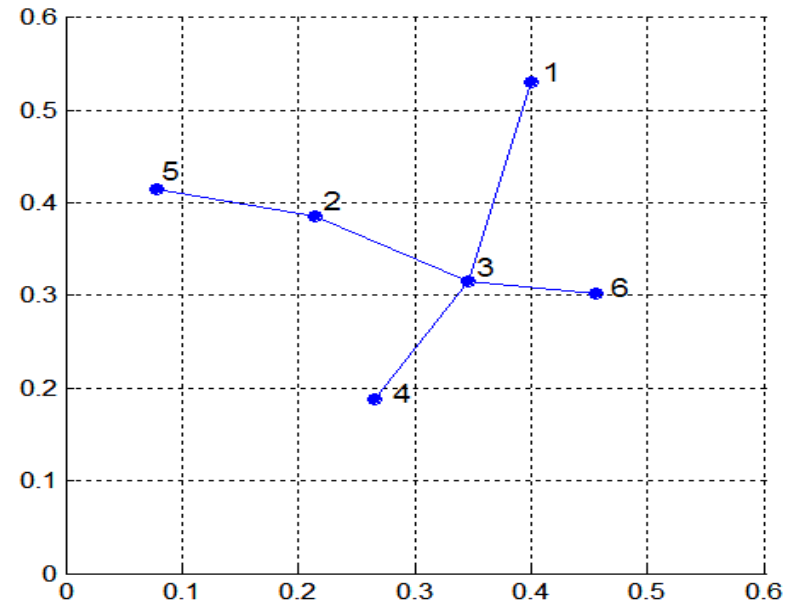
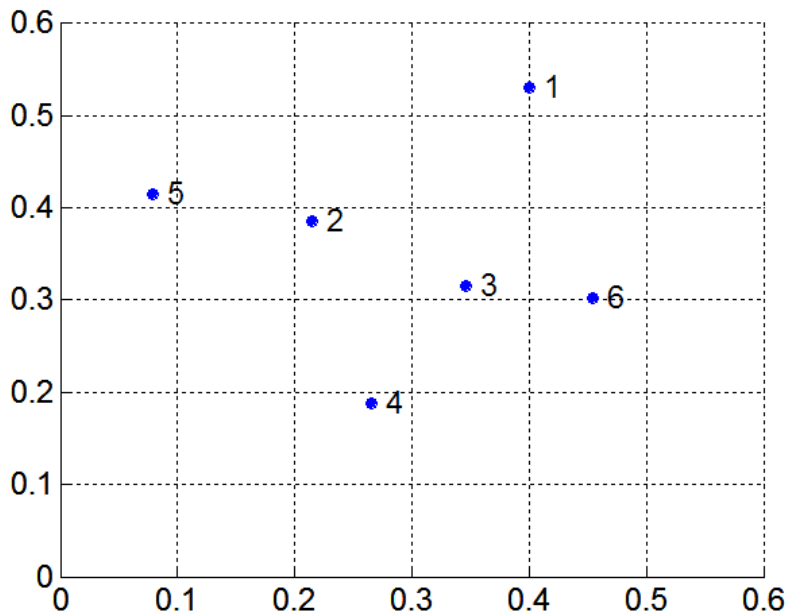


Clustering III

Wei Pang

MST: Divisive Hierarchical Clustering

- Build MST (Minimum Spanning Tree)
 - Start with a tree that consists of any point
 - In successive steps, look for the closest pair of points (p, q) such that one point (p) is in the current tree but the other (q) is not
 - Add q to the tree and put an edge between p and q



Prim's Algorithm

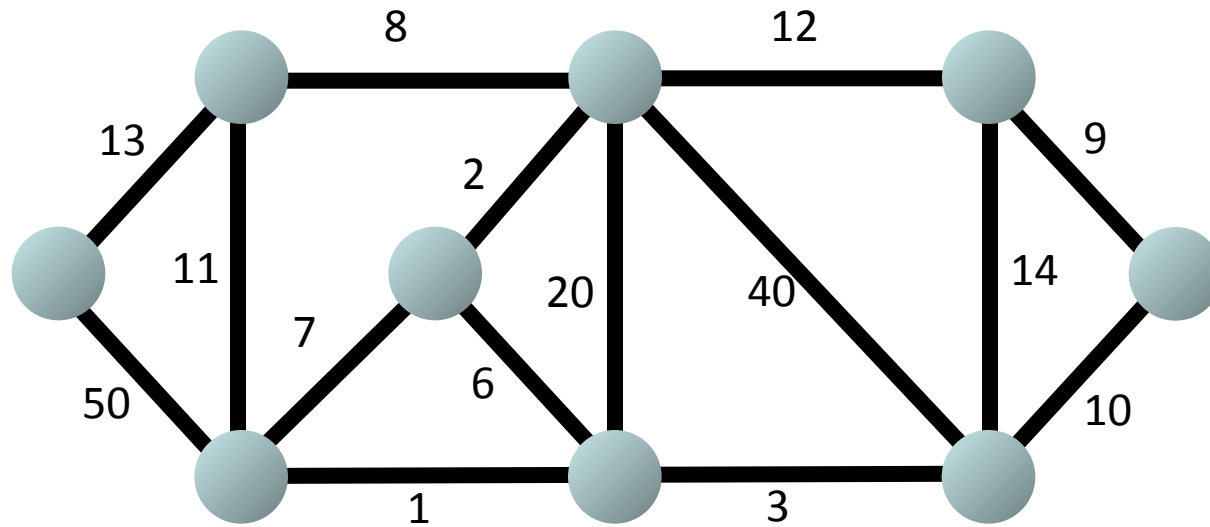


- **Robert Clay Prim**
- **Prim Approach:**
 - Choose an arbitrary start node v
 - At any point in time, we have connected component N containing v and other nodes $V-N$
 - Choose the minimum weight edge from N to $V-N$

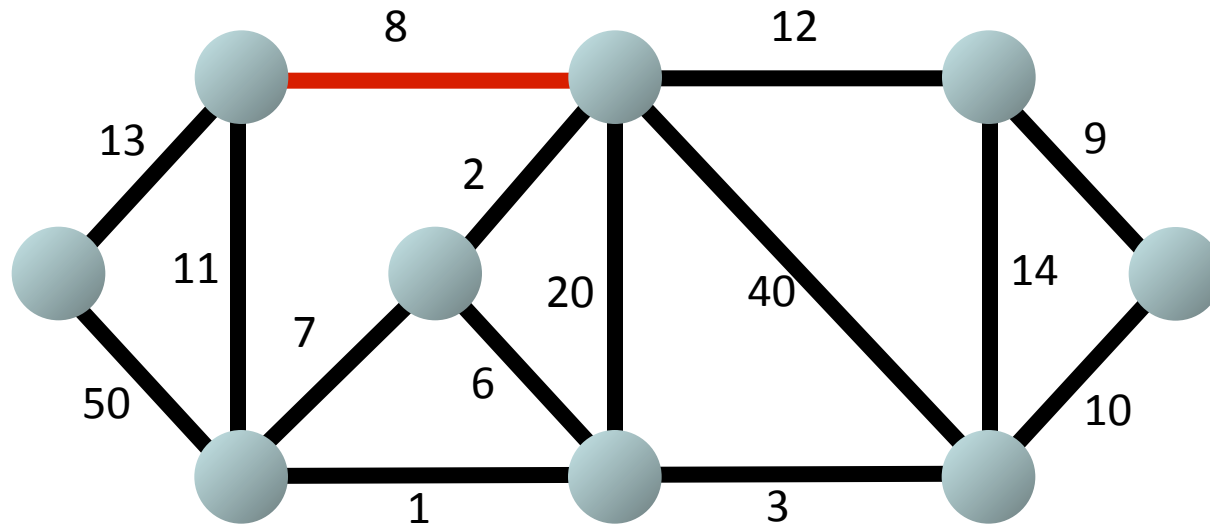
Prim's Algorithm:

```
let T be a single vertex x
while (T has fewer than n vertices)
{
    find the smallest edge connecting T to G-T
    add it to T
}
```

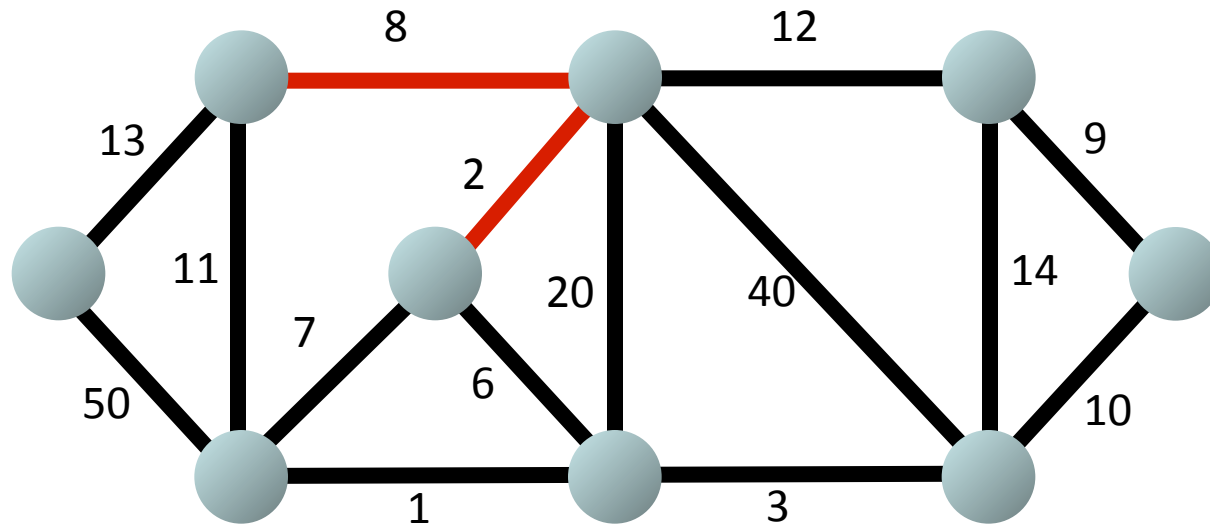
Prim's Algorithm - Example



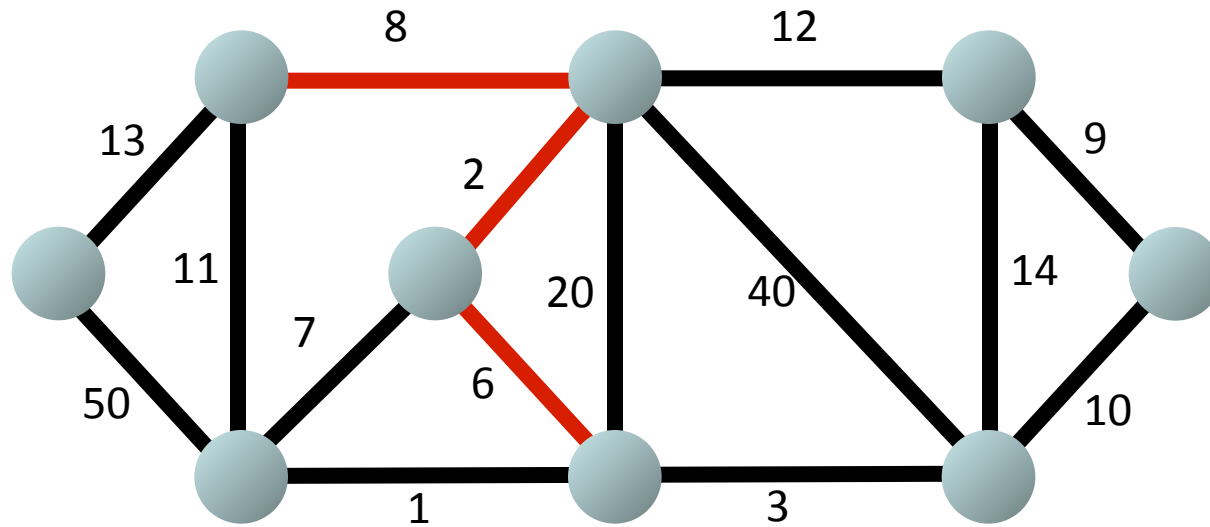
Prim's Algorithm - Example



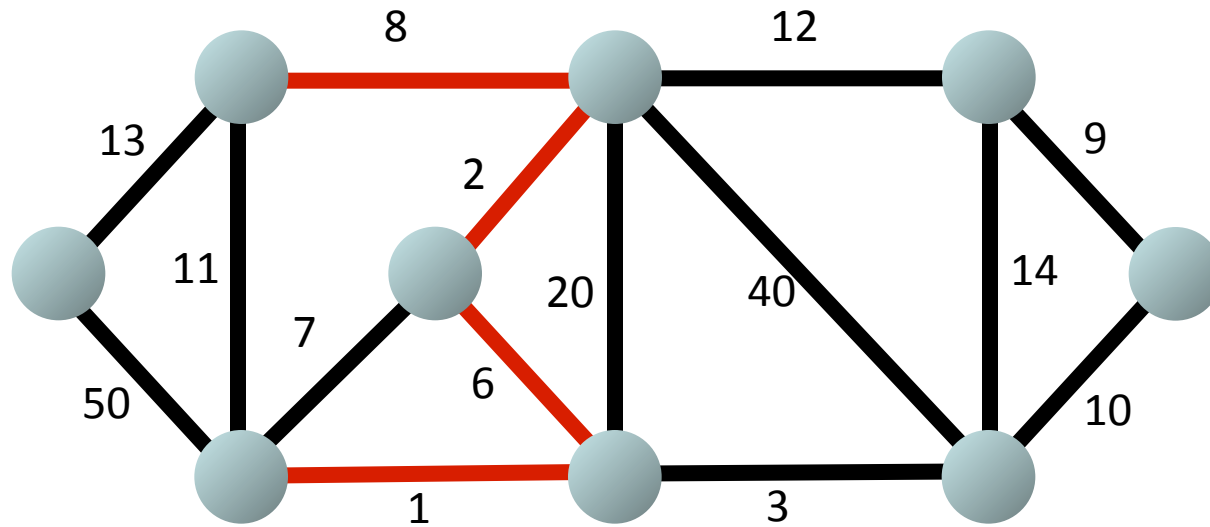
Prim's Algorithm - Example



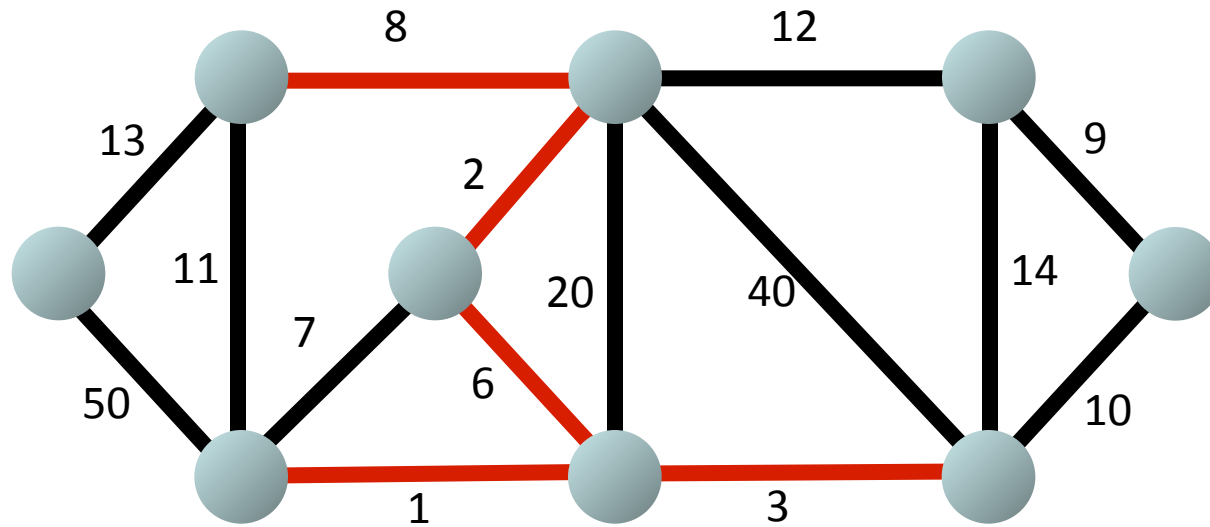
Prim's Algorithm - Example



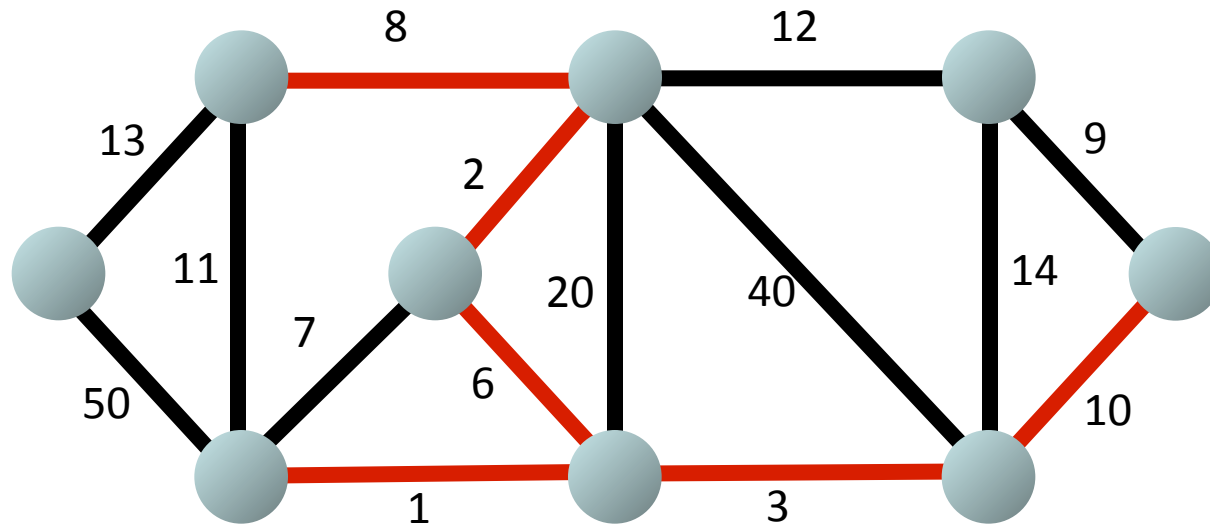
Prim's Algorithm - Example



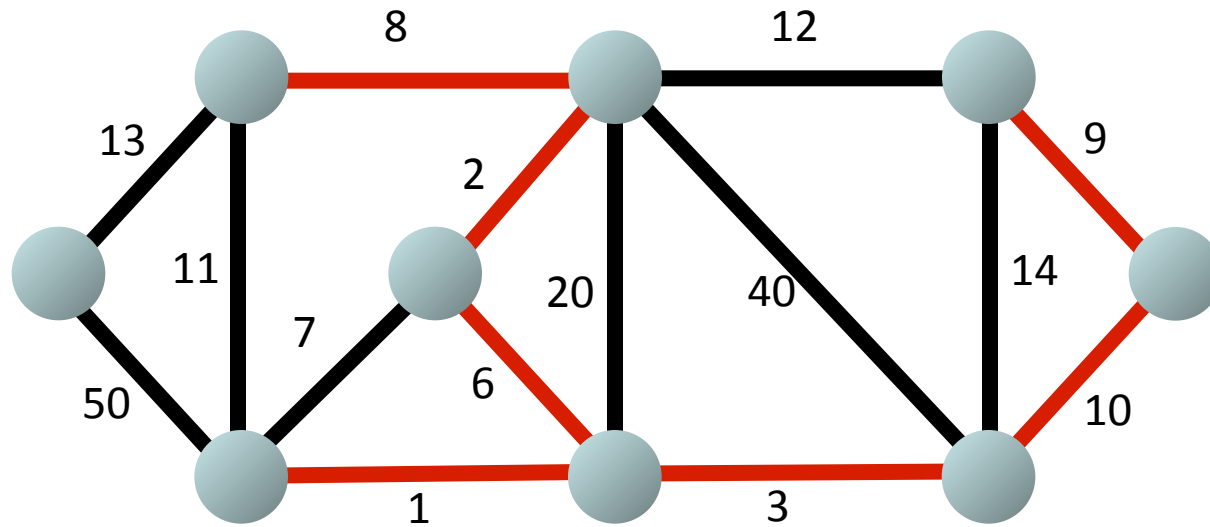
Prim's Algorithm - Example



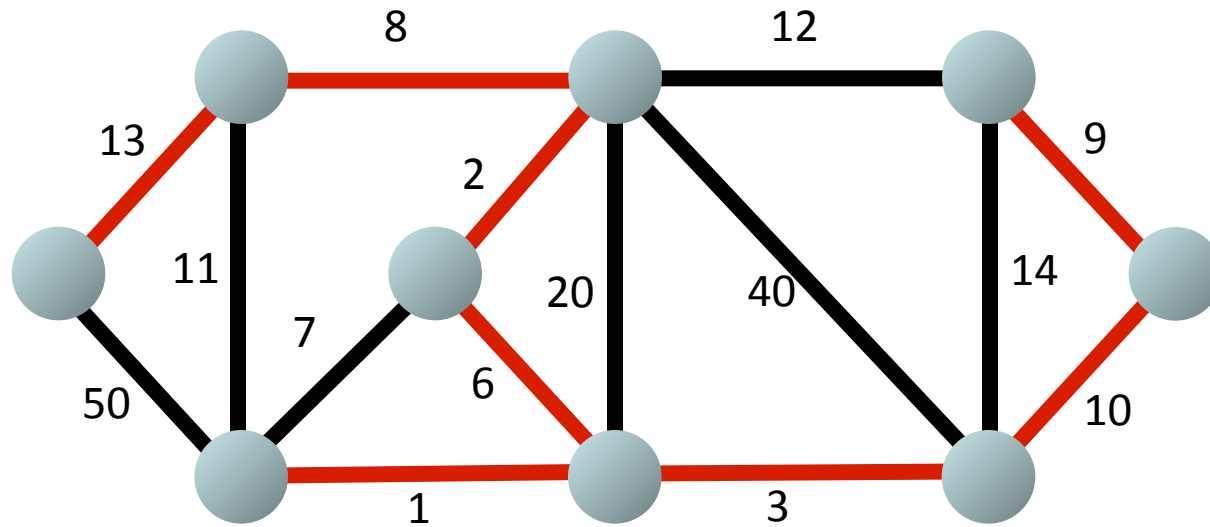
Prim's Algorithm - Example



Prim's Algorithm - Example



Prim's Algorithm - Example



MST: Divisive Hierarchical Clustering

- Use MST for constructing hierarchy of clusters

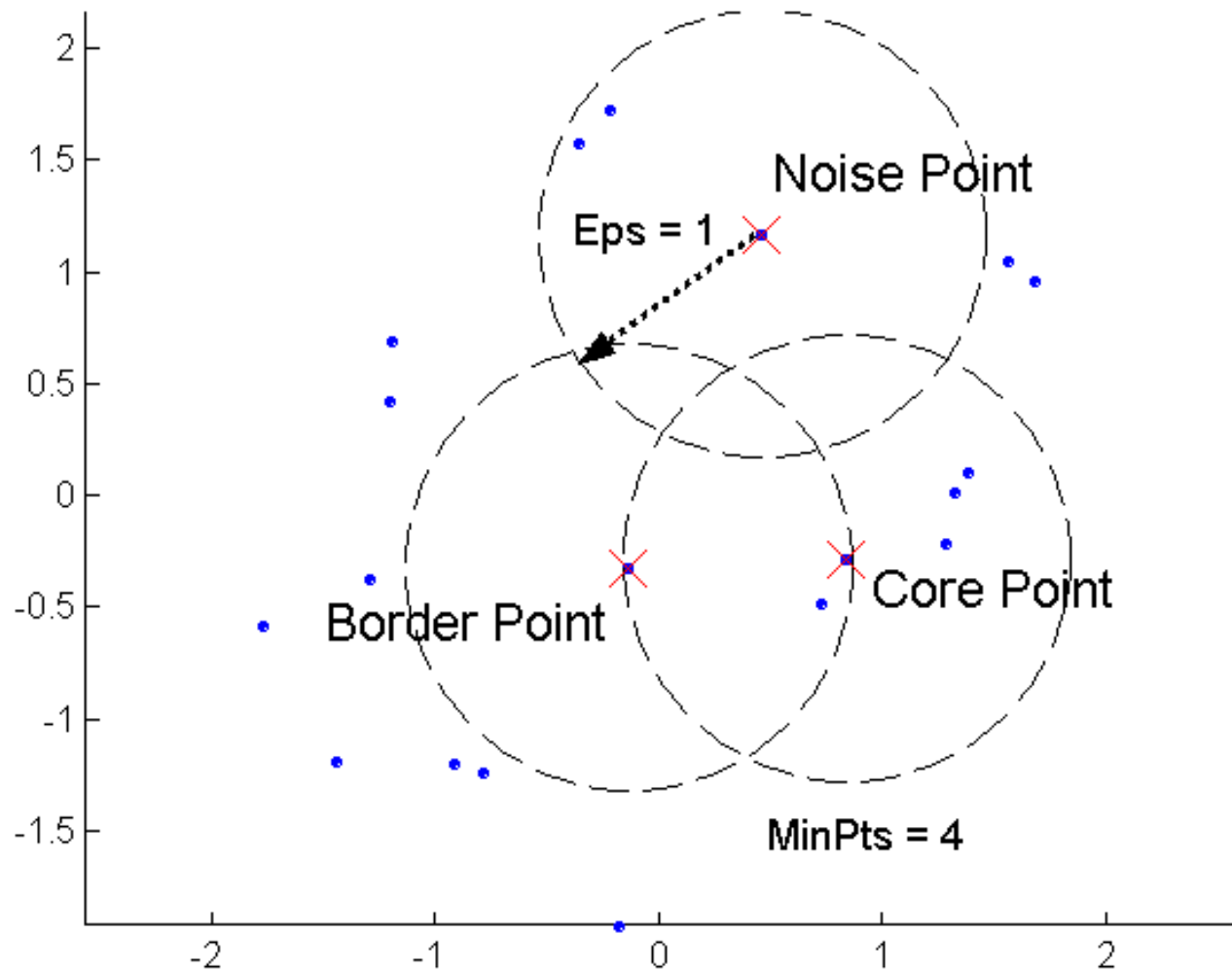
Algorithm 7.5 MST Divisive Hierarchical Clustering Algorithm

- 1: Compute a minimum spanning tree for the proximity graph.
 - 2: **repeat**
 - 3: Create a new cluster by breaking the link corresponding to the largest distance (smallest similarity).
 - 4: **until** Only singleton clusters remain
-

DBSCAN

- DBSCAN is a density-based algorithm.
 - Density = number of points within a specified radius (Eps)
 - A point is a **core point** if it has more than a specified number of points (MinPts) within Eps
 - These are points that are at the interior of a cluster
 - A **border point** has fewer than MinPts within Eps, but is in the neighborhood of a core point
 - A **noise point** is any point that is not a core point or a border point.

DBSCAN: Core, Border, and Noise Points



DBSCAN Algorithm

- Eliminate noise points
- Perform clustering on the remaining points

$current_cluster_label \leftarrow 1$

for all core points **do**

if the core point has no cluster label **then**

$current_cluster_label \leftarrow current_cluster_label + 1$

 Label the current core point with cluster label $current_cluster_label$

end if

for all points in the Eps -neighborhood, except i^{th} the point itself **do**

if the point does not have a cluster label **then**

 Label the point with cluster label $current_cluster_label$

end if

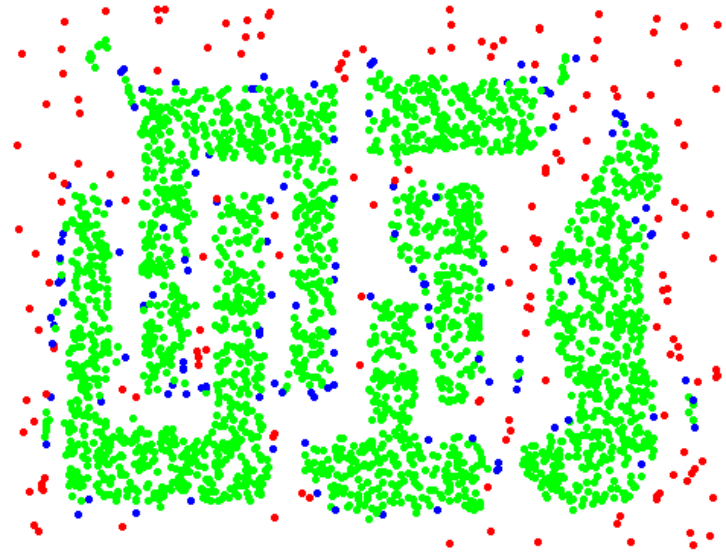
end for

end for

DBSCAN: Core, Border and Noise Points



Original Points



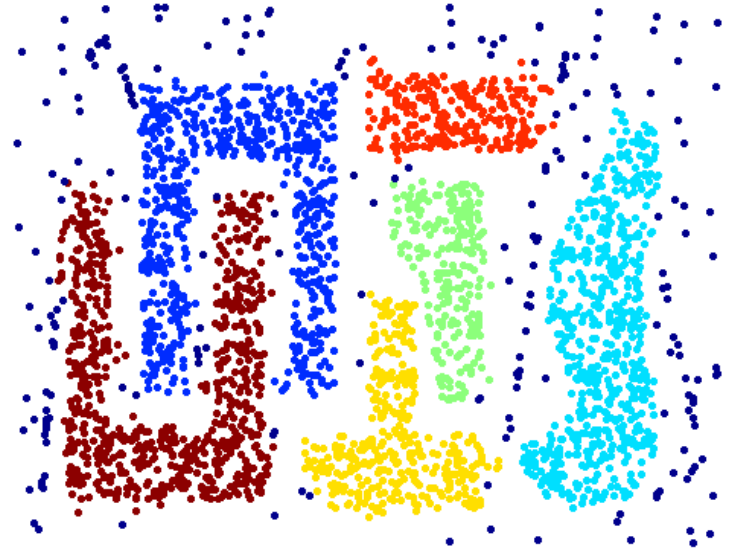
Point types: core,
border and noise

Eps = 10, MinPts = 4

When DBSCAN Works Well



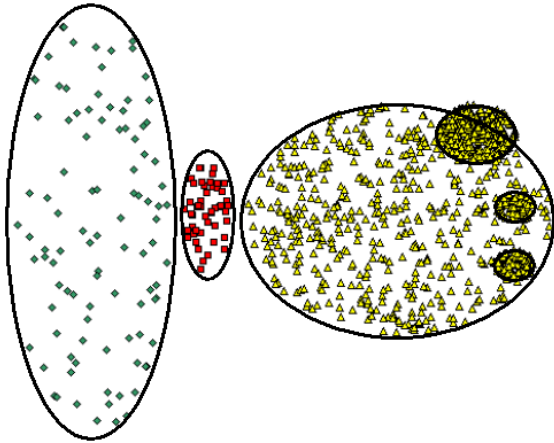
Original Points



Clusters

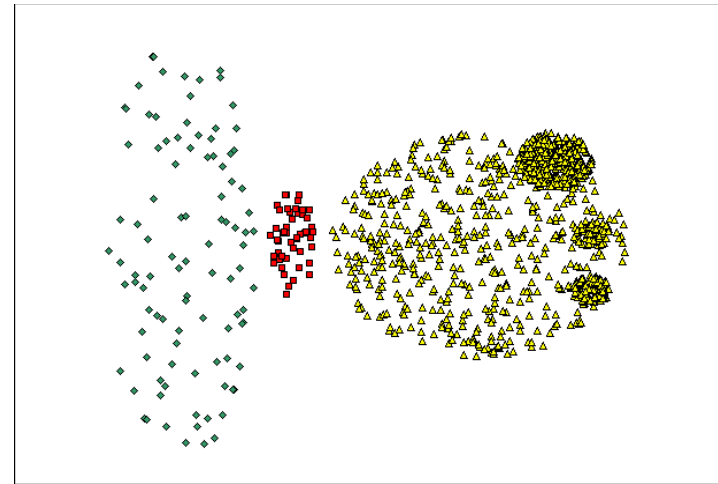
- Resistant to Noise
- Can handle clusters of different shapes and sizes

When DBSCAN Does NOT Work Well

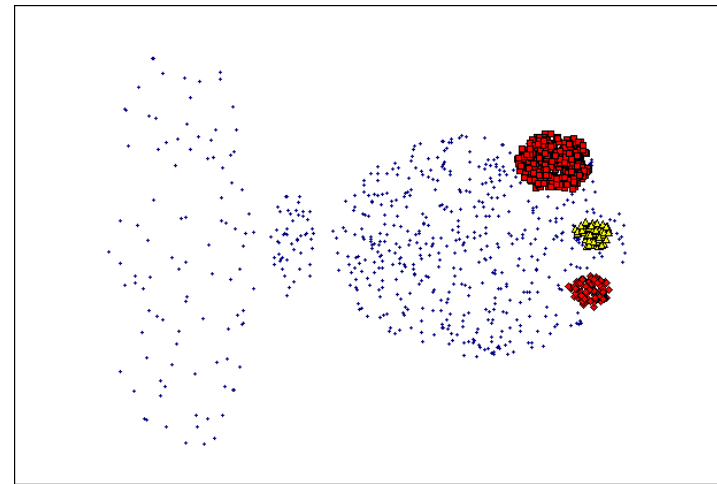


Original Points

- Varying densities
- High-dimensional data



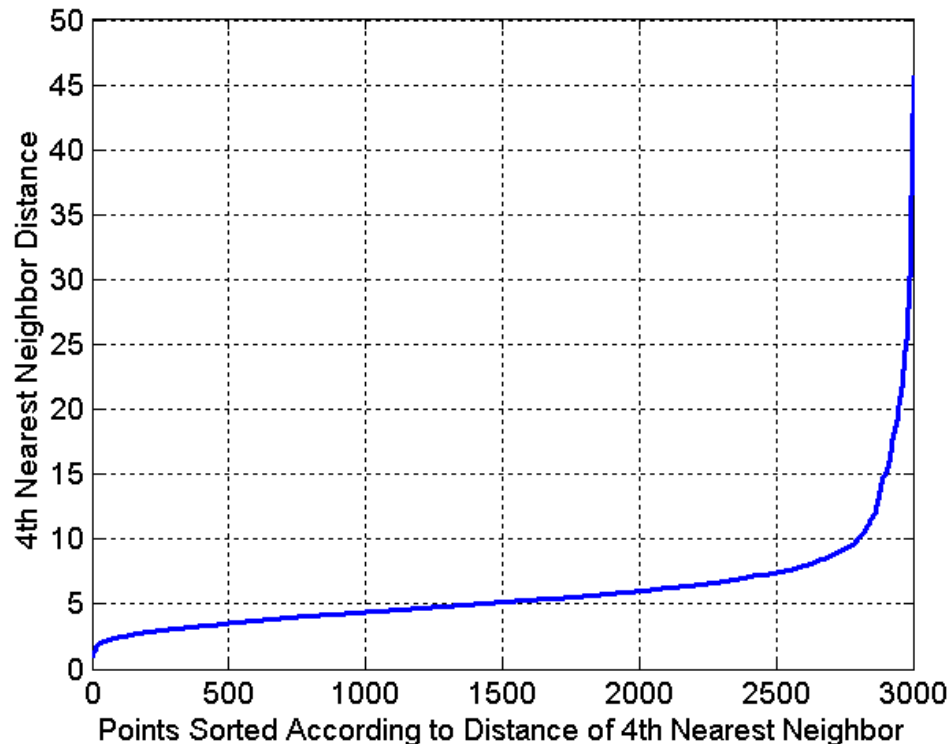
(MinPts=4, Eps=9.75).



(MinPts=4, Eps=9.92)

DBSCAN: Determining EPS and MinPts

- Idea is that for points in a cluster, their k^{th} nearest neighbors are at roughly the same distance
- Noise points have the k^{th} nearest neighbor at farther distance
- So, plot sorted distance of every point to its k^{th} nearest neighbor



Cluster Validity

- For supervised classification we have a variety of measures to evaluate how good our model is
 - Accuracy, precision, recall
- For cluster analysis, the analogous question is how to evaluate the “goodness” of the resulting clusters?
- But “clusters are in the eye of the beholder”!
- Then why do we want to evaluate them?
 - To avoid finding patterns in noise
 - To compare clustering algorithms
 - To compare two sets of clusters
 - To compare two clusters

Different Aspects of Cluster Validation

1. Determining the **clustering tendency** of a set of data, i.e., distinguishing whether non-random structure actually exists in the data.
2. Comparing the results of a cluster analysis to externally known results, e.g., to externally given class labels.
3. Evaluating how well the results of a cluster analysis fit the data *without* reference to external information.
 - Use only the data
4. Comparing the results of two different sets of cluster analyses to determine which is better.
5. Determining the 'correct' number of clusters.

For 2, 3, and 4, we can further distinguish whether we want to evaluate the entire clustering or just individual clusters.

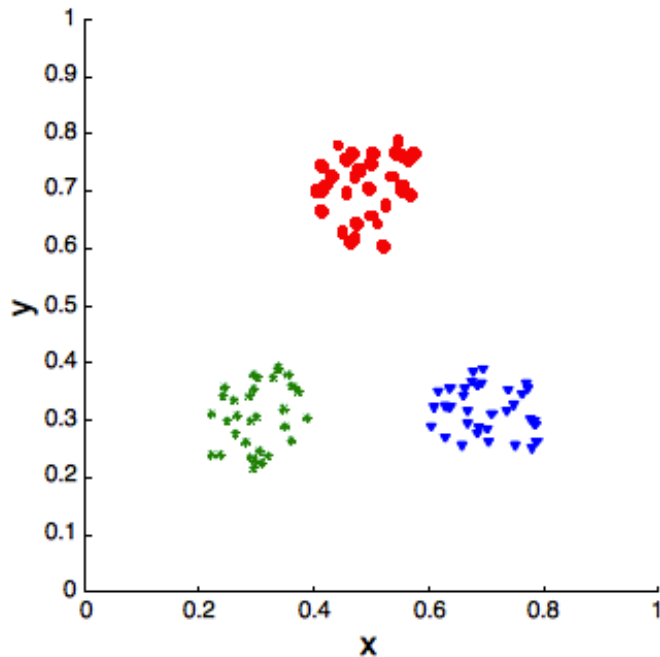
Measures of Cluster Validity

- Numerical measures that are applied to judge various aspects of cluster validity, are classified into the following three types.
 - **External Index:** Used to measure the extent to which cluster labels match externally supplied class labels.
 - Entropy
 - **Internal Index:** Used to measure the goodness of a clustering structure *without* respect to external information.
 - Sum of Squared Error (SSE)
 - **Relative Index:** Used to compare two different clusterings or clusters.
 - Often an external or internal index is used for this function, e.g., SSE or entropy
- Sometimes these are referred to as **criteria** instead of **indices**
 - However, sometimes criterion is the general strategy and index is the numerical measure that implements the criterion.

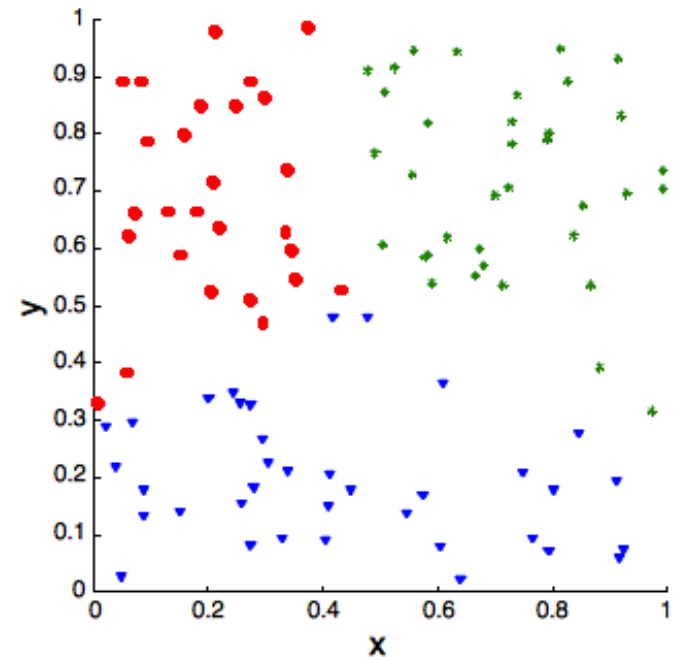
Measuring Cluster Validity Via Correlation

- Two matrices
 - Proximity Matrix
 - “Incidence” Matrix
 - One row and one column for each data point
 - An entry is 1 if the associated pair of points belong to the same cluster
 - An entry is 0 if the associated pair of points belongs to different clusters
- Compute the correlation between the two matrices
 - Since the matrices are symmetric, only the correlation between $n(n-1) / 2$ entries needs to be calculated.
- High correlation indicates that points that belong to the same cluster are close to each other.
- Not a good measure for some density or contiguity based clusters.

Measuring Cluster Validity Via Correlation



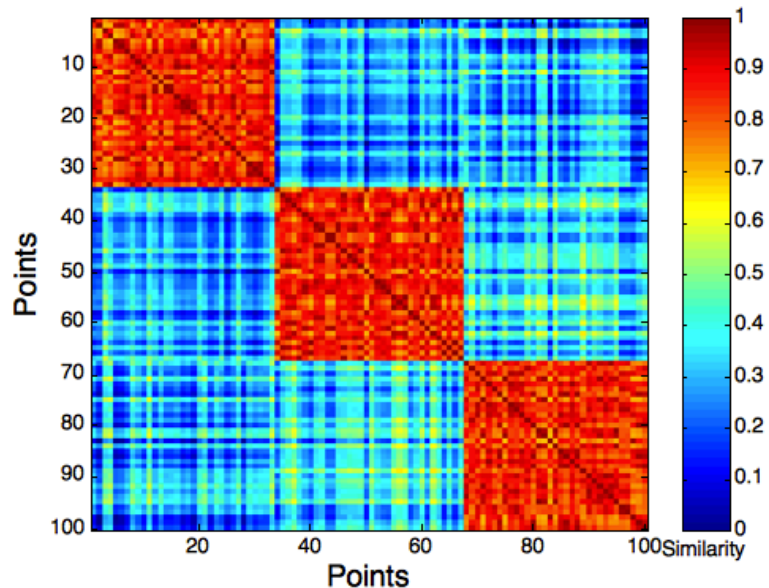
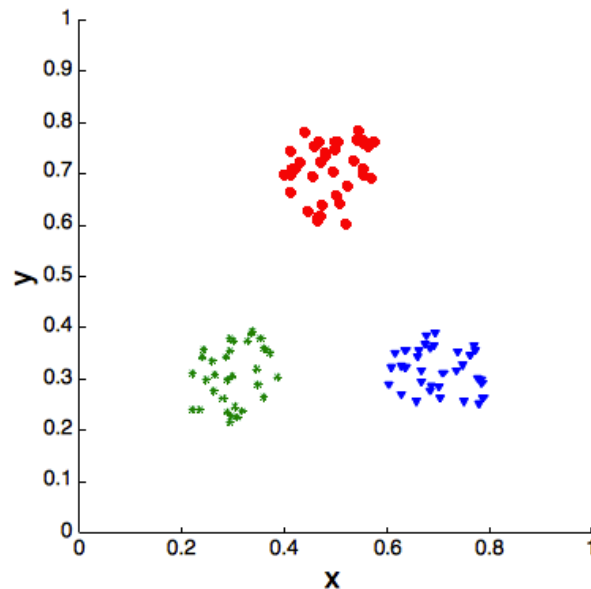
Corr = -0.9235



Corr = -0.5810

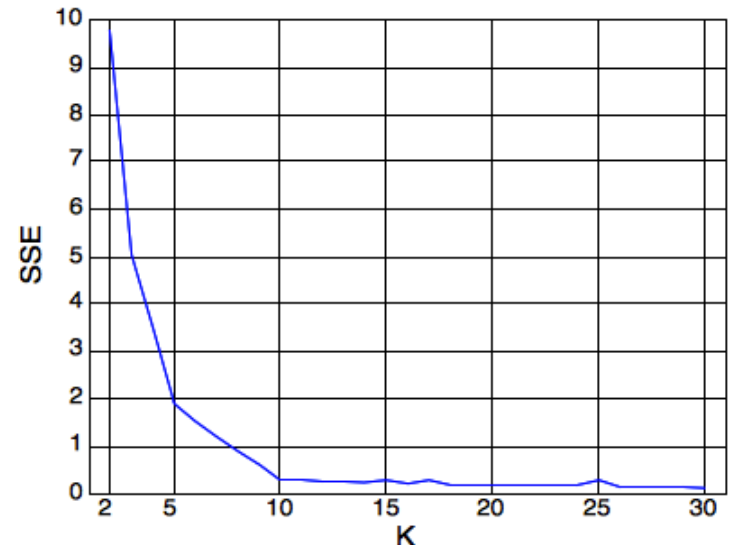
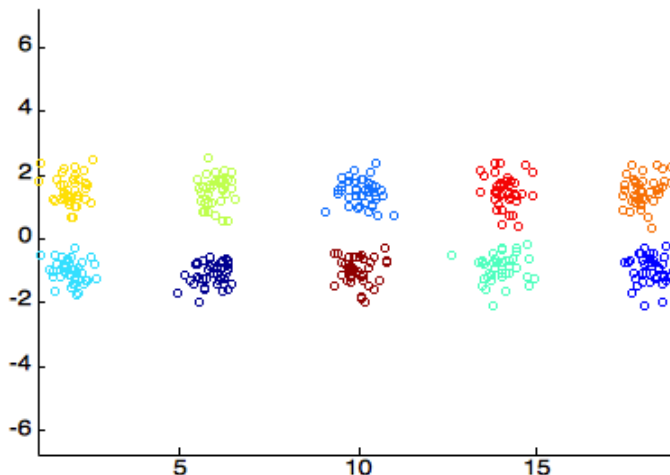
Using Similarity Matrix for Cluster Validation

- Order the similarity matrix with respect to cluster labels and inspect visually.



Internal Measures: SSE

- Clusters in more complicated figures aren't well separated
- Internal Index: Used to measure the goodness of a clustering structure without respect to external information
 - SSE
- SSE is good for comparing two clusterings or two clusters (average SSE).
- Can also be used to estimate the number of clusters



Internal Measures: Cohesion and Separation

- **Cluster Cohesion:** Measures how closely related are objects in a cluster
 - Example: SSE
- **Cluster Separation:** Measure how distinct or well-separated a cluster is from other clusters
- Example: Squared Error
 - Cohesion is measured by the within cluster sum of squares (SSE)

$$WSS = \sum_i \sum_{x \in C_i} (x - m_i)^2$$

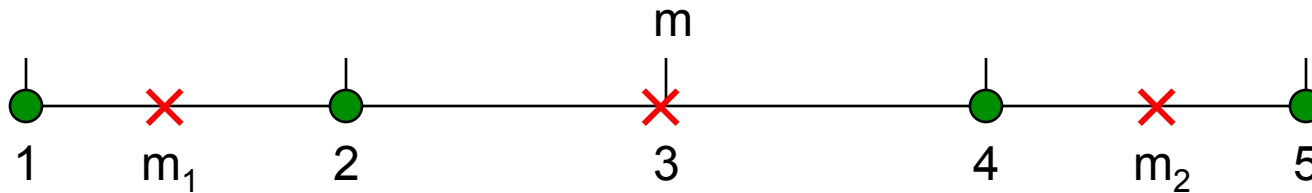
- Separation is measured by the between cluster sum of squares

$$BSS = \sum_i |C_i| (m - m_i)^2$$

- Where $|C_i|$ is the size of cluster i

Internal Measures: Cohesion and Separation

- Example: SSE
 - $BSS + WSS = \text{constant}$



K=1 cluster:

$$WSS = (1 - 3)^2 + (2 - 3)^2 + (4 - 3)^2 + (5 - 3)^2 = 10$$

$$BSS = 4 \times (3 - 3)^2 = 0$$

$$Total = 10 + 0 = 10$$

K=2 clusters:

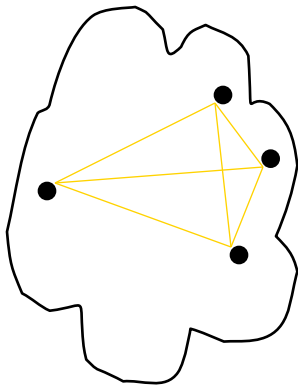
$$WSS = (1 - 1.5)^2 + (2 - 1.5)^2 + (4 - 4.5)^2 + (5 - 4.5)^2 = 1$$

$$BSS = 2 \times (3 - 1.5)^2 + 2 \times (4.5 - 3)^2 = 9$$

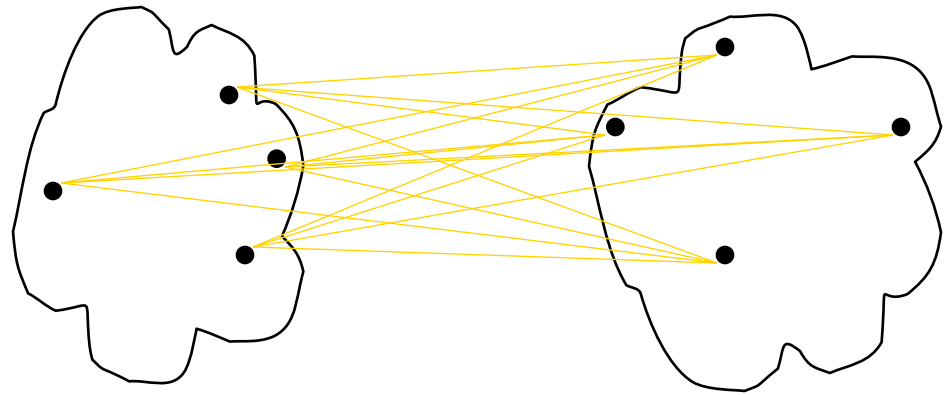
$$Total = 1 + 9 = 10$$

Internal Measures: Cohesion and Separation

- A proximity graph based approach can also be used for cohesion and separation.
 - Cluster cohesion is the sum of the weight of all links within a cluster.
 - Cluster separation is the sum of the weights between nodes in the cluster and nodes outside the cluster.



cohesion



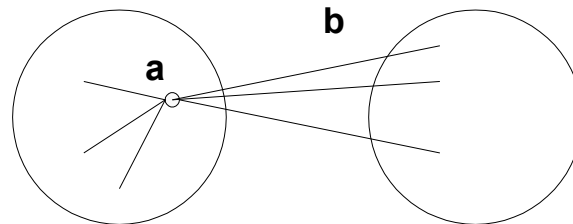
separation

Internal Measures: Silhouette Coefficient

- Silhouette Coefficient **combine ideas of both cohesion and separation**, but for individual points, as well as clusters and clusterings
- For an individual point, i
 - Calculate a = average distance of i to the points in its cluster
 - Calculate b = min (average distance of i to points in another cluster)
 - The silhouette coefficient for a point is then given by

$$s = 1 - a/b \quad \text{if } a < b, \quad (\text{or } s = b/a - 1 \quad \text{if } a \geq b, \text{ not the usual case})$$

- Typically between 0 and 1.
- The closer to 1 the better.



- Can calculate the Average Silhouette width for a cluster or a clustering

Final Comment on Cluster Validity

“The validation of clustering structures is the most difficult and frustrating part of cluster analysis.

Without a strong effort in this direction, cluster analysis will remain a black art accessible only to those true believers who have experience and great courage.”

Algorithms for Clustering Data, Jain and Dubes

Summary of Clustering Analysis

- Important DM techniques.
- Partitioning Clustering
 - K-Means, K-medoid
- Hierarchical Clustering
 - Agglomerative/divisive
- Density-based Clustering
 - DBSCAN
- EM/Cobweb
- Cluster Validation

Acknowledgement

- Some of the slides are based on or taken from the course slides provided by
 - Tan, Steinbach and Kumar (Introduction to Data Mining)
- Some pictures are taken from various online resources.