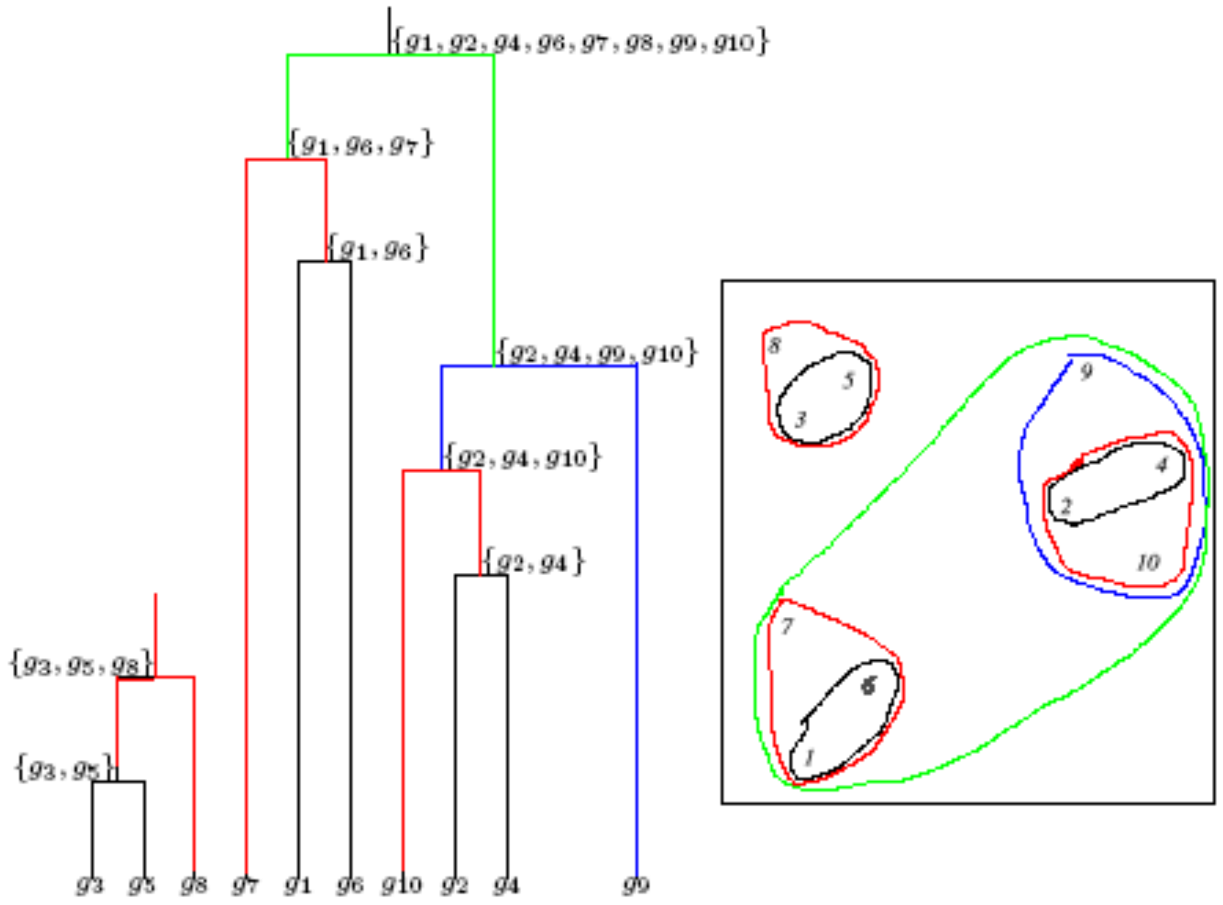
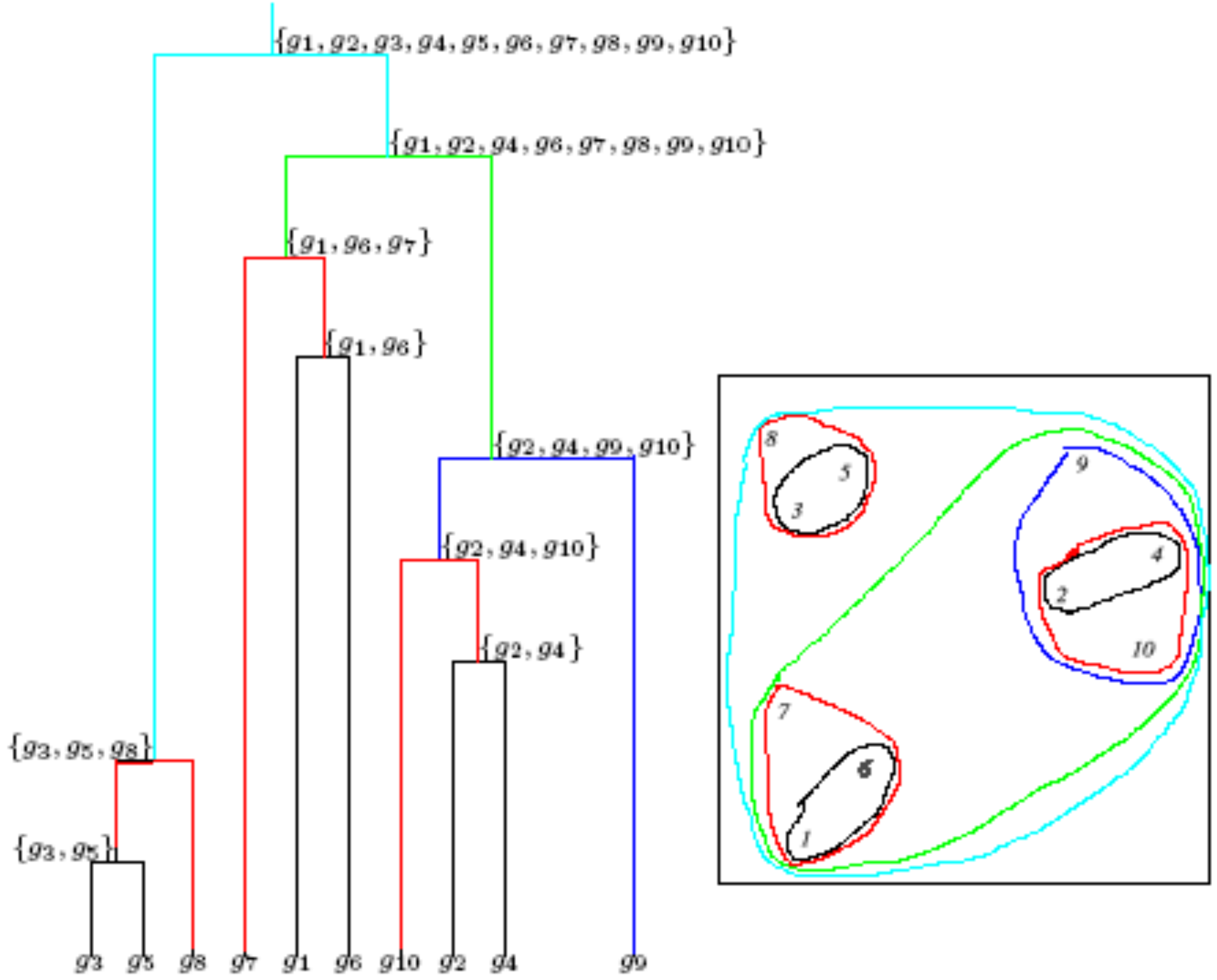
Hierarchical Clustering: Example



$\{g_1, g_2, g_4, g_6, g_7, g_8, g_9, g_{10}\}$
$\{g_1, g_6, g_7\}$
$\{g_1, g_6\}$
$\{g_2, g_4, g_9, g_{10}\}$
$\{g_2, g_4, g_{10}\}$
$\{g_2, g_4\}$
$\{g_3, g_5, g_8\}$
$\{g_3, g_5\}$
g_3 g_5 g_8 g_7 g_1 g_6 g_{10} g_2 g_4 g_9
8 5 3 9 4 2 10 7 6 1

Courtesy: www.bioalgorithms.info (Pavel Pevzner)

Hierarchical Clustering:



$\{g_1, g_2, g_3, g_4, g_5, g_6, g_7, g_8, g_9, g_{10}\}$
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Courtesy: www.bioalgorithms.info (Pavel Pevzner)

Hierarchical Clustering Algorithm

The algorithm takes a *nxn* distance matrix ***d*** of pairwise distances between points as an input.

```
Hierarchical Clustering (d , n)
  Form n clusters each with one element.
  Initialize a graph T with a vertex for each cluster.
  while there is more than one cluster
    Find the two closest clusters $C_1$ and $C_2$.
    Merge $C_1$ and $C_2$ into C with $|C_1| + |C_2|$ elements.
    Compute distance from C to all other clusters.
    Add a new vertex C to T and connect to vertices $C_1$ and $C_2$.
    Remove rows and columns of d corresponding to $C_1$ and $C_2$.
    Add a row and column to d corresponding to the new cluster C.
  return T
```

Different ways to define distances between clusters may lead to different clustering.

Courtesy: www.bioalgorithms.info (Pavel Pevzner)

Computing distance between a pair of clusters.

- $d_{min}(C, C^*) = \min d(x,y)$
  *for all elements x in C and y in C**

  - Distance between two clusters is the **smallest** distance between any pair of their elements.

- $d_{avg}(C, C^*) = (1 / (|C^*||C|)) \sum d(x,y)$
  *for all elements x in C and y in C**

  - Distance between two clusters is the **average** distance between all pairs of their elements.

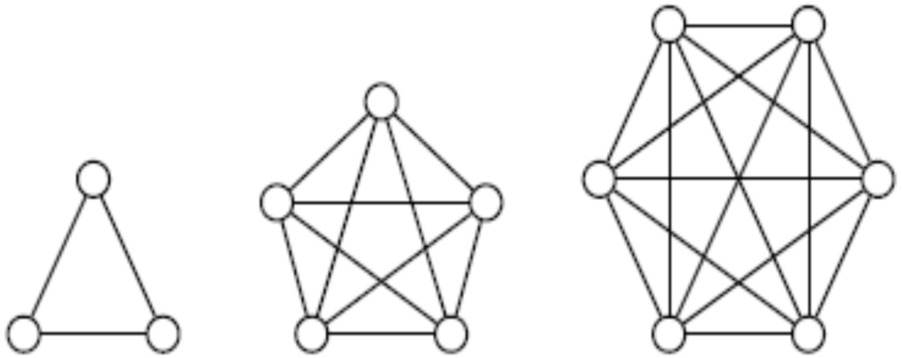
Courtesy: www.bioalgorithms.info (Pavel Pevzner)

Graph based approaches

- Form a graph from the input data.
  - May not be explicit.
- Compute cliques, connected components, etc.

Clique Graphs

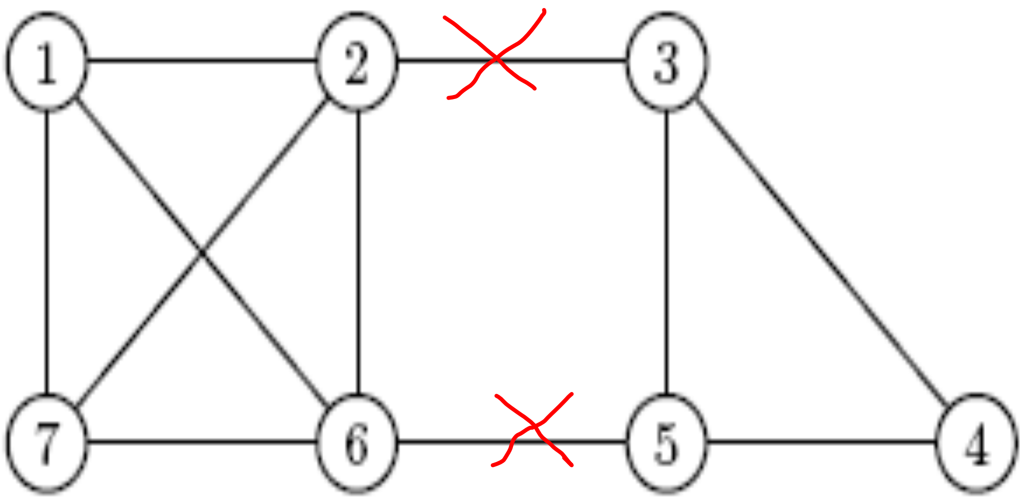
- A **clique** is a graph with every vertex connected to every other vertex.
- A **clique graph** is a graph where each connected component is a clique.



Courtesy: www.bioalgorithms.info (Pavel Pevzner)

Transforming an Arbitrary Graph into a Clique Graphs

- A graph can be transformed into a clique graph by adding or removing edges.



Courtesy: www.bioalgorithms.info (Pavel Pevzner)

Corrupted Cliques Problem

Input: A graph *G*

Output: The smallest number of additions and removals of edges that will transform *G* into a clique graph.

Courtesy: www.bioalgorithms.info (Pavel Pevzner)

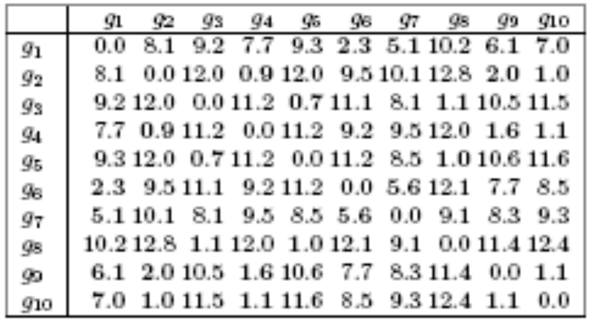
Distance Graphs

- Feature vectors represented as vertices in the graph.
- Choose a distance threshold *θ.*
- If the distance between two vertices is below *θ,* draw an edge between them.
- The resulting graph may contain cliques.
- These cliques represent clusters of closely located data points!

Courtesy: www.bioalgorithms.info (Pavel Pevzner)

Transforming into Clique Graph

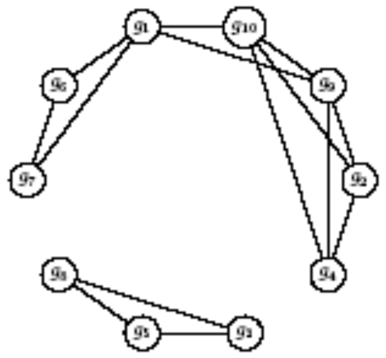
The distance graph (threshold θ=7) is transformed into a clique graph after removing the two highlighted edges



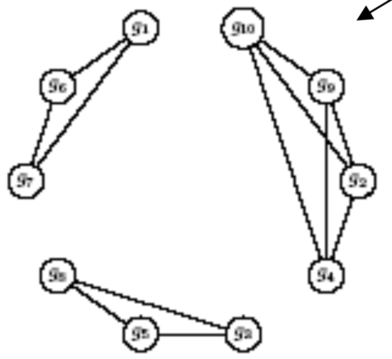
	g_1	g_2	g_3	g_4	g_5	g_6	g_7	g_8	g_9	g_{10}
g_1	**0.0**	8.1	9.2	7.7	9.3	**2.3**	**5.1**	10.2	**6.1**	7.0
g_2	8.1	**0.0**	12.0	**0.9**	12.0	9.5	10.1	12.8	**2.0**	**1.0**
g_3	9.2	12.0	**0.0**	11.2	**0.7**	11.1	8.1	**1.1**	10.5	11.5
g_4	7.7	**0.9**	11.2	**0.0**	11.2	9.2	9.5	12.0	**1.6**	**1.1**
g_5	9.3	12.0	**0.7**	11.2	**0.0**	11.2	8.5	**1.0**	10.6	11.6
g_6	**2.3**	9.5	11.1	9.2	11.2	**0.0**	**5.6**	12.1	7.7	8.5
g_7	**5.1**	10.1	8.1	9.5	8.5	**5.6**	**0.0**	9.1	8.3	9.3
g_8	10.2	12.8	**1.1**	12.0	**1.0**	12.1	9.1	**0.0**	11.4	12.4
g_9	**6.1**	**2.0**	10.5	**1.6**	10.6	7.7	8.3	11.4	**0.0**	**1.1**
g_{10}	7.0	**1.0**	11.5	**1.1**	11.6	8.5	9.3	12.4	**1.1**	**0.0**

(a) Distance matrix, d (distances shorter than 7 are shown in bold).

After transforming the distance graph into the clique graph, the dataset is partitioned into three clusters



(b) Distance graph for $\theta = 7$.



(c) Clique graph.

Figure 10.6 The distance graph (b) for $\theta = 7$ is not quite a clique graph. However, it can be transformed into a clique graph (c) by removing edges (g_1, g_{10}) and (g_1, g_9).

Corrupted Clique Problem

- Corrupted Cliques problem is NP-Hard, some heuristics exist to approximately solve it:
- **Two approximate methods:**

  1. Parallel Classification with Cores (PCC).

  - (Amir Ben-Dor et. al (1999))

  2. Cluster Affinity Search Technique (CAST)

Courtesy: www.bioalgorithms.info (Pavel Pevzner)

Parallel Classification with cores (PCC)

- Suppose S' is a subset of S.
- Let, $\{C_1, C_2, \ldots, C_k\}$ be a clustering on S'.
- How do you extend the clustering to S ?
- Let $j \in S\text{-}S'$ and $N(j, C_i)$ be no. of edges from j to C_i.
- $Affinity(j, C_i) = N(j, C_i)/|C_i|$
- Assign j to the cluster which has maximum affinity.

Algorithm for PCC

Algorithm PCC(S, G, k)

S: Set of n elements (say, feature vectors forming vertices of G).

G: Distance graph , k: No. of clusters

1. Randomly select S', a subset from S, and S'', a subset from S-S',

    s.t. $|S'|=log(log(n))$ and $|S''|=log(n)$.

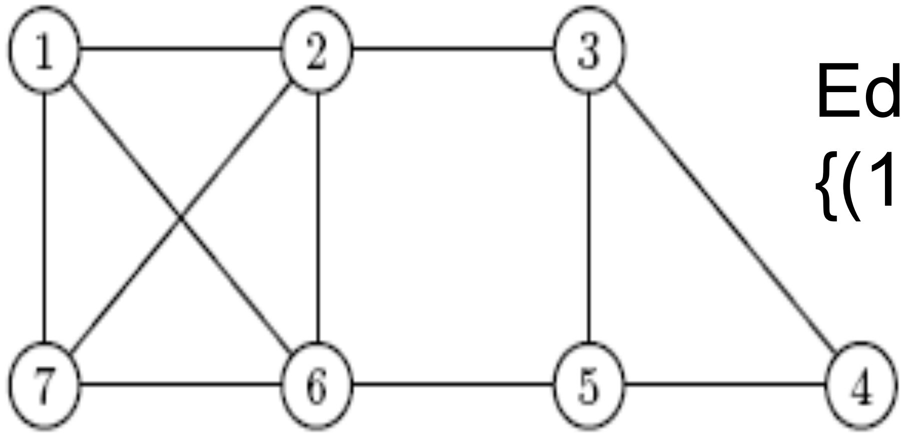
2. For all k partitions in S'

    2.1 Obtain extended partition in S through two stages of extensions i.e. $S' \rightarrow S'' \rightarrow (S-(S' \cup S''))$

    2.2 Choose the one which has minimum score , i.e. the no. of edges reqd. to add or remove from G to get a Clique graph as per the partition.

End PCC.

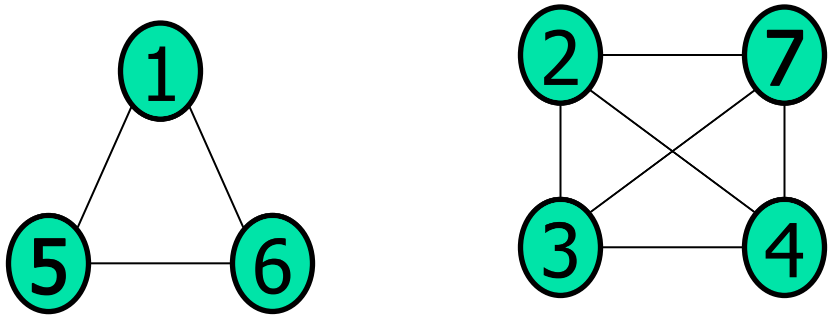
Example of computing score



Edges to be added in G: {(1,5),(2,4),(3,7),(4,7)}

Edges to be deleted in G: {(1,2),(1,7),(6,7),(4,5),(2,6),(3,5)}

Let a partition P with k=2: {1,5,6}, {2,3,7,4}.



Score: 10

Clique graph w.r.t .P

PCC: Time complexity

- No. of partitions in $S' = k^{|S'|}$

$$= k^{\log(\log(n))}$$

$$= (\log(n))^{\log_2(k)}$$

- In each iteration $O(n^2)$ operations for extension and score computation.
- Total time complexity: $O(n^2 (\log(n))^{\log_2(k)})$

CAST

- **CAST** (Cluster Affinity Search Technique): a practical and fast algorithm:
  - **CAST** is based on the notion of features *close* to cluster *C* or *distant* from cluster *C.*
  - Distance between feature *i* and cluster *C*:

    d(i,C) = average distance between feature *i* and all other features in *C*

Gene *i* is ***close*** to cluster *C*, if $d(i,C) < \theta$

and ***distant*** otherwise.

Courtesy: www.bioalgorithms.info (Pavel Pevzner)

CAST Algorithm

***S* – set of elements, *G* – distance graph, *θ* – distance threshold**

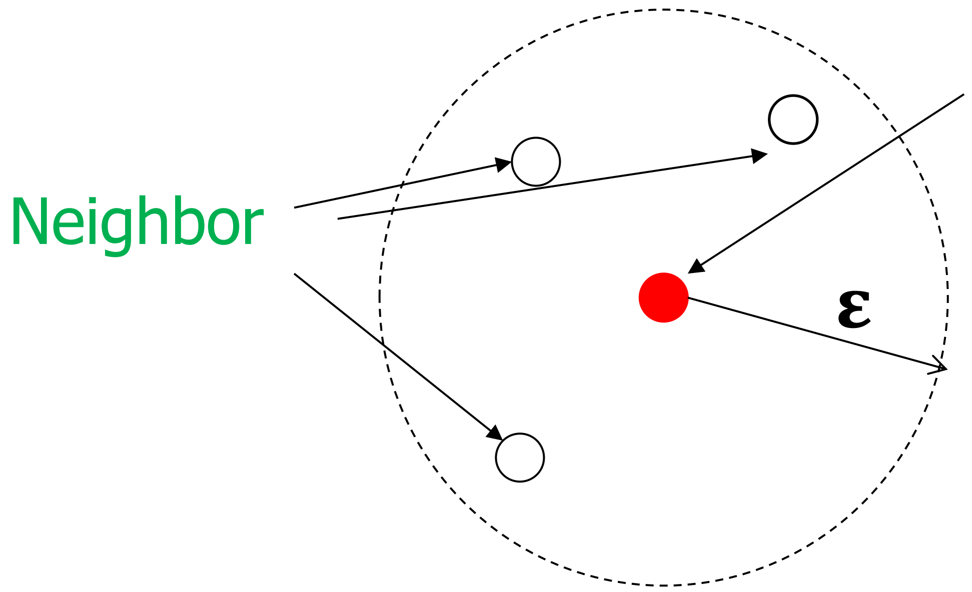
```
CAST($S, G, \theta$)
  $P \leftarrow \emptyset$
  while $S \neq \emptyset$
    $V \leftarrow$ vertex of maximal degree in the distance graph $G$.
    $C \leftarrow \{v\}$
    while a close feature $i$ not in $C$ or distant feature $i$ in $C$ exists
      {
      Find the nearest close feature $i$ not in $C$ and add it to $C$.
      Remove the farthest distant feature $i$ in $C$.
      }
    Add cluster $C$ to partition $P$.
    $S \leftarrow S \setminus C$
    Remove vertices of cluster $C$ from the distance graph $G$.
  return $P$
```

Courtesy: www.bioalgorithms.info (Pavel Pevzner)

DBSCAN

Density-based spatial clustering of applications with noise (DBSCAN) (Ester, Kriegel, Sander and Xu'96)

- No explicit computation of distance graph.



Core point: number of point within ε more than a threshold k.

Forms clusters of arbitrary shape.

Use of R-tree for efficient search.

- Grow regions of connected core points from a seed.

A neighbor but not a core point called a border point.

Summary

- Clustering techniques
  - Semi-parametric approaches.
    - K-means algorithm
      - No explicit parameter estimation
    - Expectation Maximization
      - Mixture of Gaussian
  - Hierarchical clustering method
    - Builds a tree hierarchy following a bottom-up approach.
    - Uses distance matrix instead of explicit feature representation.

Summary

- Graph based approaches.
  - A clique: A graph with every vertex connected to every other vertex.
  - A clique graph: Each component is a clique.
  - Distance graphs: Feature Vectors represented as vertices and edges if distance less than a threshold.
    - Corrupted clique problem
      - Smallest number of additions and removals of edge to transform a graph into a clique graph.
      - PCC and CAST
  - Without explicit computation of distance graph
    - DBSCAN

Thank you!