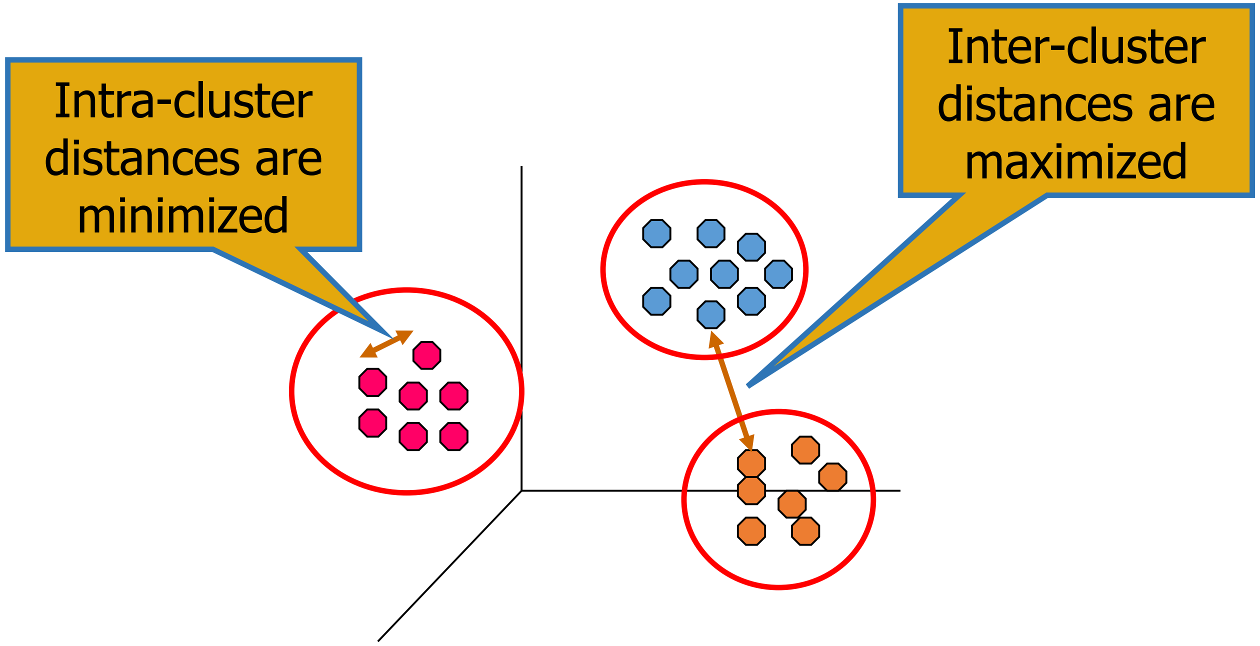
Clustering Model

Agenda

- **Introduction to Clustering**
- Partitioning Methods
- Hierarchical Methods
- Density-Based Methods
- Model Evaluation and Selection

What is
Cluster Analysis?

- Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups.

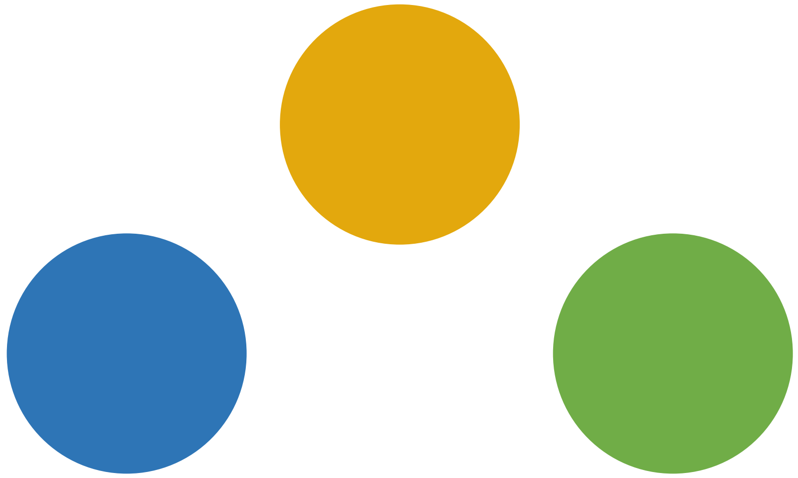


What is not Cluster Analysis?

- Supervised classification
  - Have class label information
- Simple segmentation
  - Dividing students into different registration groups alphabetically, by last name
- Results of a query
  - Groupings are a result of an external specification
- Graph partitioning
  - Some mutual relevance and synergy, but areas are not identical

Types of Clusters:
Well-Separated

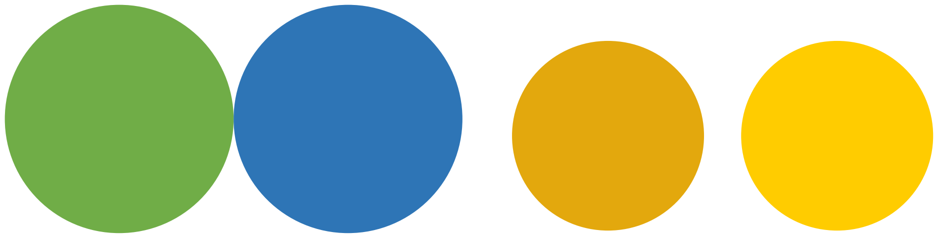
- Well-Separated Clusters:
    - A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.



3 well-separated clusters

Types of Clusters:
Center-Based

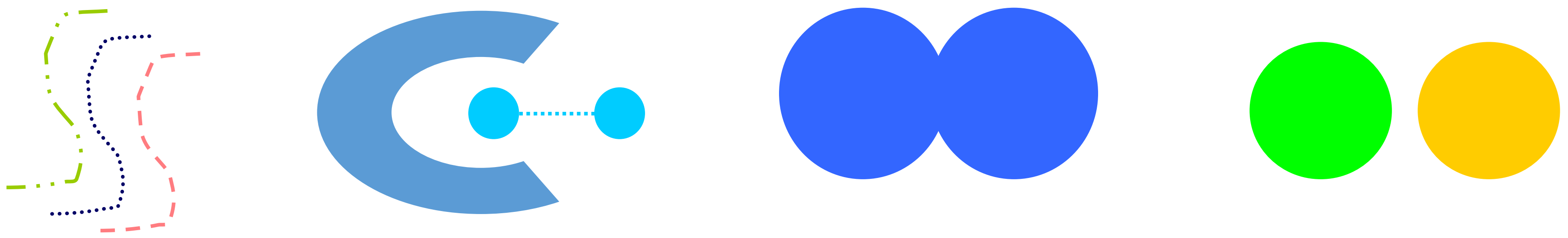
- Center-based
  - A cluster is a set of objects such that an object in a cluster is closer (more similar) to the "center" of a cluster, than to the center of any other cluster
  - The center of a cluster is often a centroid, the average of all the points in the cluster, or a medoid i.e. the most "representative" point of a cluster



4 center-based clusters

Types of Clusters: Contiguity-Based

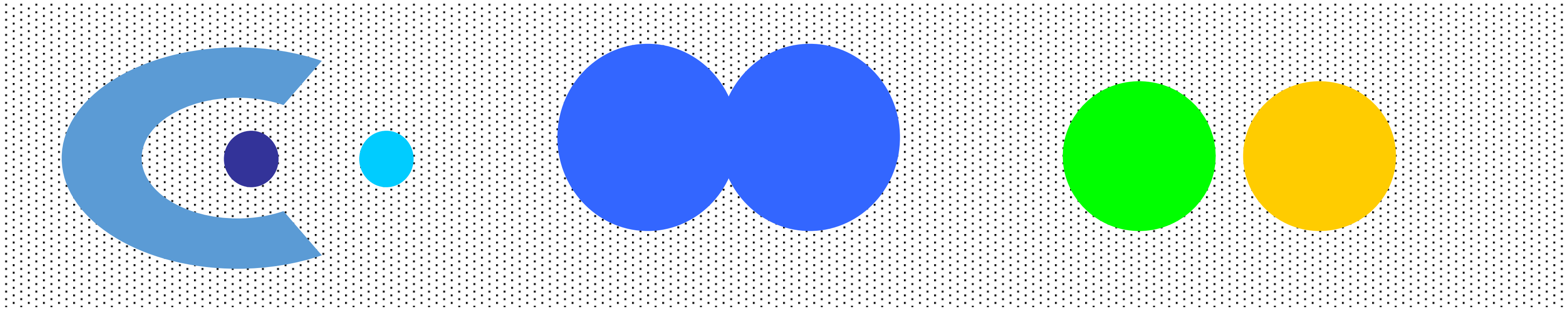
- Contiguous Cluster (Nearest neighbor or Transitive)
  - A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.



8 contiguous clusters

Types of Clusters:
Density-Based

- Density-based
  - A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
  - Used when the clusters are irregular or intertwined, and when noise and outliers are present.



6 density-based clusters

Types of Clusters:
Objective Function

Clusters Defined by an Objective Function

- Finds clusters that minimize or maximize an objective function.
- Enumerate all possible ways of dividing the points into clusters and evaluate the `goodness' of each potential set of clusters by using the given objective function. (NP Hard)
- Can have global or local objectives.
  - Hierarchical clustering algorithms typically have local objectives
  - Partitional algorithms typically have global objectives

Types of Clusters:
Objective Function

Clusters Defined by an Objective Function

- A variation of the global objective function approach is to fit the data to a parameterized model.
  - Parameters for the model are determined from the data.
  - Mixture models assume that the data is a ‘mixture' of a number of statistical distributions.
- Map the clustering problem to a different domain and solve a related problem in that domain
  - Proximity matrix defines a weighted graph, where the nodes are the points being clustered, and the weighted edges represent the proximities between points
  - Clustering is equivalent to breaking the graph into connected components, one for each cluster.
  - Want to minimize the edge weight between clusters and maximize the edge weight within clusters

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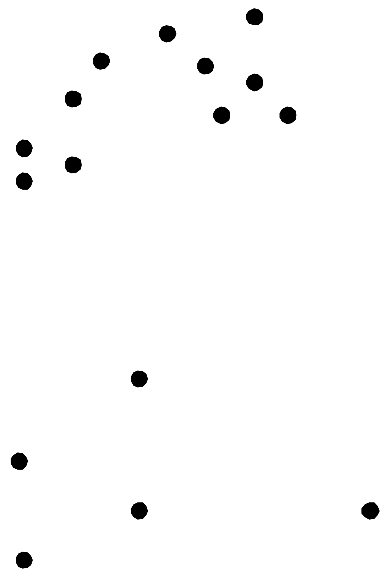
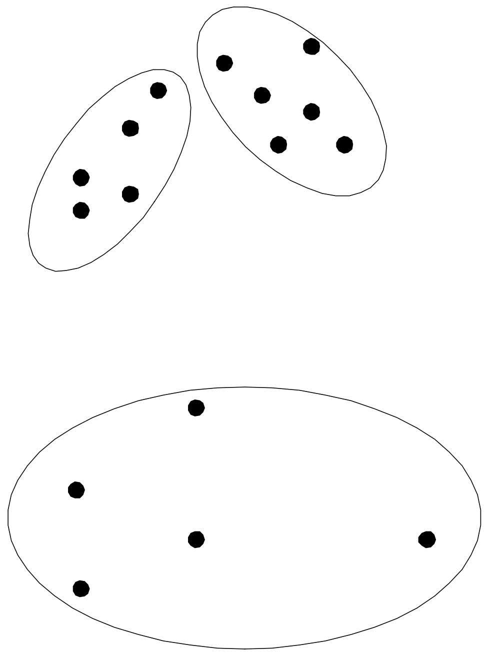
- **Partitioning Methods**
- Hierarchical Methods
- Density-Based Methods
- Model Evaluation and Selection

Partitional Clustering



Original Points



A Partitional Clustering

K-means Algorithm

- Partitional clustering approach
- Each cluster is associated with a centroid (center point)
- Each point is assigned to the cluster with the closest centroid
- Number of clusters, K, must be specified
- The basic algorithm is very simple

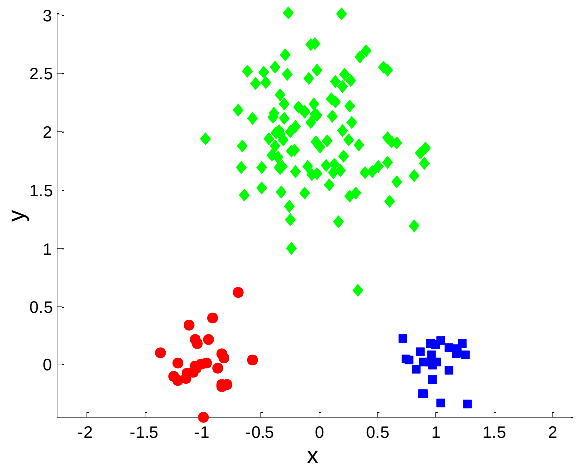
Algorithm 1 Basic K-means Algorithm.

1: Select K points as the initial centroids.
2: **repeat**
3: Form K clusters by assigning all points to the closest centroid.
4: Recompute the centroid of each cluster.
5: **until** The centroids don't change

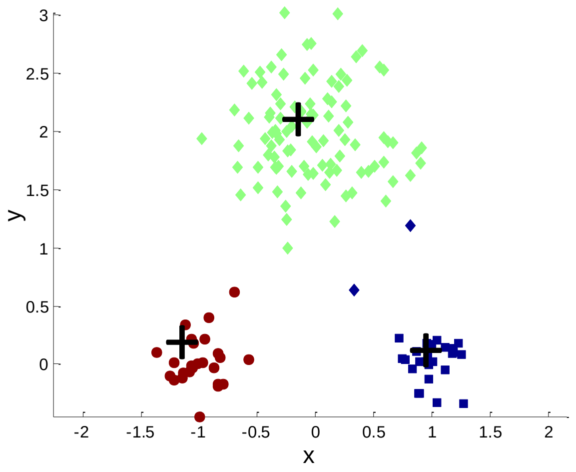
K-means Clustering - Details

- Initial centroids are often chosen randomly.
  - Clusters produced vary from one run to another.
- The centroid is (typically) the mean of the points in the cluster.
- ‘Closeness’ is commonly measured by Euclidean distance.
- K-means will converge for common similarity measures mentioned above.
- Most of the convergence happens in the first few iterations.
  - Often the stopping condition is changed to ‘Until relatively few points change clusters’
- Complexity is O(n * K * I * d)
  - n = number of points, K = number of clusters,
I = number of iterations, d = number of attributes

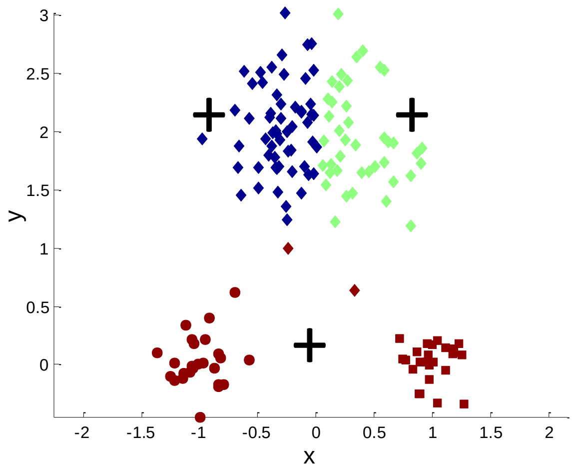
Two different
K-means Clusterings



Original Points

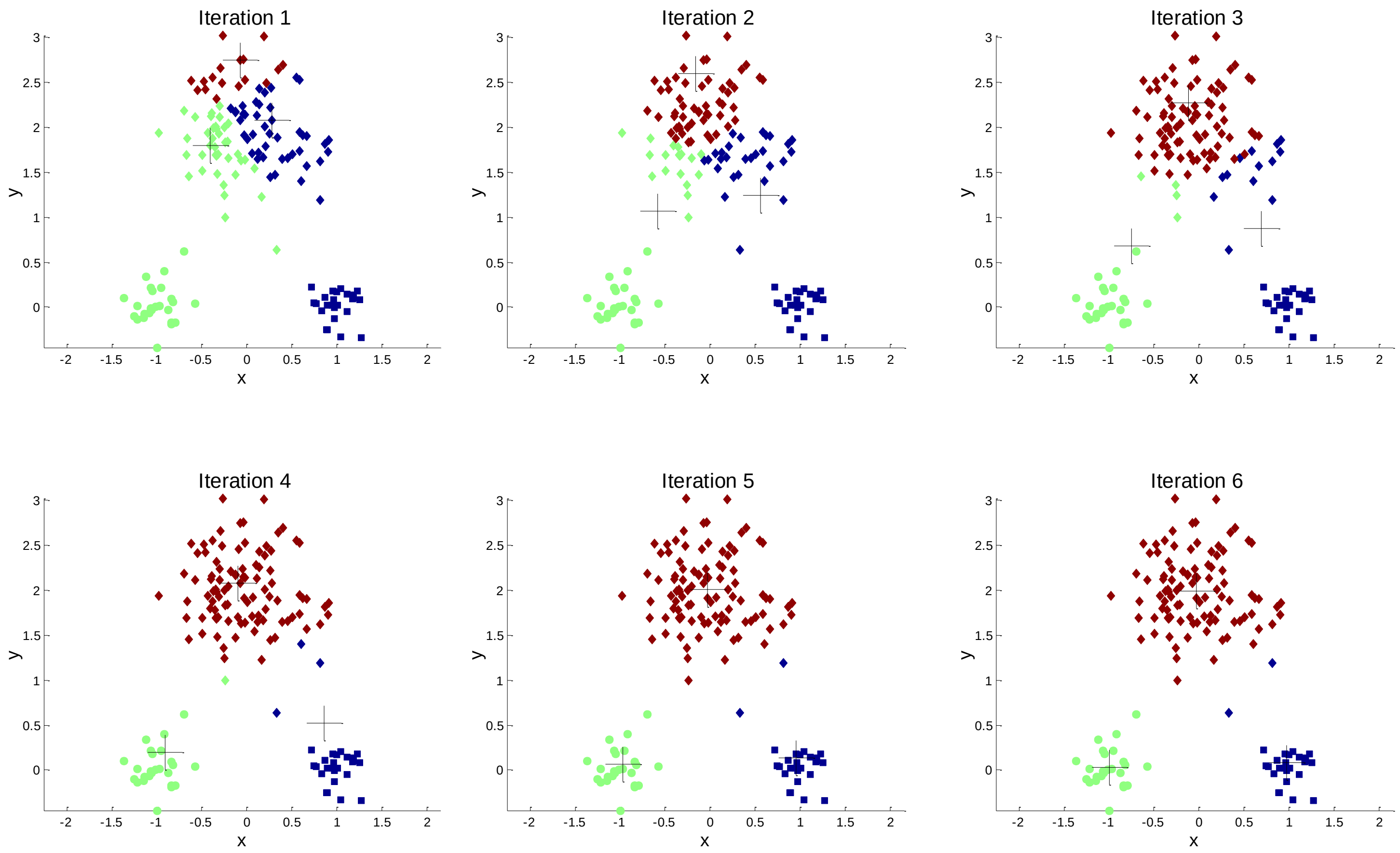


Optimal Clustering



Sub-optimal Clustering

Importance of
Choosing Initial Centroids



Evaluating
K-means Clusters

Most common measure is Sum of Squared Error (SSE)

- For each point, the error is the distance to the nearest cluster
- To get SSE, we square these errors and sum them.

$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(m_i, x)$$

- x is a data point in cluster Ci and mi is the representative point for cluster Ci
  - can show that mi corresponds to the center (mean) of the cluster
- Given two clusters, we can choose the one with the smallest error
- One easy way to reduce SSE is to increase K, the number of clusters
  - A good clustering with smaller K can have a lower SSE than a poor clustering with higher K

Selecting Optimal
Number of Cluster

- Elbow Method
  - Compute clustering algorithm (e.g., k-means clustering) for different values of k. For instance, by varying k from 1 to 10 clusters.
  - For each k, calculate the total within-cluster sum of square (wss).
  - Plot the curve of wss according to the number of clusters k.
  - The location of a bend (knee) in the plot is generally considered as an indicator of the appropriate number of clusters.

- Average silhouette method
  - Compute clustering algorithm (e.g., k-means clustering) for different values of k. For instance, by varying k from 1 to 10 clusters.
  - For each k, calculate the average silhouette of observations (avg.sil).
  - Plot the curve of avg.sil according to the number of clusters k.
  - The location of the maximum is considered as the appropriate number of clusters.

Selecting Optimal
Number of Cluster

These methods include direct methods and statistical testing methods:

- Direct methods: consists of optimizing a criterion, such as the within cluster sums of squares or the average silhouette. The corresponding methods are named elbow and silhouette methods, respectively.
- Statistical testing methods: consists of comparing evidence against null hypothesis. An example is the gap statistic.

Problems with
Selecting Initial Points

If there are K ‘real’ clusters then the chance of selecting one centroid from each cluster is small.

- Chance is relatively small when K is large
- If clusters are the same size, n, then

$$P = \frac{\text{number of ways to select one centroid from each cluster}}{\text{number of ways to select } K \text{ centroids}} = \frac{K!n^K}{(Kn)^K} = \frac{K!}{K^K}$$

For example, if K = 10, then probability = 10!/1010 = 0.00036

- Sometimes the initial centroids will readjust themselves in ‘right’ way, and sometimes they don’t
- Consider an example of five pairs of clusters

Solutions to
Initial Centroids Problem

- Multiple runs
  - Helps, but probability is not on your side
- Sample and use hierarchical clustering to determine initial centroids
- Select more than k initial centroids and then select among these initial centroids
  - Select most widely separated
- Post-processing
- Bisecting K-means
  - Not as susceptible to initialization issues

Pre-processing and Post-processing

Pre-processing

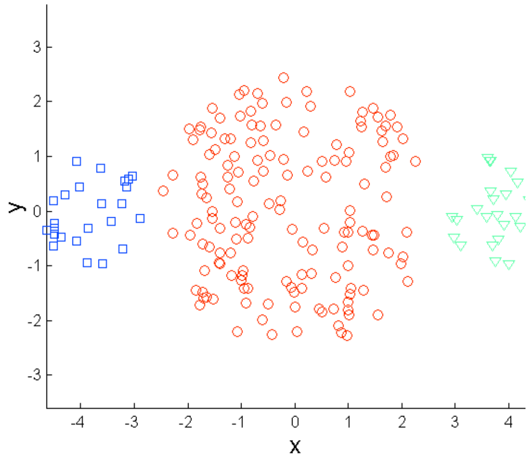
- Normalize the data
- Eliminate outliers

Post-processing

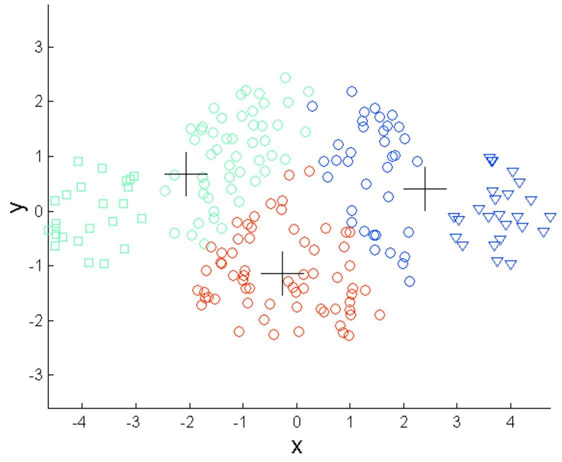
- Eliminate small clusters that may represent outliers
- Split 'loose' clusters, i.e., clusters with relatively high SSE
- Merge clusters that are 'close' and that have relatively low SSE

Limitations & Overcoming of K-means:
Differing Sizes

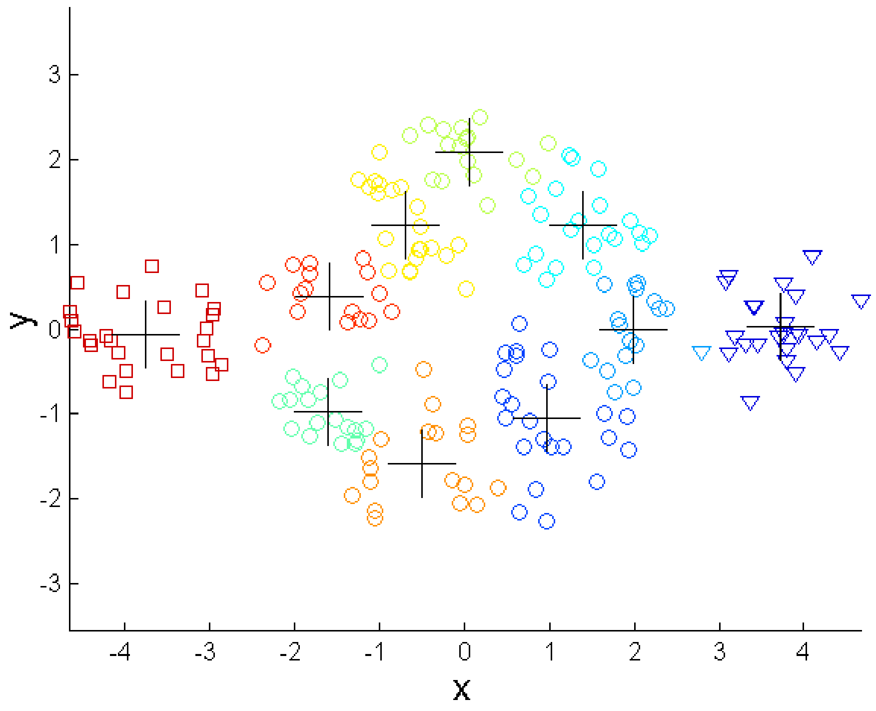
One solution is to use many clusters.
Find parts of clusters, but need to put together.



Original Points

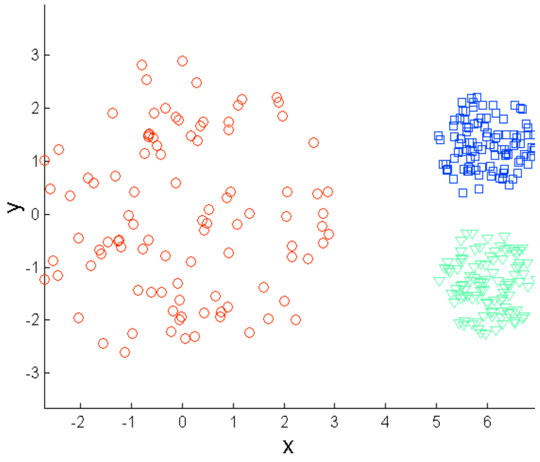


K-means (3 Clusters)

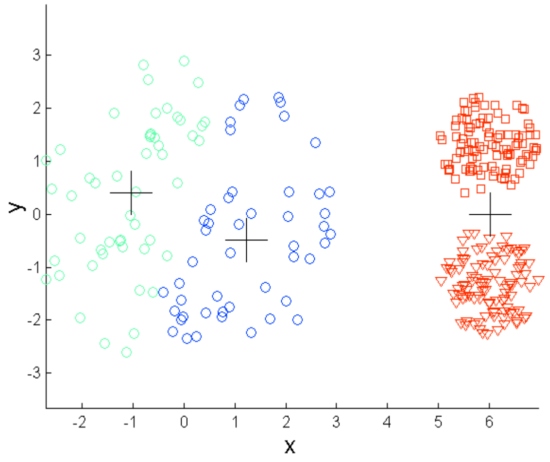


Overcoming K-means

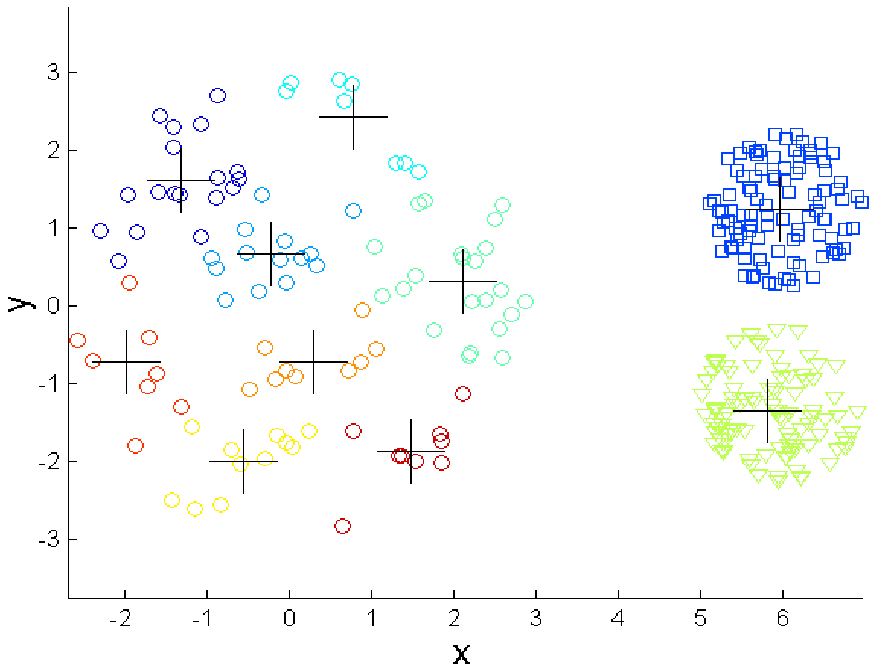
Limitations & Overcoming of K-means:
Differing Density



Original Points

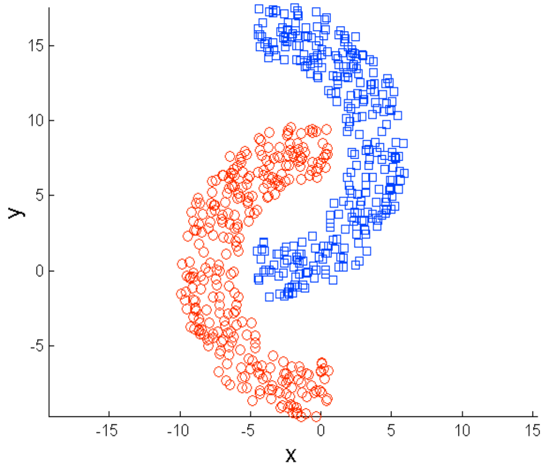


K-means (3 Clusters)

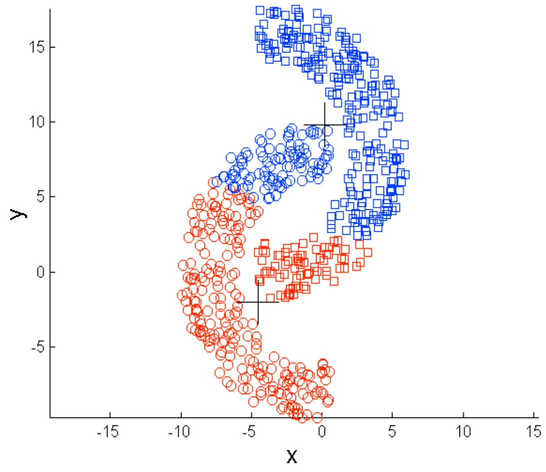


Overcoming K-means

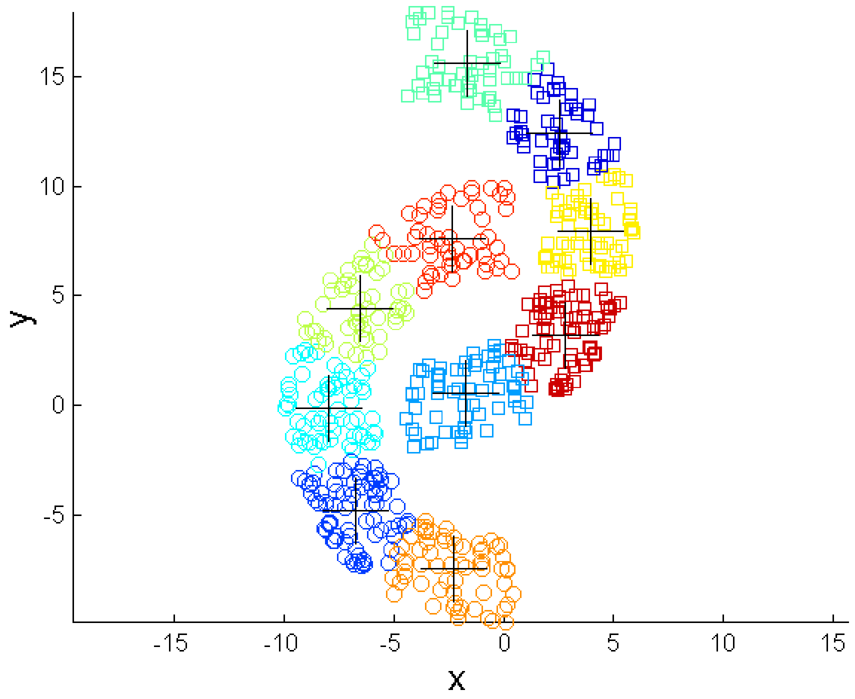
Limitations & Overcoming of K-means:
Non-globular Shapes



Original Points



K-means (2 Clusters)



Overcoming K-means

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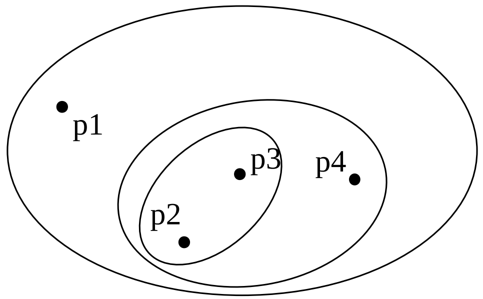
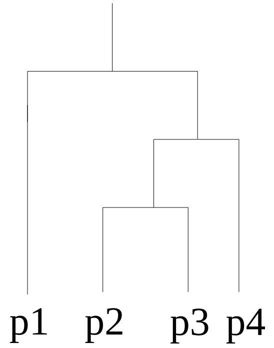
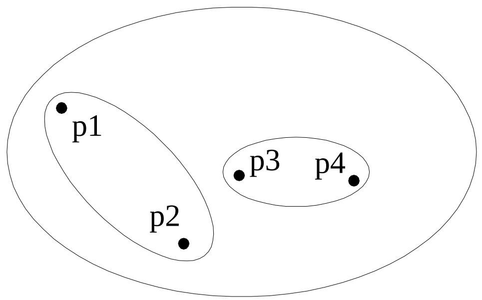
Hierarchical Clustering



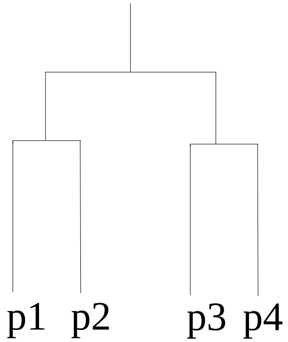
Traditional Hierarchical Clustering



Traditional dendogram



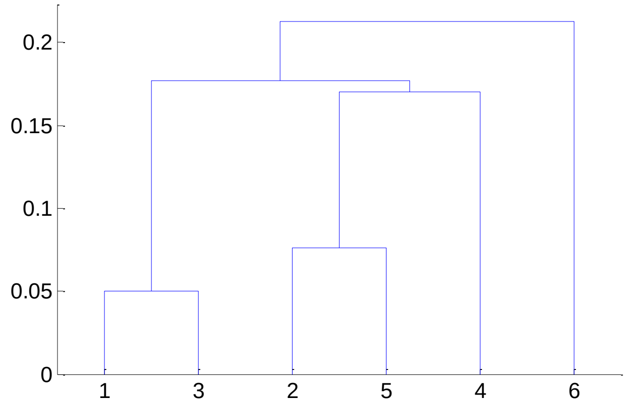
Non-traditional Hierarchical Clustering

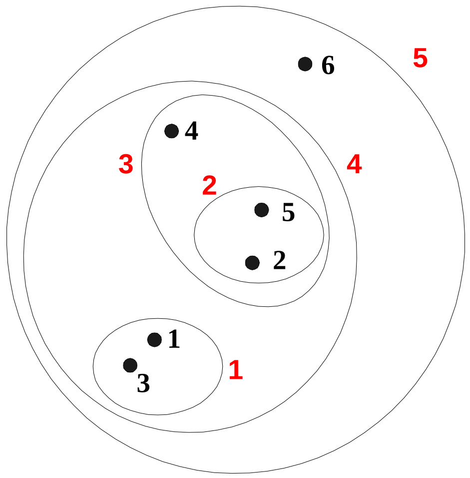


Non-traditional dendogram

Hierarchical Clustering

- Produces a set of nested clusters organized as a hierarchical tree
  - Can be visualized as a dendogram
  - A tree like diagram that records the sequences of merges or splits





Strengths of Hierarchical Clustering

- Do not have to assume any particular number of clusters
  - Any desired number of clusters can be obtained by 'cutting' the dendogram at the proper level
- They may correspond to meaningful taxonomies
  - Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, …)

Hierarchical Clustering

Two main types of hierarchical clustering

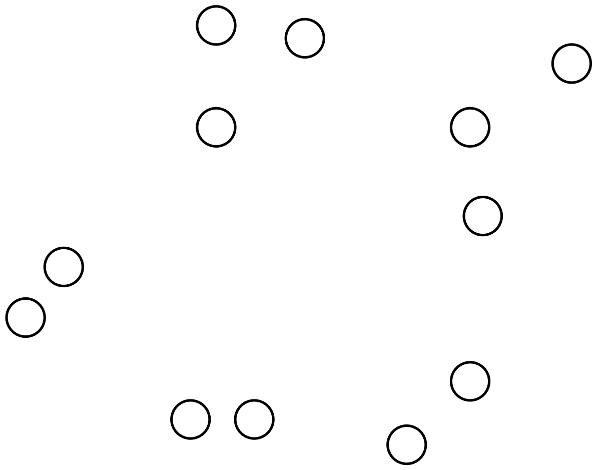
- Agglomerative:
  - Start with the points as individual clusters
  - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
- Divisive:
  - Start with one, all-inclusive cluster
  - At each step, split a cluster until each cluster contains a point (or there are k clusters)
- Traditional hierarchical algorithms use a similarity or distance matrix
  - Merge or split one cluster at a time

Agglomerative Clustering Algorithm

- More popular hierarchical clustering technique
- Basic algorithm is straightforward
  1. Compute the proximity matrix
  2. Let each data point be a cluster
  3. Repeat
  4. Merge the two closest clusters
  5. Update the proximity matrix
  6. Until only a single cluster remains
- Key operation is the computation of the proximity of two clusters
  - Different approaches to defining the distance between clusters distinguish the different algorithms

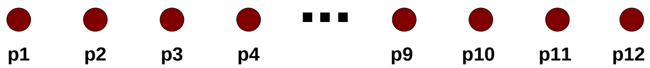
Starting Situation

- Start with clusters of individual points and a proximity matrix



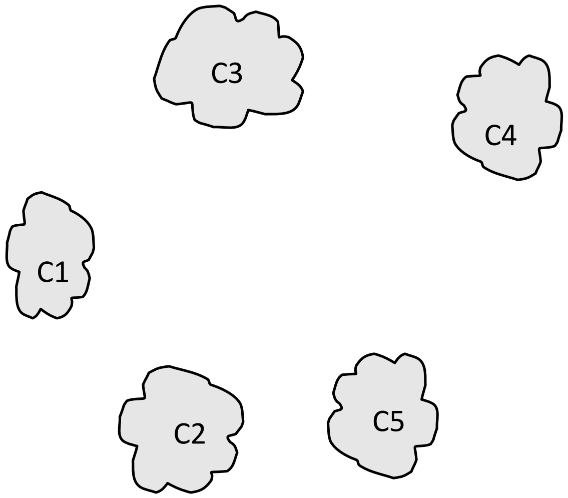
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix



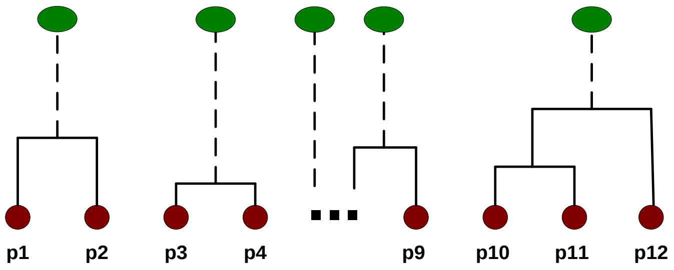
Intermediate Situation

- After some merging steps, we have some clusters



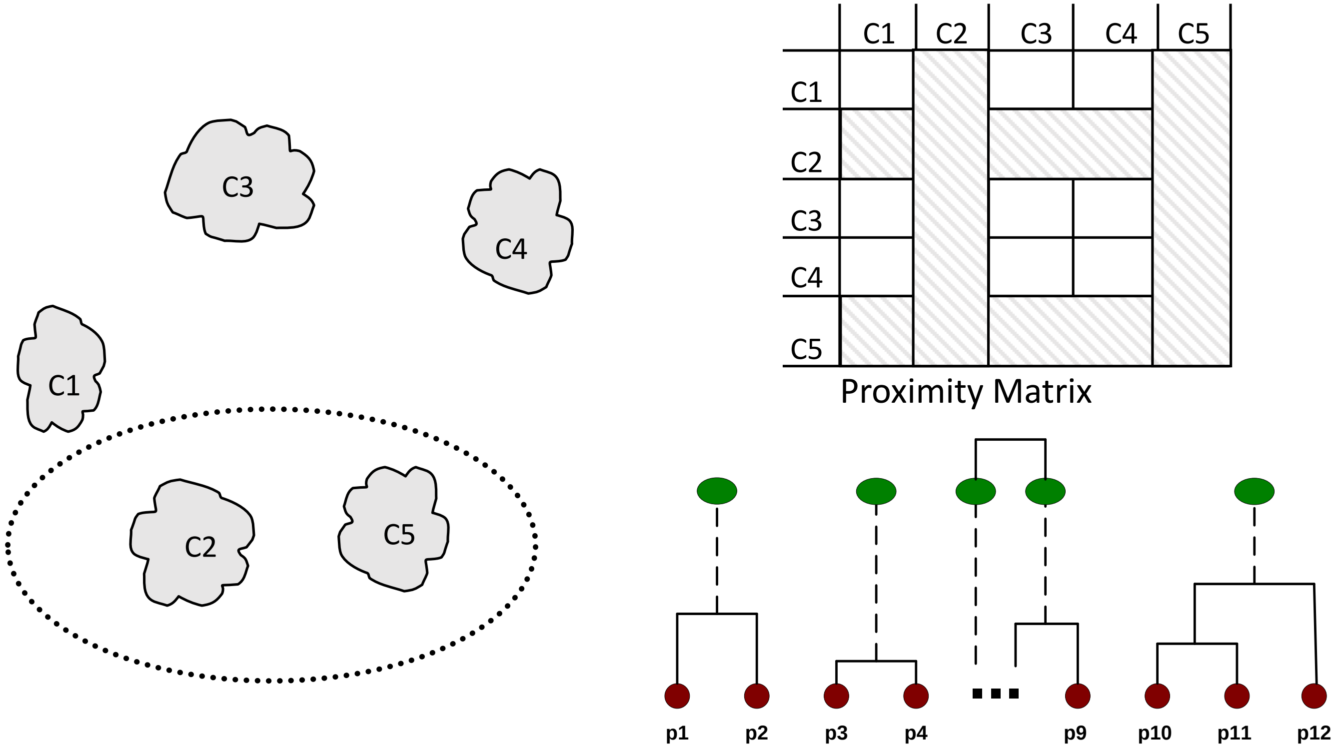
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Proximity Matrix



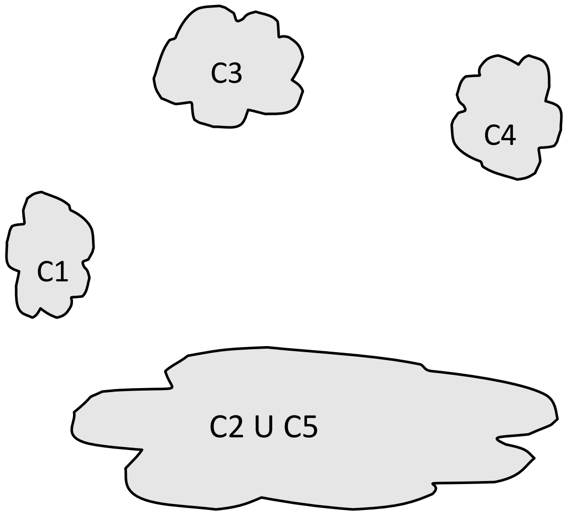
Intermediate Situation

- We want to merge the two closest clusters (C2 and C5) and update the proximity matrix.



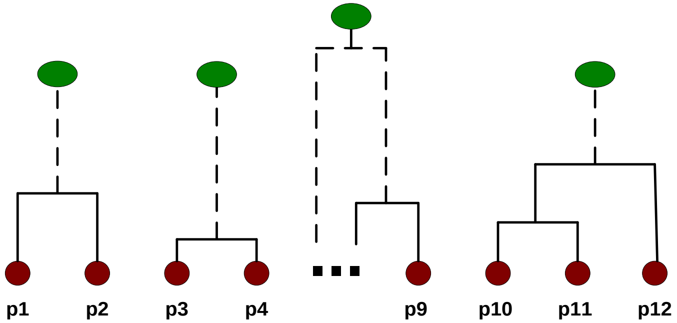
After Merging

- The question is “How do we update the proximity matrix?”



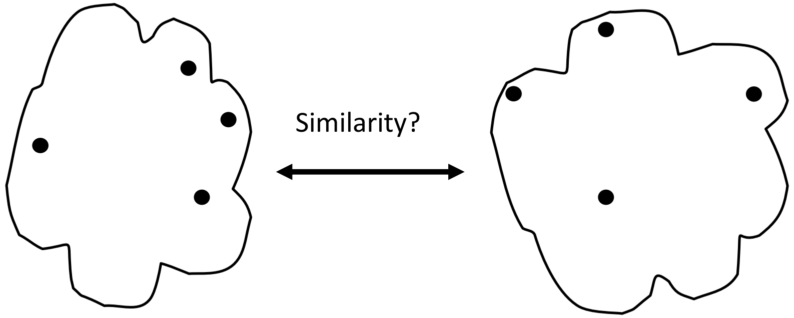
	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	? ?	?	
C3		?		
C4		?		

Proximity Matrix



How to Define
Inter-Cluster Similarity

- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
  - Ward's Method uses squared error

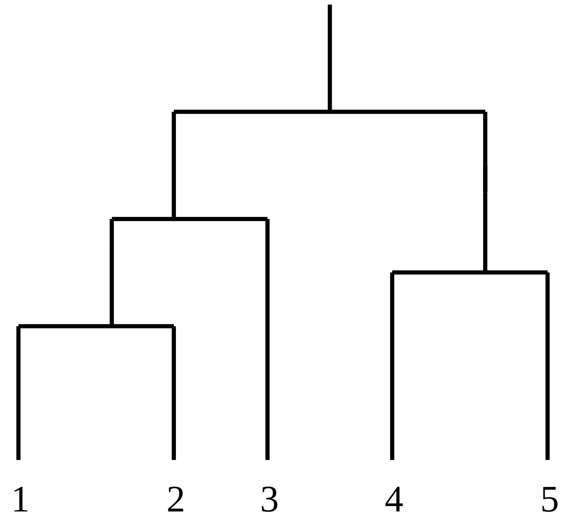


	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Cluster Similarity:
MIN or Single Link

- Similarity of two clusters is based on the two most similar (closest) points in the different clusters
  - Determined by one pair of points, i.e., by one link in the proximity graph.

	I1	I2	I3	I4	I5
I1	1.00	0.90	0.10	0.65	0.20
I2	0.90	1.00	0.70	0.60	0.50
I3	0.10	0.70	1.00	0.40	0.30
I4	0.65	0.60	0.40	1.00	0.80
I5	0.20	0.50	0.30	0.80	1.00

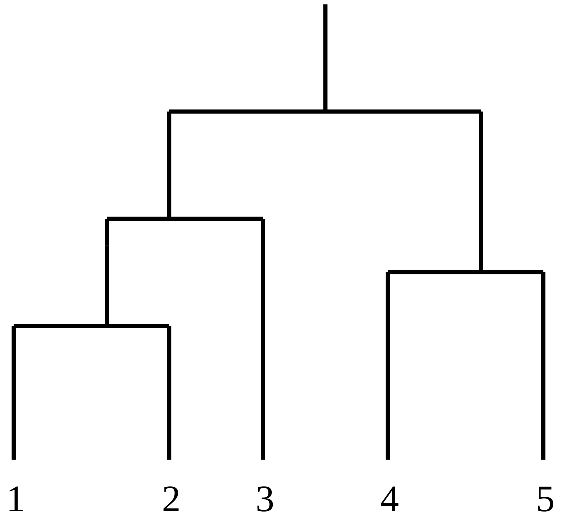


*Proximity matrix is based on Correlation

Cluster Similarity:
MAX or Complete Linkage

- Similarity of two clusters is based on the two least similar (most distant) points in the different clusters
  - Determined by all pairs of points in the two clusters

	I1	I2	I3	I4	I5
I1	1.00	0.90	0.10	0.65	0.20
I2	0.90	1.00	0.70	0.60	0.50
I3	0.10	0.70	1.00	0.40	0.30
I4	0.65	0.60	0.40	1.00	0.80
I5	0.20	0.50	0.30	0.80	1.00



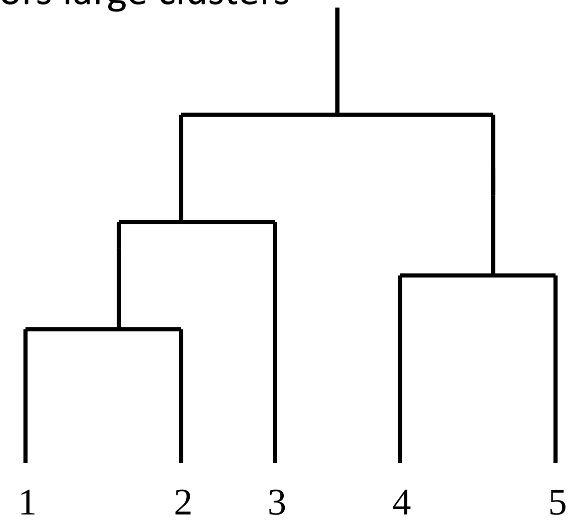
Cluster Similarity:
Group Average

- Proximity of two clusters is the average of pairwise proximity between points in the two clusters.

$$\text{proximity}(\text{Cluster}_i, \text{Cluster}_j) = \frac{\sum\limits_{\substack{p_i \in \text{Cluster}_i \\ p_j \in \text{Cluster}_j}} \text{proximity}(p_i, p_j)}{|\text{Cluster}_i| * |\text{Cluster}_j|}$$

- Need to use average connectivity for scalability since total proximity favors large clusters

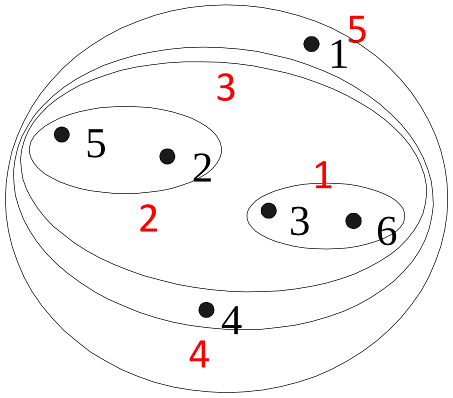
	I1	I2	I3	I4	I5
I1	1.00	0.90	0.10	0.65	0.20
I2	0.90	1.00	0.70	0.60	0.50
I3	0.10	0.70	1.00	0.40	0.30
I4	0.65	0.60	0.40	1.00	0.80
I5	0.20	0.50	0.30	0.80	1.00



Cluster Similarity:
Ward's Method

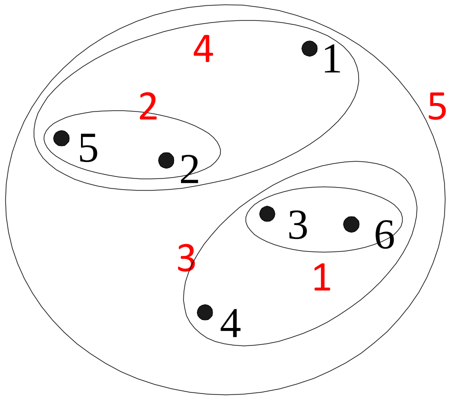
- Similarity of two clusters is based on the increase in squared error when two clusters are merged
  - Similar to group average if distance between points is distance squared
- Less susceptible to noise and outliers
- Biased towards globular clusters
- Hierarchical analogue of K-means
  - Can be used to initialize K-means

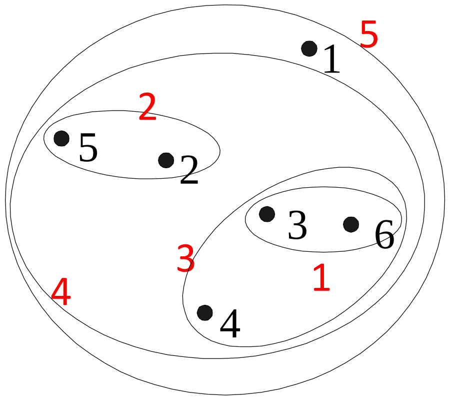
Hierarchical Clustering:
Comparison



MIN

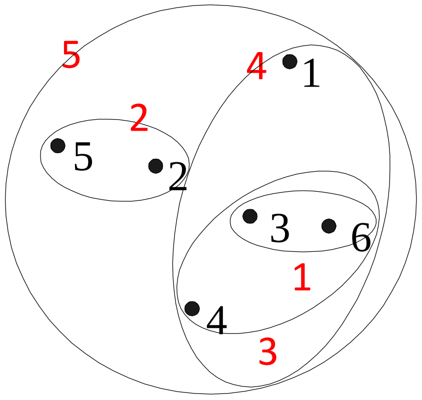
MAX





Group Average

Ward's Method



Hierarchical Clustering: Comparison

STRENGTH

- MIN :
  - Can handle non-elliptical shapes
- MAX :
  - Less susceptible to noise and outliers
- GROUP AVG :
  - Less susceptible to noise and outliers

LIMITATION

- MIN:
  - Sensitive to noise and outliers
- MAX :
  - Tends to break large clusters
  - Biased towards globular clusters
- GROUP AVG :
  - Biased towards globular clusters

Hierarchical Clustering:
Problems and Limitations

- Once a decision is made to combine two clusters, it cannot be undone
- No objective function is directly minimized
- Different schemes have problems with one or more of the following:
    - Sensitivity to noise and outliers
    - Difficulty handling different sized clusters and convex shapes
    - Breaking large clusters

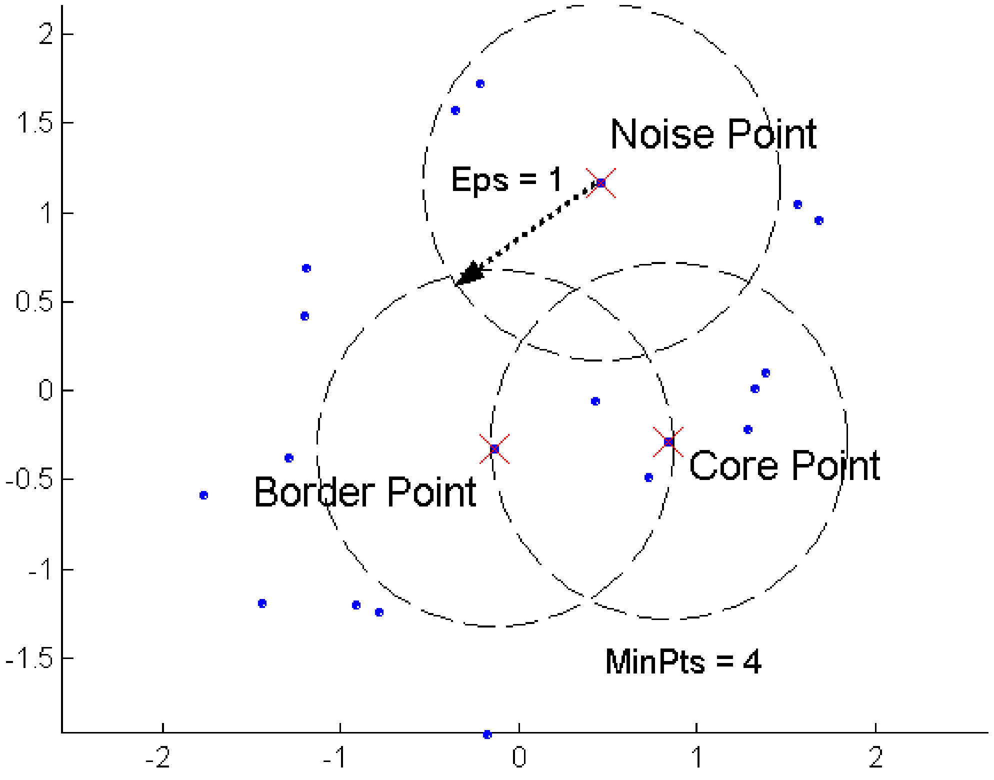
Agenda

- Introduction to Clustering
- Partitioning Methods
- Hierarchical Methods
- **Density-Based Methods**
- Model Evaluation and Selection

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.



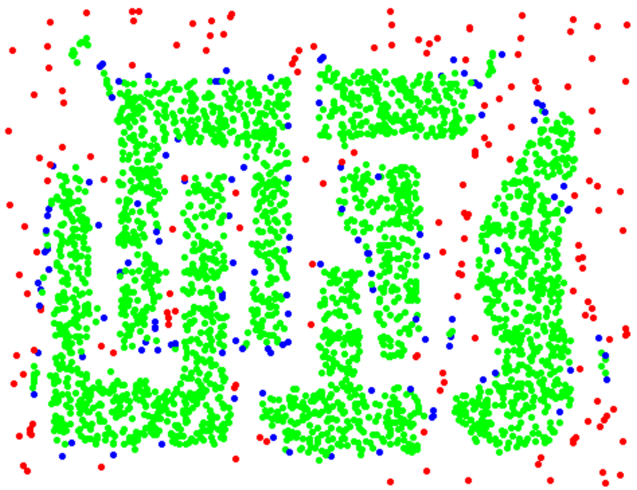
DBSCAN
Algorithm

- 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

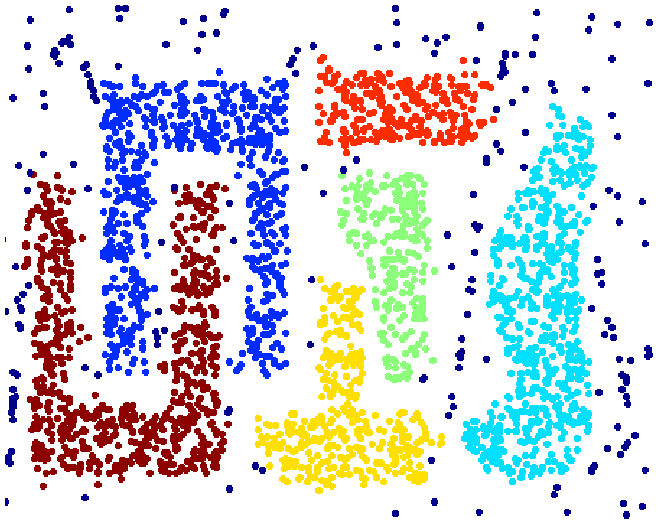


Point types: core, border and noise

Eps = 10, MinPts = 4

When DBSCAN
Works Well

Original Points



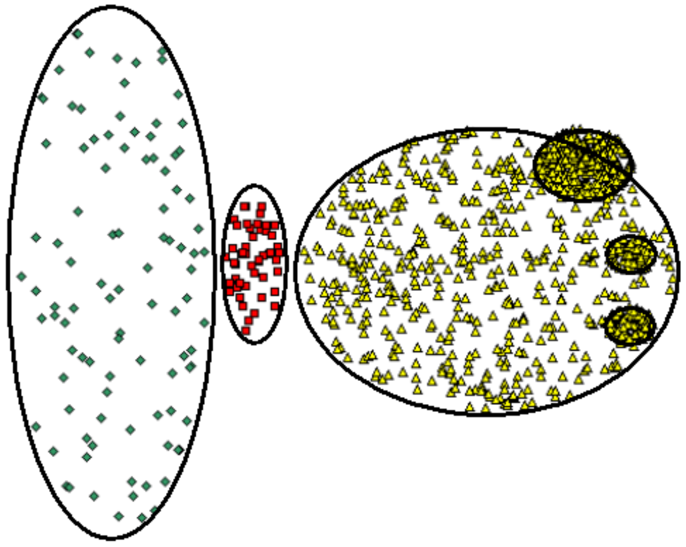
Clusters

Resistant to Noise

Can handle clusters of different shapes and sizes

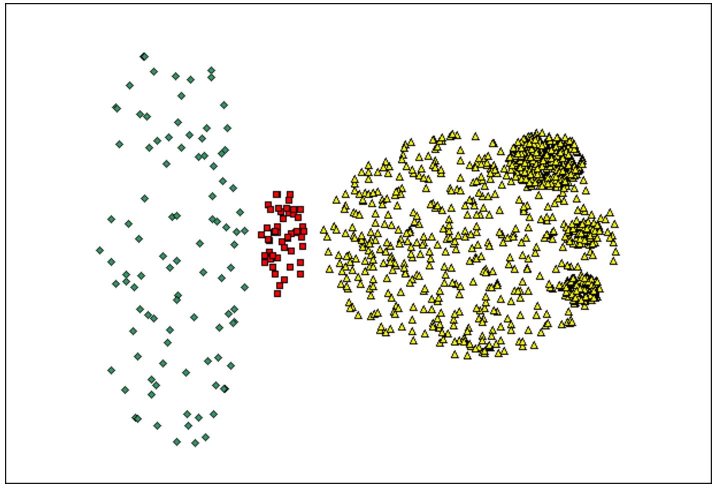
When DBSCAN

Does NOT Works Well

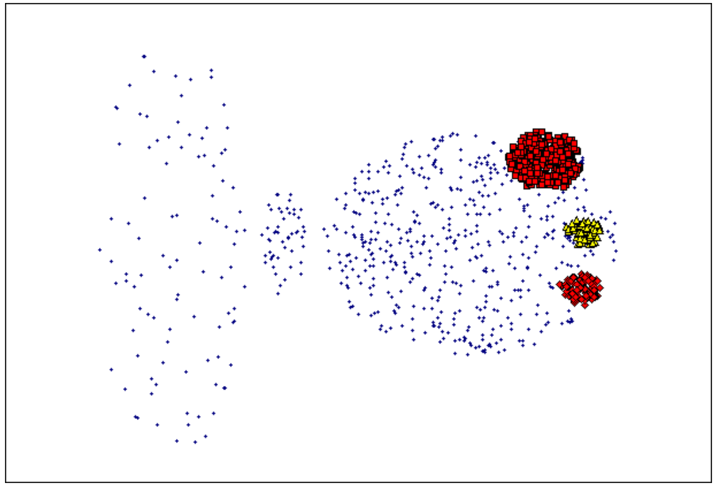


Original Points

- Varying densities
- High-dimensional data



(MinPts=4, Eps=9.75).



(MinPts=4, Eps=9.92)

Agenda

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

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

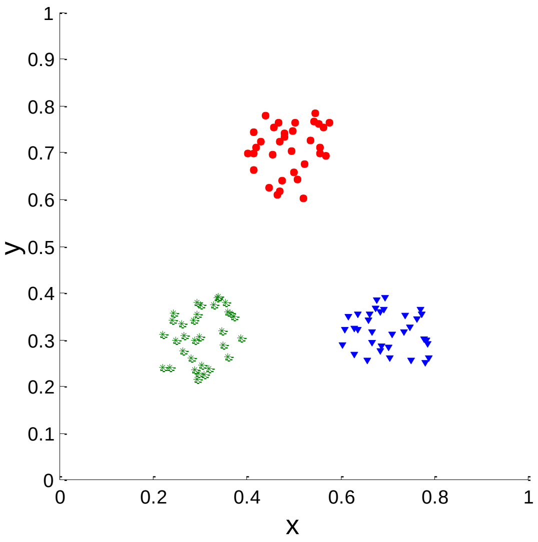
- However, sometimes criterion is the general strategy and index is the numerical measure that implements the criterion.

Validity Measurement
Via Correlation

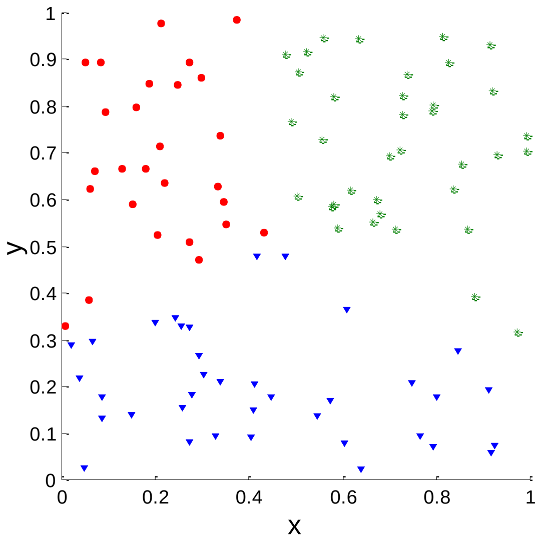
- Two matrices
  - Proximity Matrix – distance between any pair of points
  - “Incidence” Matrix – association pair of points
    - One row and one column for each data point
    - An entry is 1 if the associated pair of points belong to the same cluster
    - An entry is 0 if the associated pair of 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.

Validity Measurement
Via Correlation

- Correlation of incidence and proximity matrices for the K-means clusterings of the following two data sets.



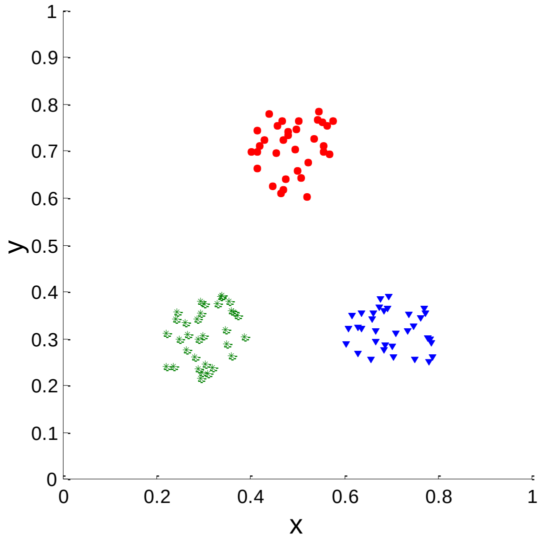
Corr = -0.9235

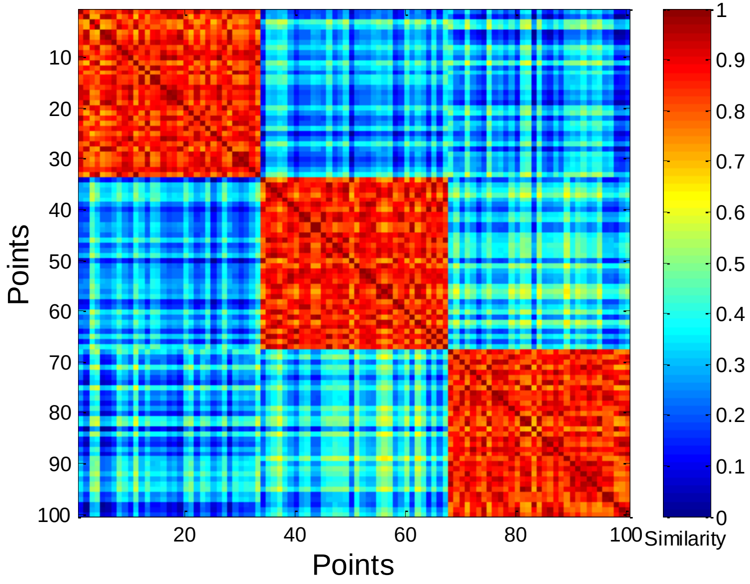


Corr = -0.5810

Validity Measurement
Using Similarity Matrix

- Order the similarity matrix with respect to cluster labels and inspect visually.
- Clusters in random data are not so crisp





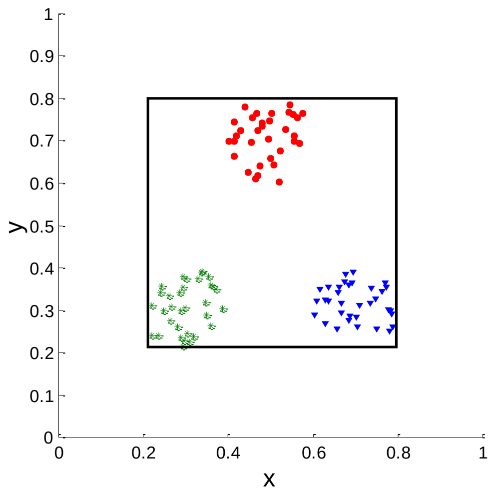
Framework for Cluster Validity

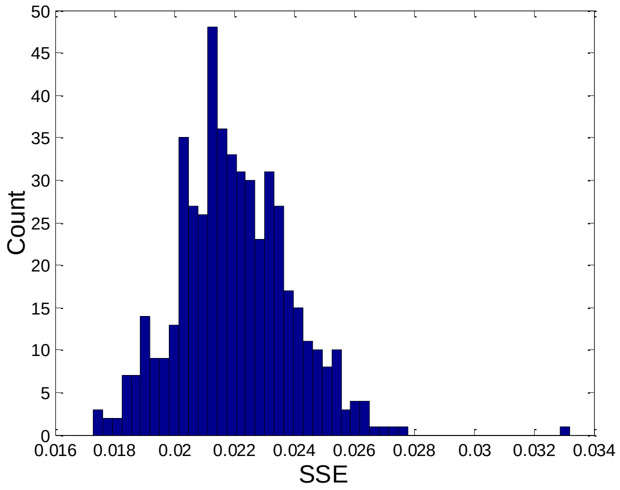
- Need a framework to interpret any measure.
  - For example, if our measure of evaluation has the value, 10, is that good, fair, or poor?
- Statistics provide a framework for cluster validity
  - The more "atypical" a clustering result is, the more likely it represents valid structure in the data
  - Can compare the values of an index that result from random data or clusterings to those of a clustering result.
    - If the value of the index is unlikely, then the cluster results are valid
  - These approaches are more complicated and harder to understand.
- For comparing the results of two different sets of cluster analyses, a framework is less necessary.
  - However, there is the question of whether the difference between two index values is significant

Statistical Framework
for SSE

Example

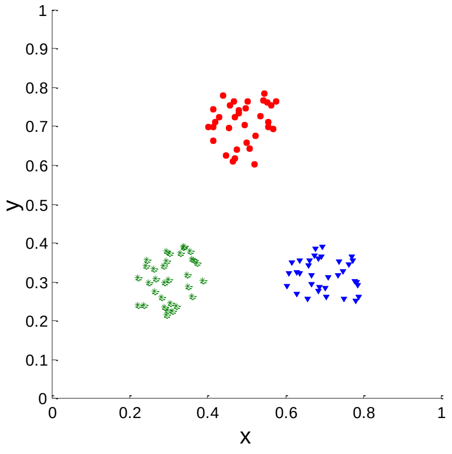
- Compare SSE of 0.005 against three clusters in random data
- Histogram shows SSE of three clusters in 500 sets of random data points of size 100 distributed over the range 0.018 – 0.028 for x and y values



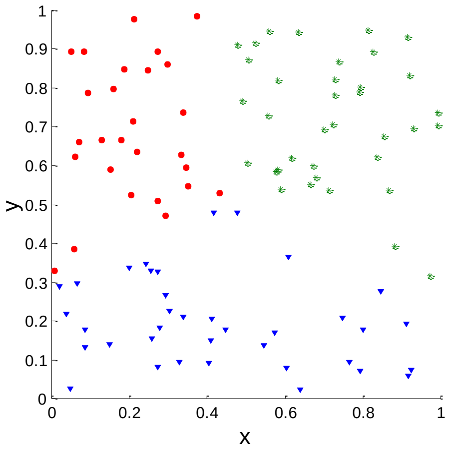


Statistical Framework
for Correlation

- Correlation of incidence and proximity matrices for the K-means clusterings of the following two data sets.



Corr = -0.9235



Corr = -0.5810