CLUSTERING

UNIT 4

CONTENT

Cluster Analysis	
Partitioning Methods	k-Means and k-Medoids
Hierarchical Methods	Agglomerative versus Divisive Hierarchical Clustering Distance Measures in Algorithmic Methods BIRCH
Density-Based Method	DBSCAN, Grid-Based Methods STING Evaluation of Clustering

Similarity and Dissimilarity

Similarity

Numerical measure of how alike two data objects are.

Is higher when objects are more alike.

Often falls in the range [0,1]

Dissimilarity

Numerical measure of how different are two data objects

Lower when objects are more alike

Minimum dissimilarity is often 0

Upper limit varies

Proximity refers to a similarity or dissimilarity

Euclidean Distance

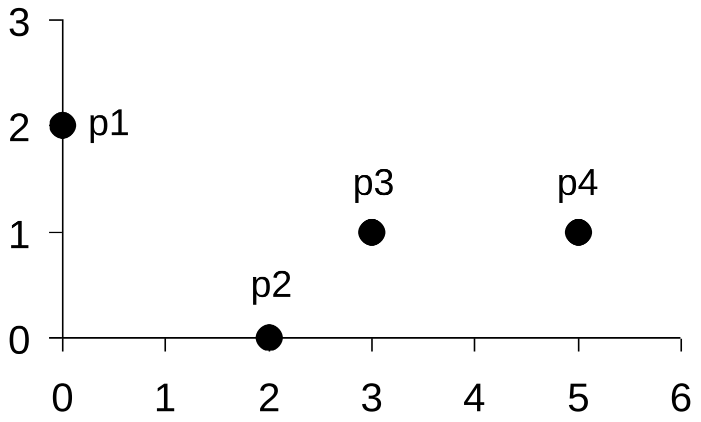
- Euclidean Distance

$$dist = \sqrt{\sum_{k=1}^{n} (p_k - q_k)^2}$$

Where *n* is the number of dimensions (attributes) and p_k and q_k are, respectively, the k^{th} attributes (components) or data objects *p* and *q*.

- Standardization is necessary, if scales differ.

Euclidean Distance



point	x	y
p1	0	2
p2	2	0
p3	3	1
p4	5	1

	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

Distance Matrix

Minkowski Distance

- Minkowski Distance is a generalization of Euclidean Distance

$$dist = \left(\sum_{k=1}^{n} | p_k - q_k |^r \right)^{\frac{1}{r}}$$

Where r is a parameter, n is the number of dimensions (attributes) and p_k and q_k are, respectively, the kth attributes (components) or data objects p and q.

Minkowski Distance: Examples

r = 1. City block (Manhattan, taxicab, L_1 norm) distance.

A common example of this is the Hamming distance, which is just the number of bits that are different between two binary vectors

r = 2. Euclidean distance

$r \rightarrow \infty$. "supremum" (L_{max} norm, L_∞ norm) distance.

This is the maximum difference between any component of the vectors

Example: L_infinity of (1, 0, 2) and (6, 0, 3) = ??

Do not confuse *r* with *n*, i.e., all these distances are defined for all numbers of dimensions.

Minkowski Distance

point	x	y
p1	0	2
p2	2	0
p3	3	1
p4	5	1

L1	p1	p2	p3	p4
p1	0	4	4	6
p2	4	0	2	4
p3	4	2	0	2
p4	6	4	2	0

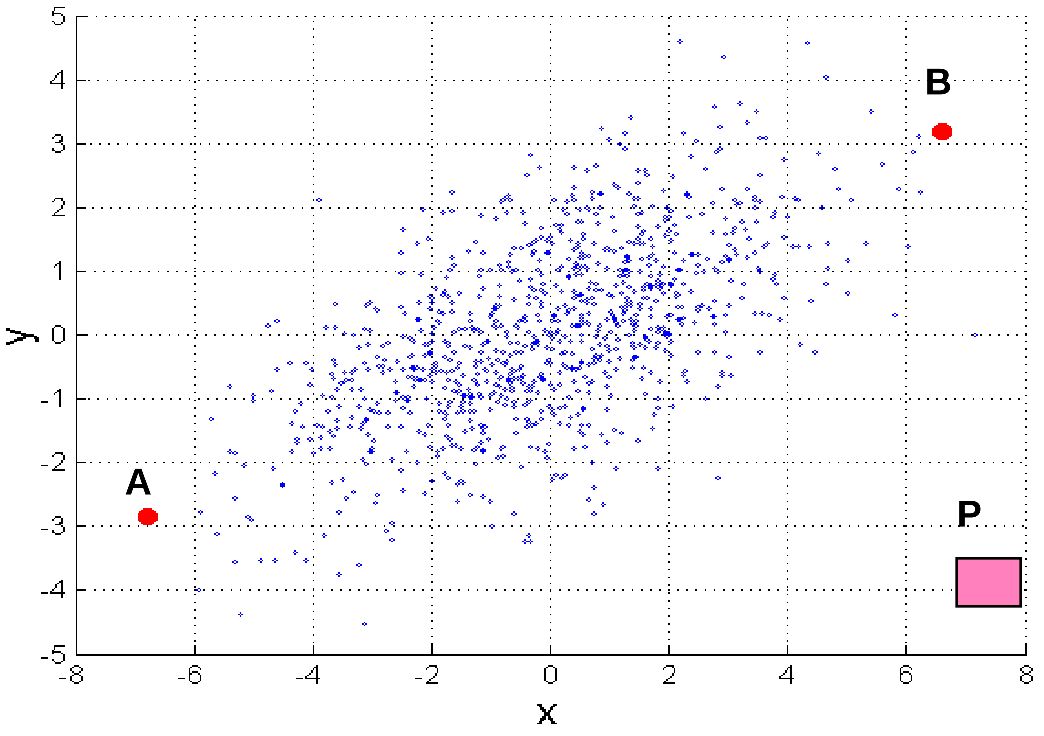
L2	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

L_∞	p1	p2	p3	p4
p1	0	2	3	5
p2	2	0	1	3
p3	3	1	0	2
p4	5	3	2	0

Distance Matrix

Mahalanobis Distance

$$mahalanobis(p,q) = (p-q)\Sigma^{-1}(p-q)^T$$



Σ is the covariance matrix of the input data *X*

$$\Sigma_{j,k} = \frac{1}{n-1}\sum_{i=1}^{n}(X_{ij}-\overline{X}_j)(X_{ik}-\overline{X}_k)$$

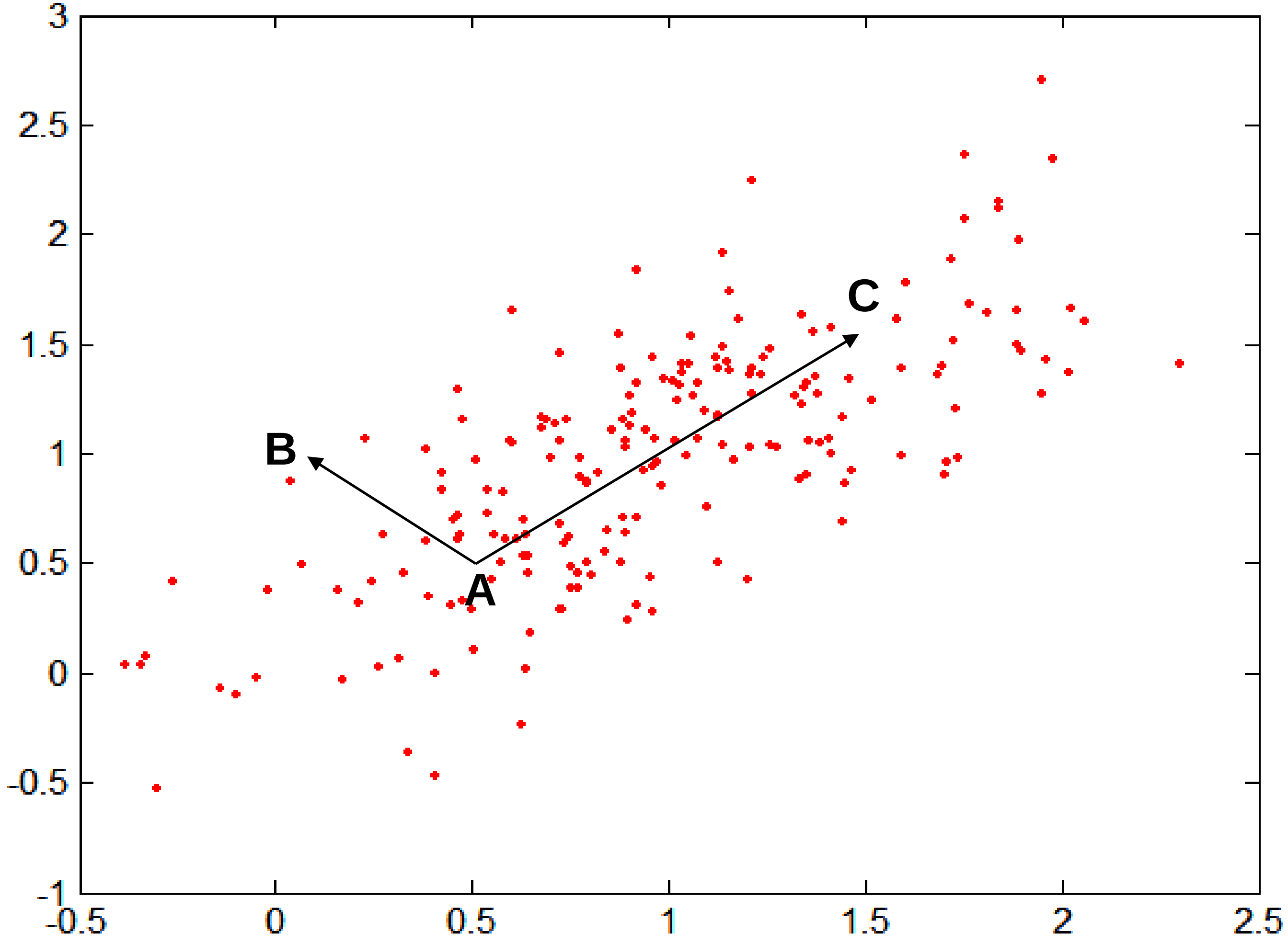
When the covariance matrix is identity Matrix, the mahalanobis distance is the same as the Euclidean distance.

Useful for detecting outliers.

Q: what is the shape of data when covariance matrix is identity?
Q: A is closer to P or B?

For red points, the Euclidean distance is 14.7, Mahalanobis distance is 6.

Mahalanobis Distance



Covariance Matrix:

$$\Sigma = \begin{bmatrix} 0.3 & 0.2 \\ 0.2 & 0.3 \end{bmatrix}$$

A: (0.5, 0.5)

B: (0, 1)

C: (1.5, 1.5)

Mahal(A,B) = 5

Mahal(A,C) = 4

Common Properties of a Distance

Distances, such as the Euclidean distance, have some well known properties.

1. $d(p, q) \geq 0$ for all p and q and $d(p, q) = 0$ only if $p = q$. (Positive definiteness)

2. $d(p, q) = d(q, p)$ for all p and q. (Symmetry)

3. $d(p, r) \leq d(p, q) + d(q, r)$ for all points p, q, and r. (Triangle Inequality)

where $d(p, q)$ is the distance (dissimilarity) between points (data objects), p and q.

A distance that satisfies these properties is a metric, and a space is called a metric space

Common Properties of a Similarity

- Similarities, also have some well known properties.

1. $s(p, q) = 1$ (or maximum similarity) only if $p = q$.
2. $s(p, q) = s(q, p)$ for all p and q. (Symmetry)

where $s(p, q)$ is the similarity between points (data objects), p and q.

Cosine Similarity

- If d_1 and d_2 are two document vectors, then

  $$\cos(d_1, d_2) = (d_1 \bullet d_2) / \|d_1\| \, \|d_2\| ,$$

  where $\bullet$ indicates vector dot product and $\| d \|$ is the length of vector d.

- Example:

  d_1 **= 3 2 0 5 0 0 0 2 0 0**
  d_2 **= 1 0 0 0 0 0 0 1 0 2**

$d_1 \bullet d_2 = 3*1 + 2*0 + 0*0 + 5*0 + 0*0 + 0*0 + 0*0 + 2*1 + 0*0 + 0*2 = 5$

$\|d_1\| = (3*3+2*2+0*0+5*5+0*0+0*0+0*0+2*2+0*0+0*0)^{\mathbf{0.5}} = (42)^{\mathbf{0.5}} = 6.481$

$\|d_2\| = (1*1+0*0+0*0+0*0+0*0+0*0+0*0+1*1+0*0+2*2)^{\mathbf{0.5}} = (6)^{\mathbf{0.5}} = 2.245$

$\cos(d_1, d_2) = .3150$, distance=1-cos(d1,d2)

CLUSTERING: BASIC CONCEPTS

VIDEO TO EXPLAIN CLUSTERING

https://youtu.be/wk2yli1qgu0?si=pgct4muxo_nyssgs

INTRODUCTION

Algorithm Diversity

- Clustering algorithms are diverse and tailored to specific data types or clusters due to the variability in data characteristics.

Subjective Nature of Cluster Evaluation:

- Defining optimal clusters is subjective, lacking a universally agreed-upon measure for evaluating cluster quality.

Computational Complexity and Feasibility:

- Precisely defining clusters can lead to computationally infeasible problems, adding complexity to finding optimal clustering solutions.

Key Issues in Cluster Analysis:

- Understanding data, clusters, and algorithms significantly influences the outcomes of clustering techniques.

INTRODUCTION

Algorithm Selection Criteria:

- Choosing an appropriate algorithm involves considering factors like complexity, scalability, and suitability for specific data sizes.

Exploration of Clustering Techniques:

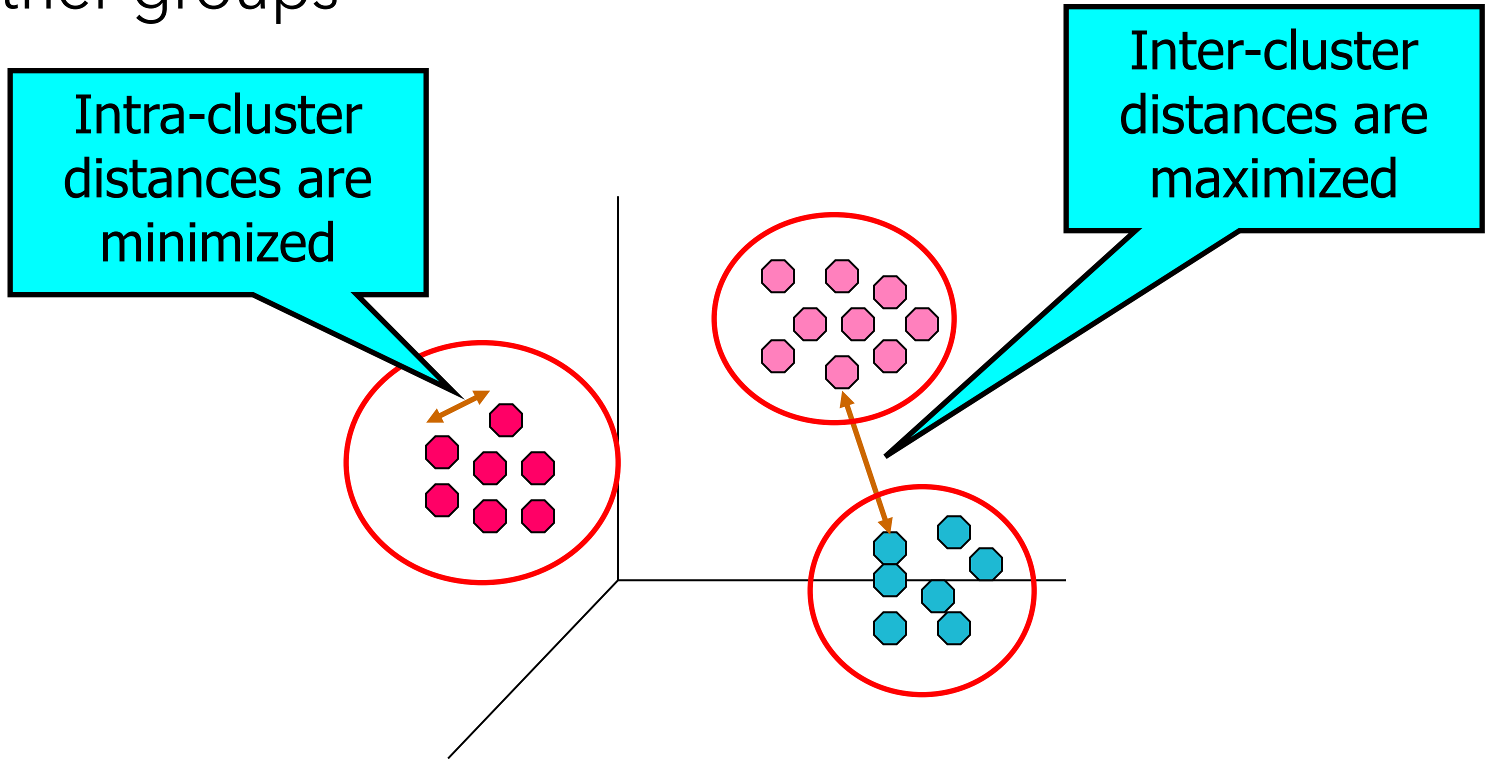
- Various techniques address specific problems related to data, clusters, or algorithms in cluster analysis.

Guidelines for Algorithm Selection:

- General guidelines assist in selecting suitable clustering algorithms by considering data characteristics, feasibility, and specific task requirements.

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

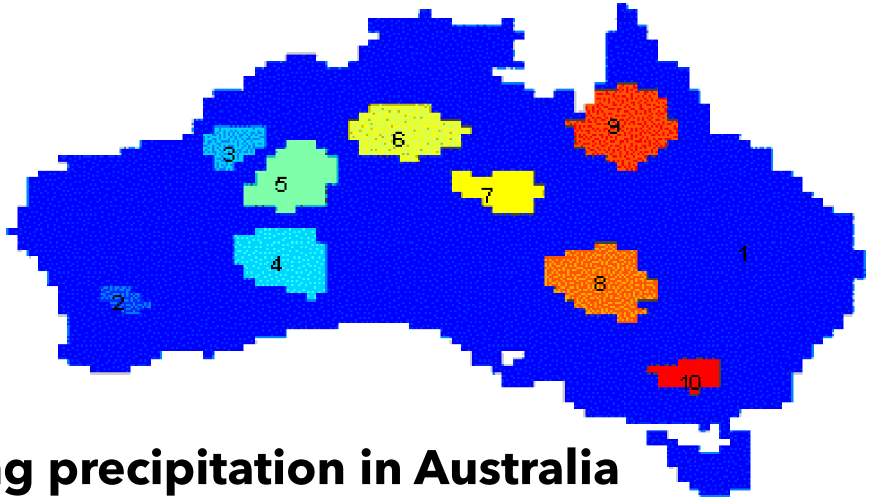


Applications of Cluster Analysis

- **Understanding**
  - Group related documents for browsing, group genes and proteins that have similar functionality, or group stocks with similar price fluctuations

- **Summarization**
  - Reduce the size of large data sets

	Discovered Clusters	*Industry Group*
1	Applied-Matl-DOWN,Bay-Network-Down,3-COM-DOWN, Cabletron-Sys-DOWN,CISCO-DOWN,HP-DOWN, DSC-Comm-DOWN,INTEL-DOWN,LSI-Logic-DOWN, Micron-Tech-DOWN,Texas-Inst-Down,Tellabs-Inc-Down, Natl-Semiconduct-DOWN,Oracl-DOWN,SGI-DOWN, Sun-DOWN	Technology1-DOWN
2	Apple-Comp-DOWN,Autodesk-DOWN,DEC-DOWN, ADV-Micro-Device-DOWN,Andrew-Corp-DOWN, Computer-Assoc-DOWN,Circuit-City-DOWN, Compaq-DOWN, EMC-Corp-DOWN, Gen-Inst-DOWN, Motorola-DOWN,Microsoft-DOWN,Scientific-Atl-DOWN	Technology2-DOWN
3	Fannie-Mae-DOWN,Fed-Home-Loan-DOWN, MBNA-Corp-DOWN,Morgan-Stanley-DOWN	Financial-DOWN
4	Baker-Hughes-UP,Dresser-Inds-UP,Halliburton-HLD-UP, Louisiana-Land-UP,Phillips-Petro-UP,Unocal-UP, Schlumberger-UP	Oil-UP



Clustering precipitation in Australia

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

Notion of a Cluster can be Ambiguous

How many clusters?

Six Clusters

Two Clusters

Four Clusters

Types of Clusterings

A clustering is a set of clusters

Important distinction between hierarchical and partitional sets of clusters

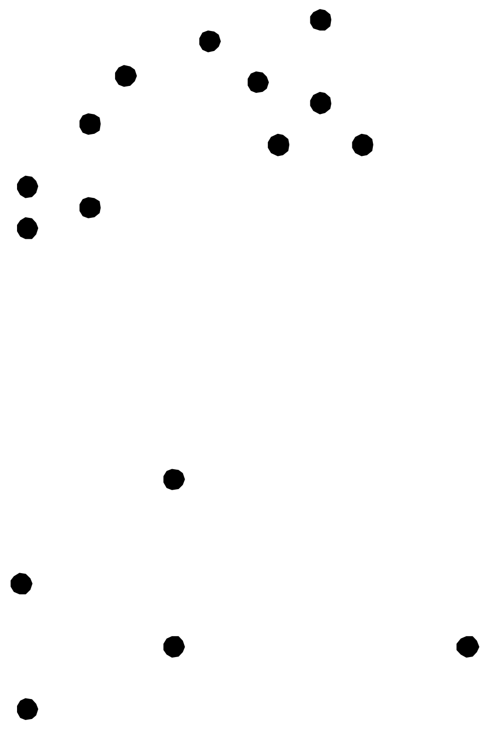
Partitional Clustering

A division data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset

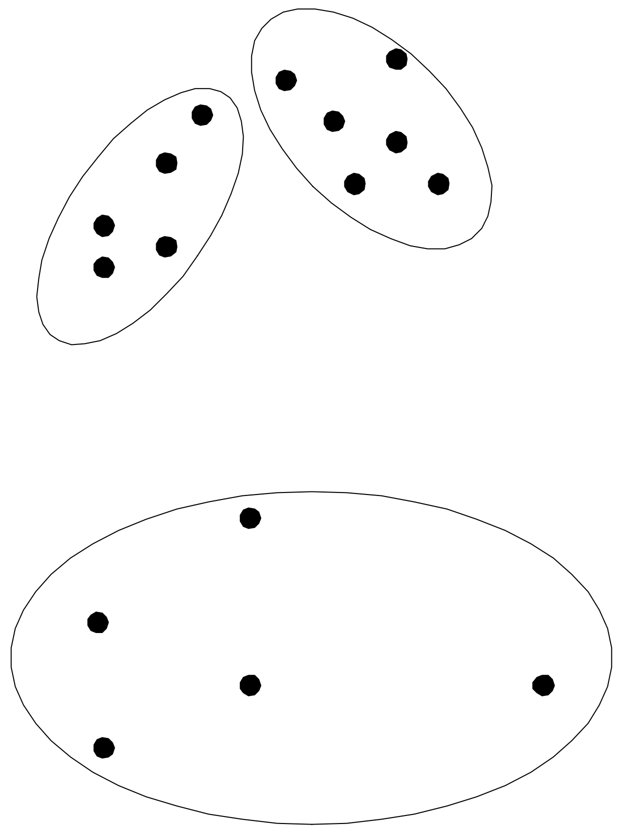
Hierarchical clustering

A set of nested clusters organized as a hierarchical tree

Partitional Clustering

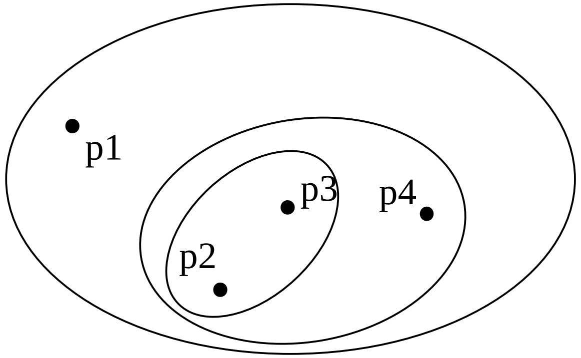


Original Points

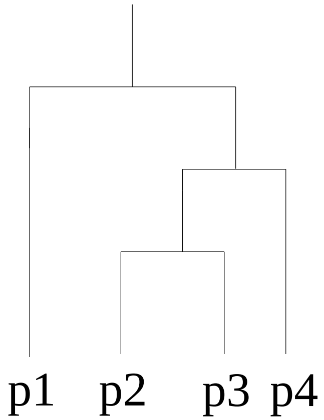


A Partitional Clustering

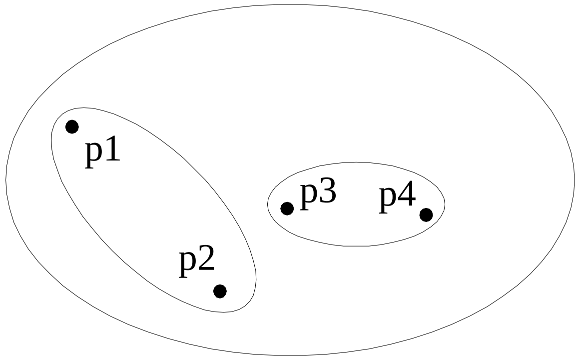
Hierarchical Clustering



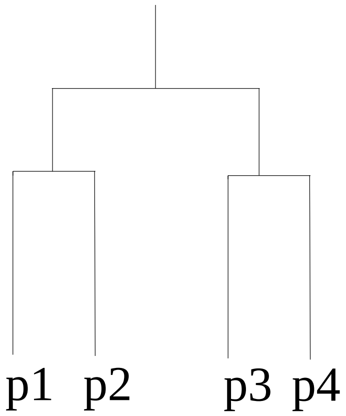
Traditional Hierarchical Clustering



Traditional Dendrogram



Non-traditional Hierarchical Clustering



Non-traditional Dendrogram

Other Distinctions Between Sets of Clusters

Exclusive versus non-exclusive

In non-exclusive clusterings, points may belong to multiple clusters.

Can represent multiple classes or 'border' points

Fuzzy versus non-fuzzy

In fuzzy clustering, a point belongs to every cluster with some weight between 0 and 1

Weights must sum to 1

Probabilistic clustering has similar characteristics

Partial versus complete

In some cases, we only want to cluster some of the data

Heterogeneous versus homogeneous

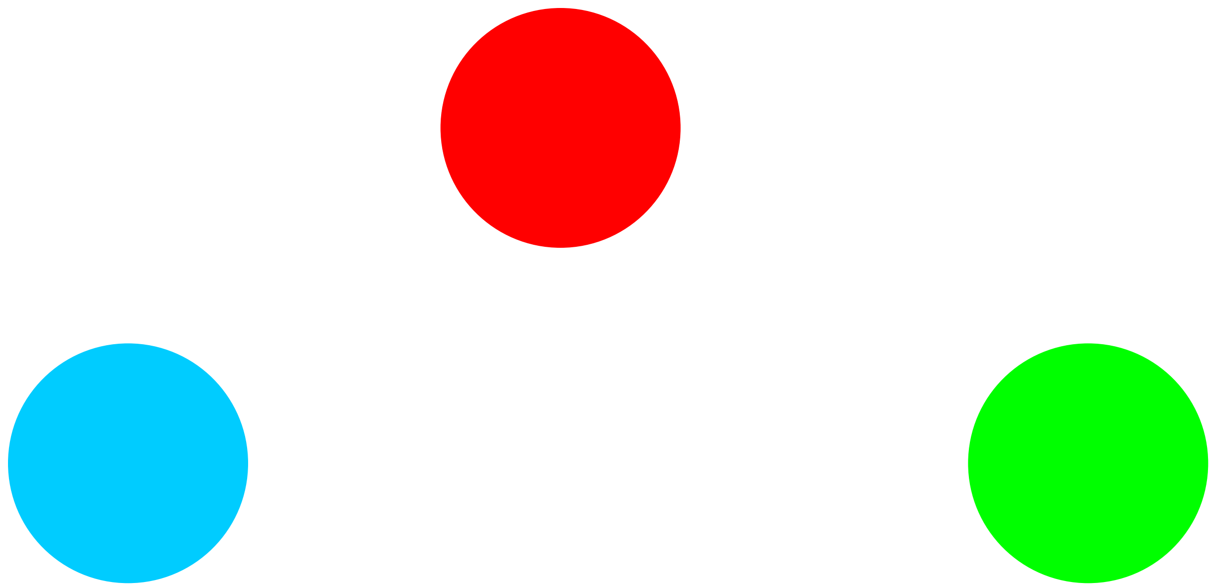
Cluster of widely different sizes, shapes, and densities

Types of Clusters

- Well-separated clusters
- Center-based clusters
- Contiguous clusters
- Density-based clusters
- Property or Conceptual
- Described by an Objective Function

Types of Clusters: Well-Separated

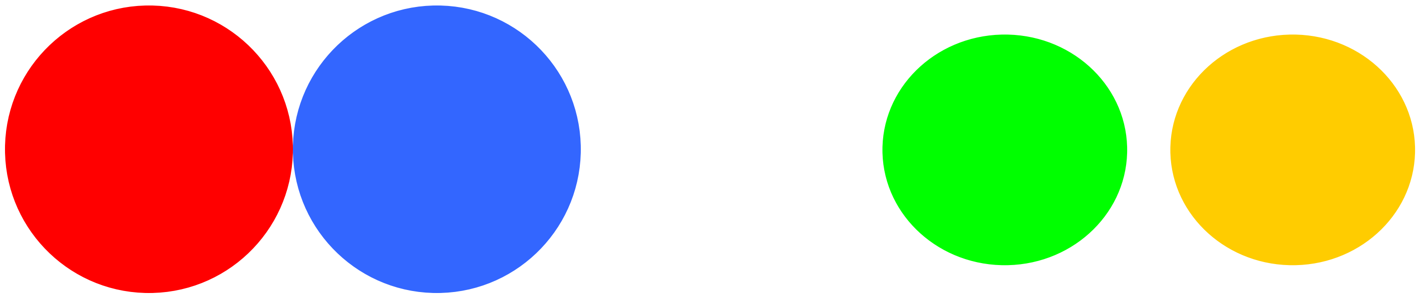
- Well-Separated Clusters:
  - A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.



3 well-separated clusters

Types of Clusters: Center-Based

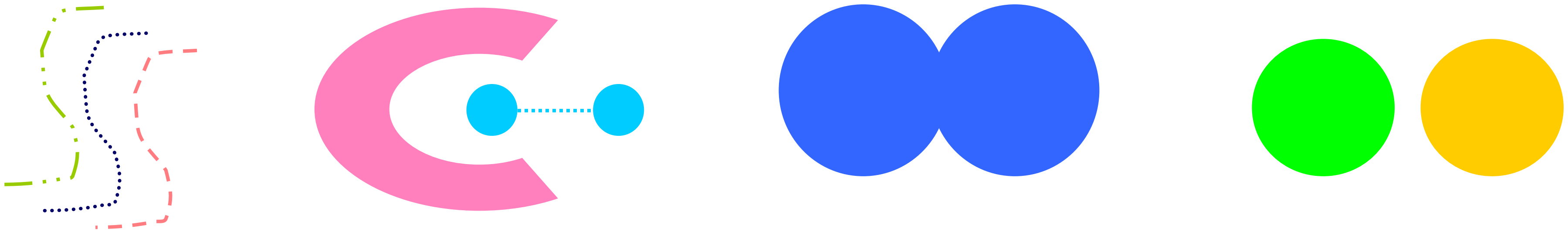
- Center-based
  - A cluster is a set of objects such that an object in a cluster is closer (more similar) to the "center" of a cluster, than to the center of any other cluster
  - The center of a cluster is often a centroid, the average of all the points in the cluster, or a medoid, the most "representative"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



4 center-based clusters

Types of Clusters: Contiguity-Based

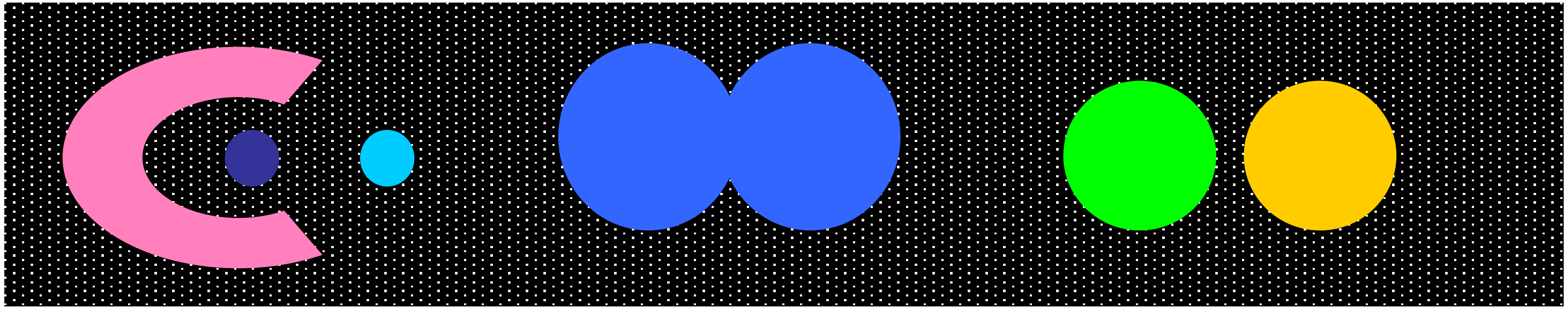
- Contiguous Cluster (Nearest neighbor or Transitive)
  - A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.



8 contiguous clusters

Types of Clusters: Density-Based

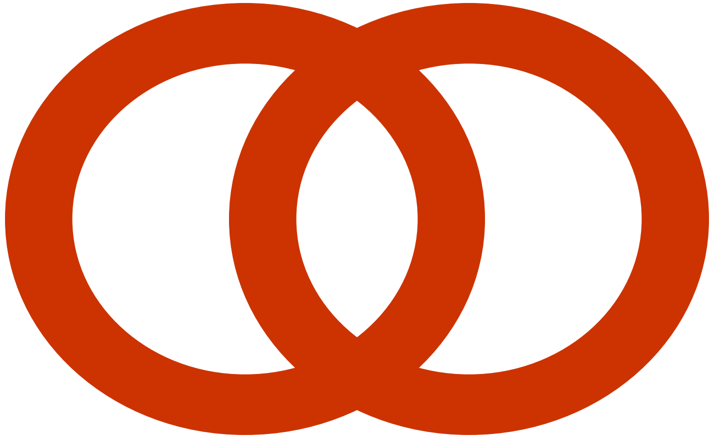
- Density-based
  - A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
  - Used when the clusters are irregular or intertwined, and when noise and outliers are present.



6 density-based clusters

Types of Clusters: Conceptual Clusters

- Shared Property or Conceptual Clusters
- Finds clusters that share some common property or represent a particular concept.
-



2 Overlapping Circles

Part 9 Deep Learning What is the Objective Function

Data Science A-Z for Beginners and Advance • 1.2K views

Deep Learning, Neural Networks, Digging Deeper, Deep Neural Networks, Overfitting, Initialization, Preprocessing, Classifying on the MNIST Dataset, Deep Learning - How to Build a Neural Network...

OBJECTIVE FUNCTION

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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

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.

Types of Clusters: Objective Function …

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

Characteristics of the Input Data Are Important

Type of proximity or density measure,
- a derived measure, but central to clustering

Sparseness –
- Dictates type of similarity
- Adds to efficiency

Attribute type-
- Dictates type of similarity

Type of Data-
- Dictates type of similarity
- Other characteristics, e.g., autocorrelation

Dimensionality

Noise and Outliers

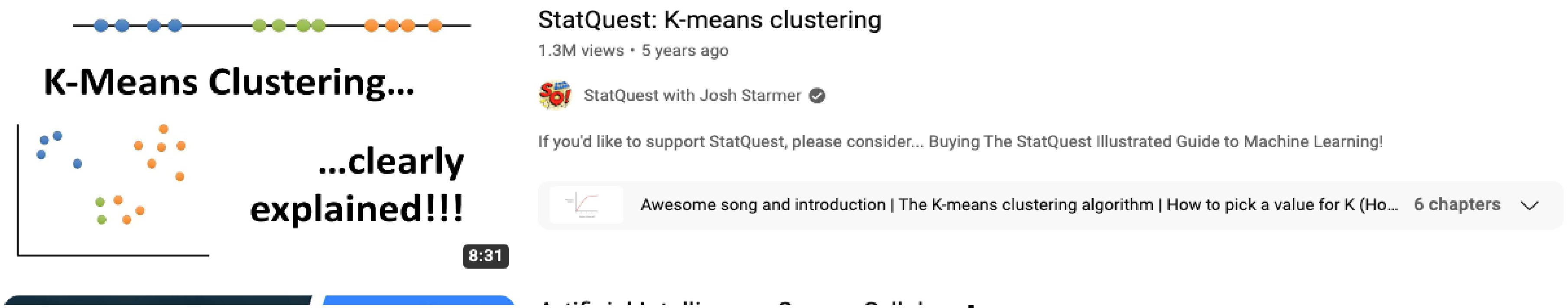
Type of Distribution

Clustering Algorithms

K-means and its variants

Hierarchical clustering

Density-based clustering



K MEANS CLUSTERING

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K-means Clustering

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

```
Select K points as the initial centroids.
repeat
    Form K clusters by assigning all points to the closest centroid.
    Recompute the centroid of each cluster.
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.

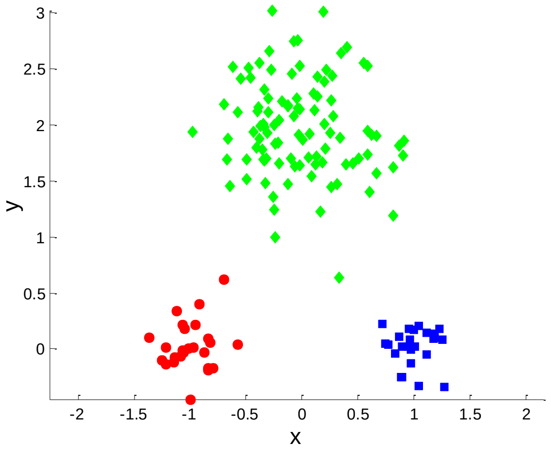
'Closeness' is measured by Euclidean distance, cosine similarity, correlation, etc.

K-means will converge for common similarity measures mentioned above.

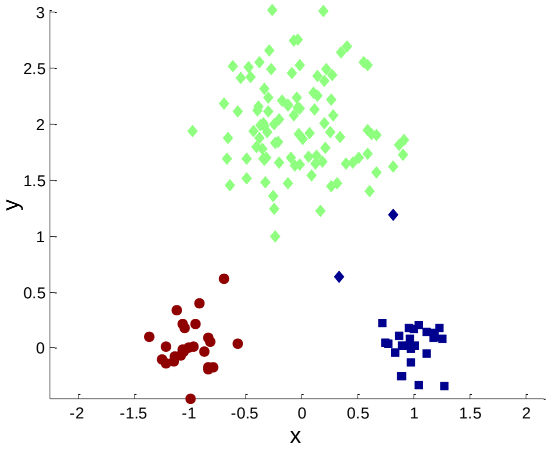
Most of the convergence happens in the first few iterations. Often the stopping condition is changed to 'Until relatively few points change clusters'

Complexity is O(n * K * I * d) n = number of points, K = number of clusters, I = number of iterations, d = number of attributes

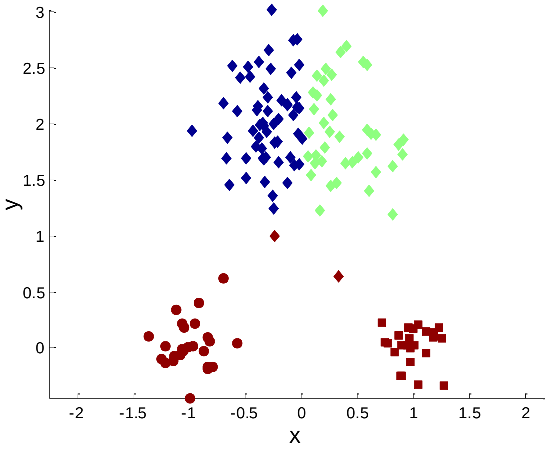
Two different K-means Clusterings



Original Points

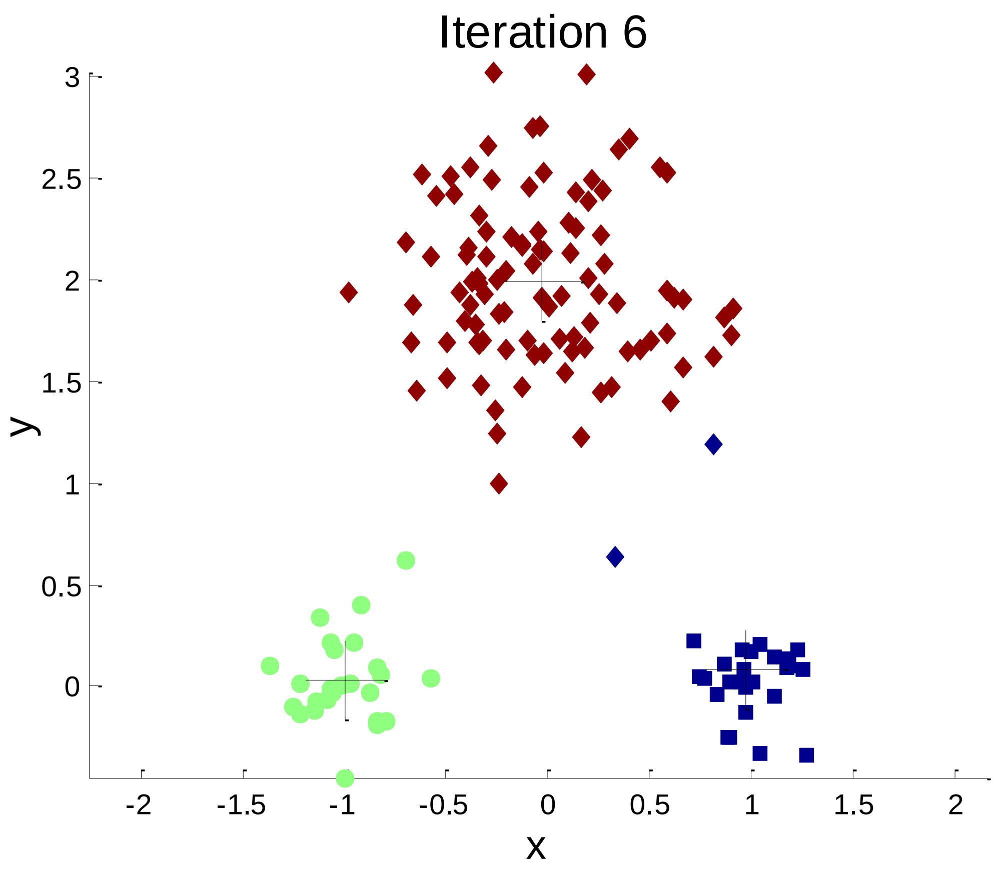


Optimal Clustering

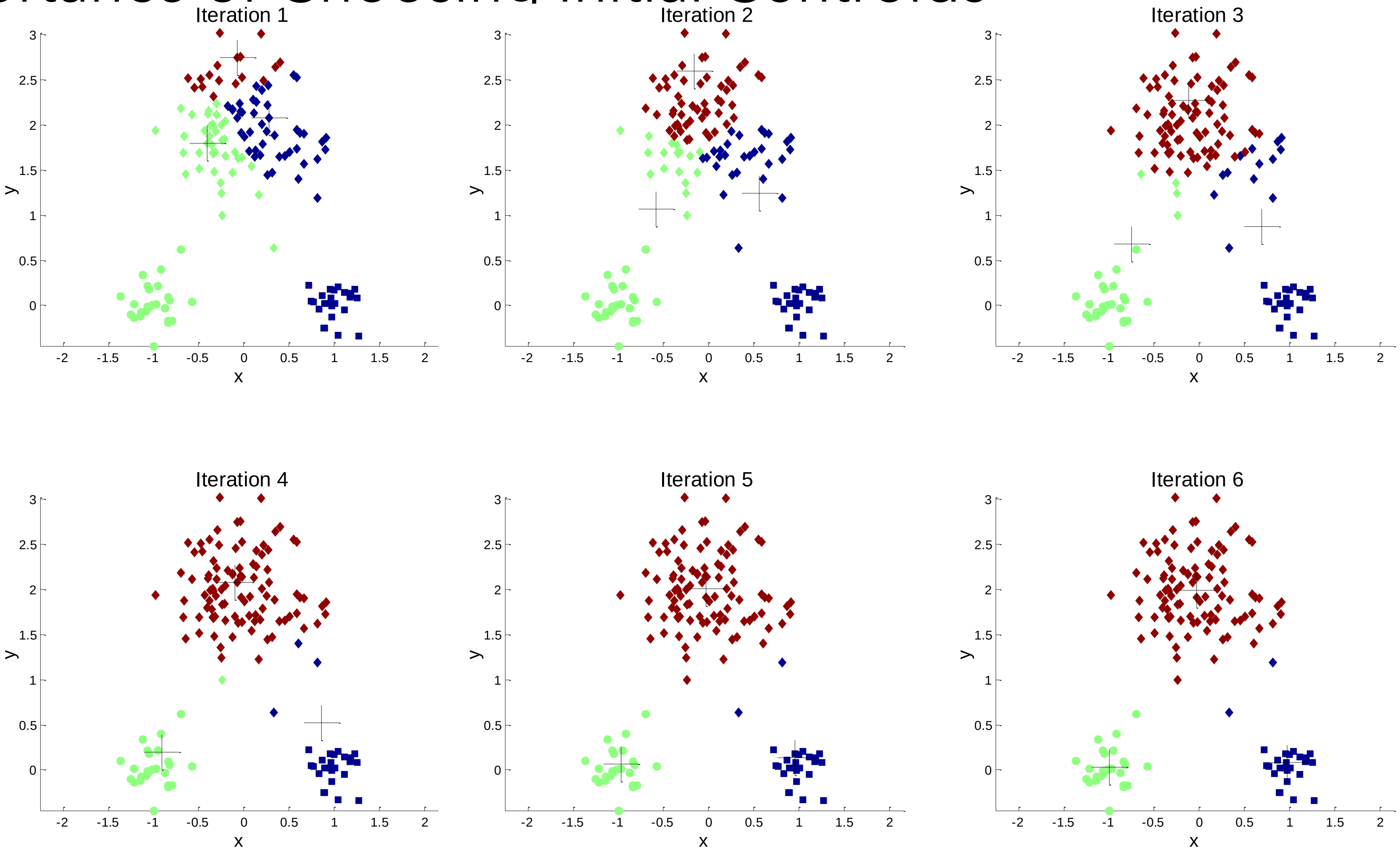


Sub-optimal Clustering

Importance of Choosing Initial Centroids



Importance of Choosing Initial Centroids



Evaluating K-means Clusters

Step 4 of K-means Algorithm: Recompute centroids of each cluster.

Centroid choice depends on proximity measure and clustering goal.

Objective function:

Expresses clustering goal, depends on data proximities.

Objective functions include minimizing squared distance to closest centroid.

Evaluating K-means Clusters- Euclidean Space Data:

- **Proximity Measure:** Euclidean distance.
- **Objective Function:** Sum of Squared Error (SSE) or scatter.
- 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 C_i and m_i is the representative point for cluster C_i
    - can show that m_i 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

Evaluating K-means Clusters- **Centroid for SSE minimization:**

- Mathematically shown to be the mean.
- Centroid calculation:

$$c_i = \frac{1}{m_i} \sum_{x \in C_i} x$$

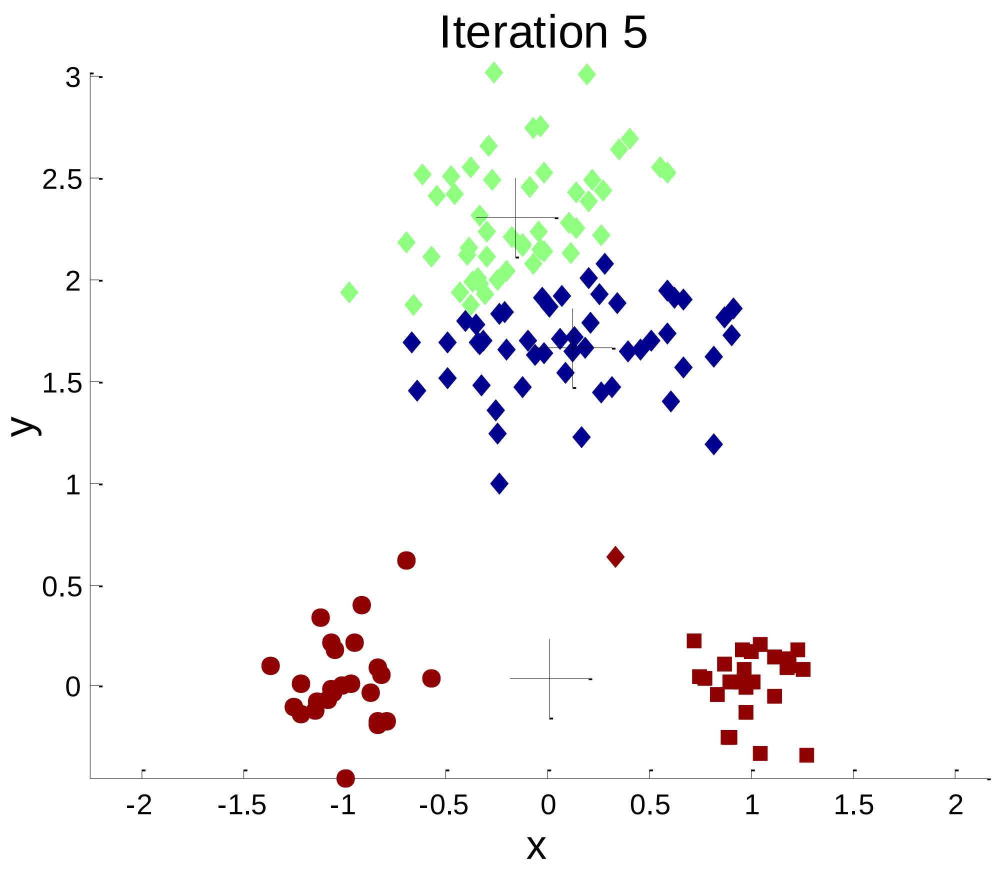
- Example: Centroid of a cluster containing points (1,1), (2,3), and (6,2) is (3, 2).
- K-means Steps and SSE Optimization:
  - Steps 3 and 4: Aim to minimize SSE.
  - Step 3 assigns points to nearest centroids, minimizing SSE.
  - Step 4 recomputes centroids to further minimize SSE.
  - K-means actions find local minimum for SSE, not global minimum due to specific centroid and cluster choices.

The General Case

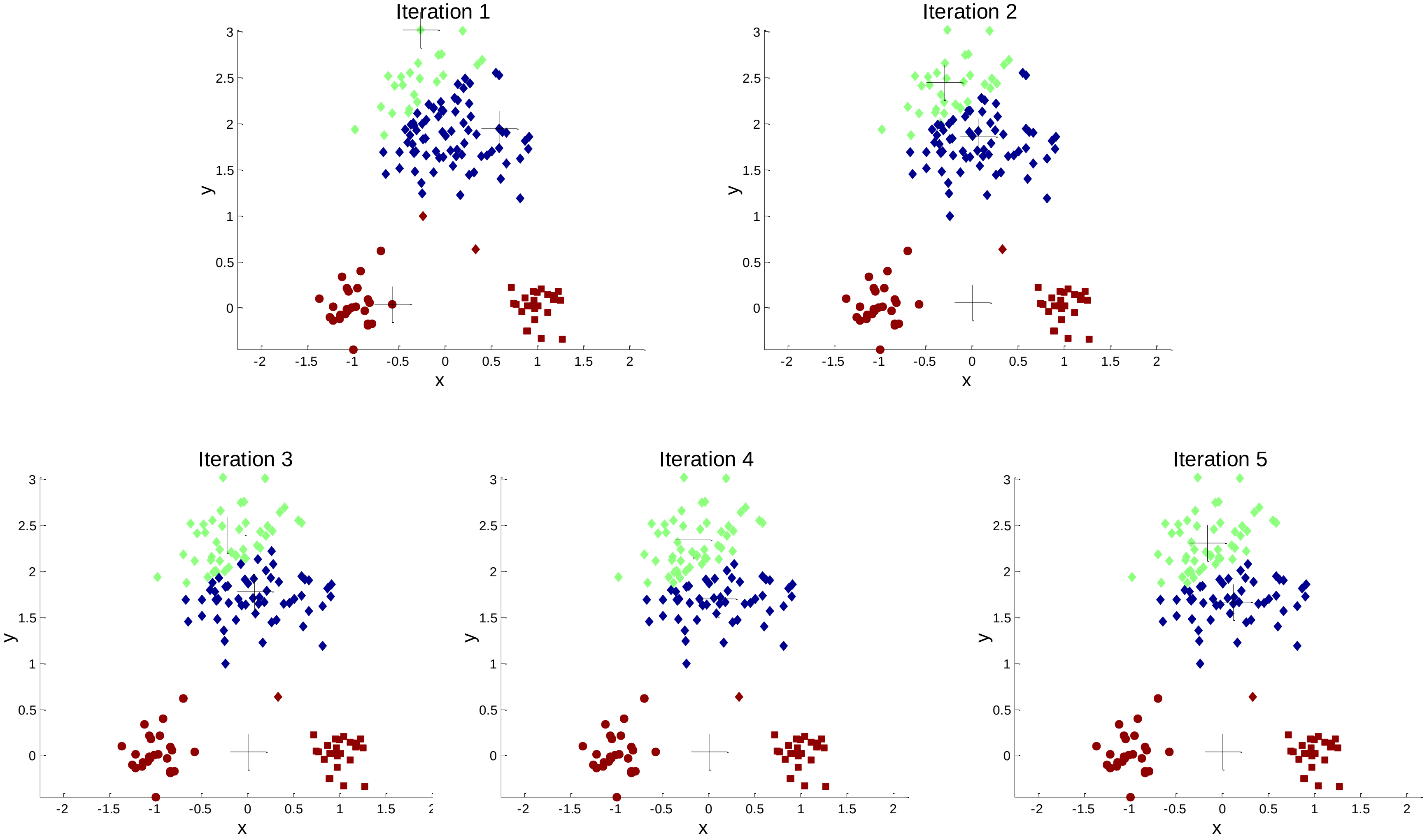
Table 5.2. K-means: Common choices for proximity, centroids, and objective functions.

Proximity Function	Centroid	Objective Function
Manhattan (L_1)	median	Minimize sum of the L_1 distance of an object to its cluster centroid
Squared Euclidean (L_2^2)	mean	Minimize sum of the squared L_2 distance of an object to its cluster centroid
cosine	mean	Maximize sum of the cosine similarity of an object to its cluster centroid
Bregman divergence	mean	Minimize sum of the Bregman divergence of an object to its cluster centroid

Importance of Choosing Initial Centroids …



Importance of Choosing Initial Centroids …



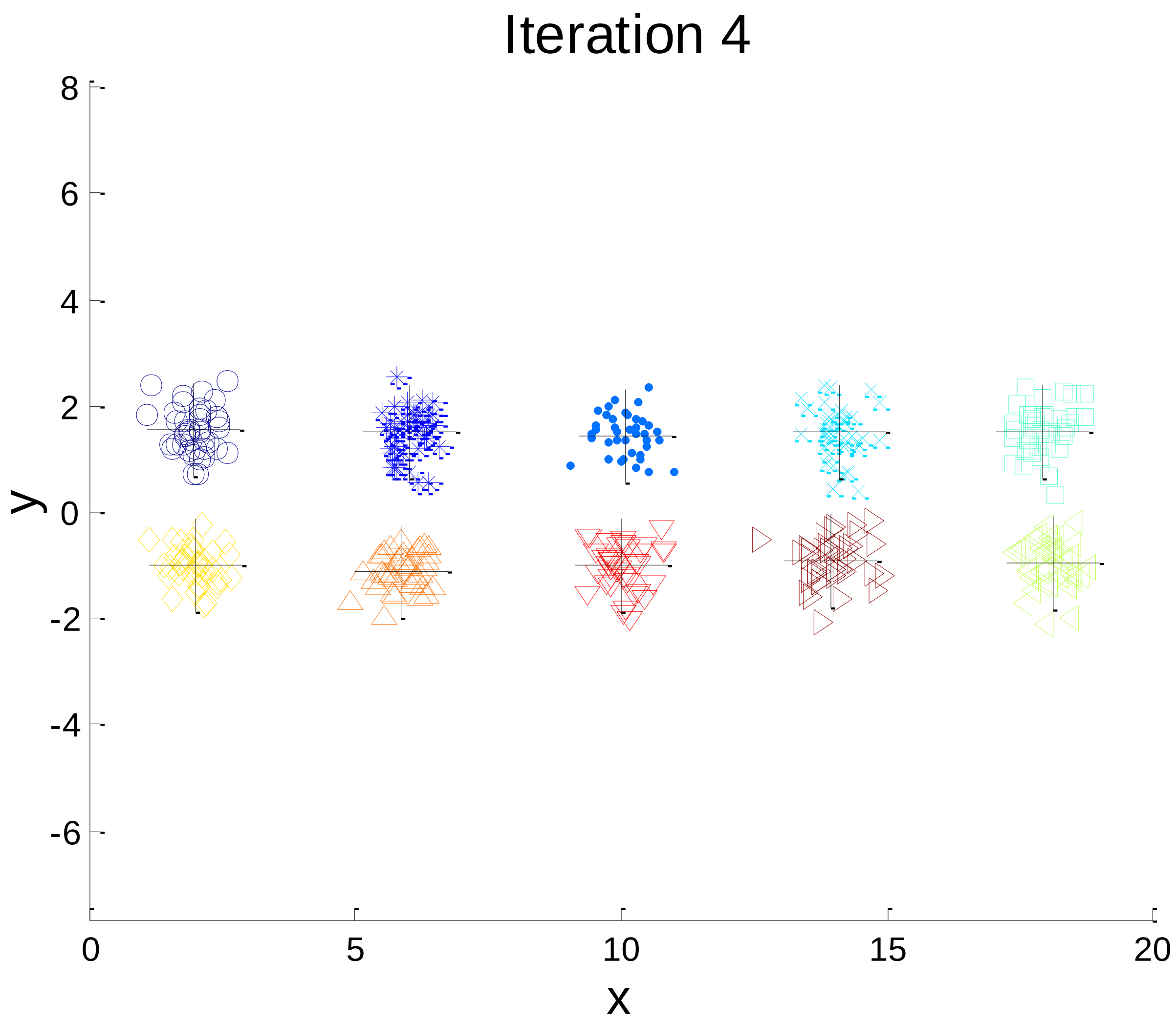
Problems with Selecting Initial Points

- 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

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

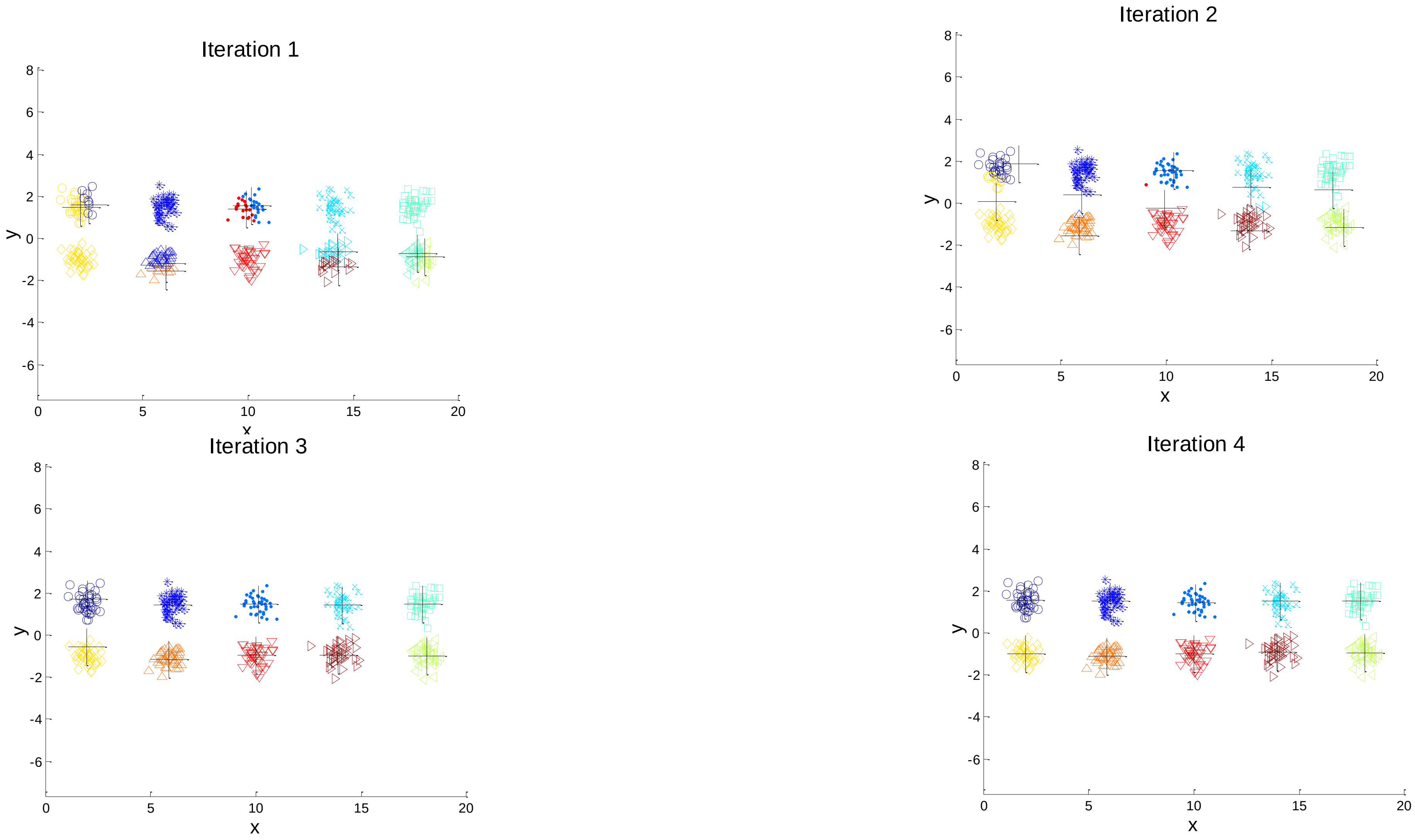
  - For example, if K = 10, then probability = $10!/10^{10} = 0.00036$
  - Sometimes the initial centroids will readjust themselves in 'right' way, and sometimes they don't
  - Consider an example of five pairs of clusters

10 Clusters Example



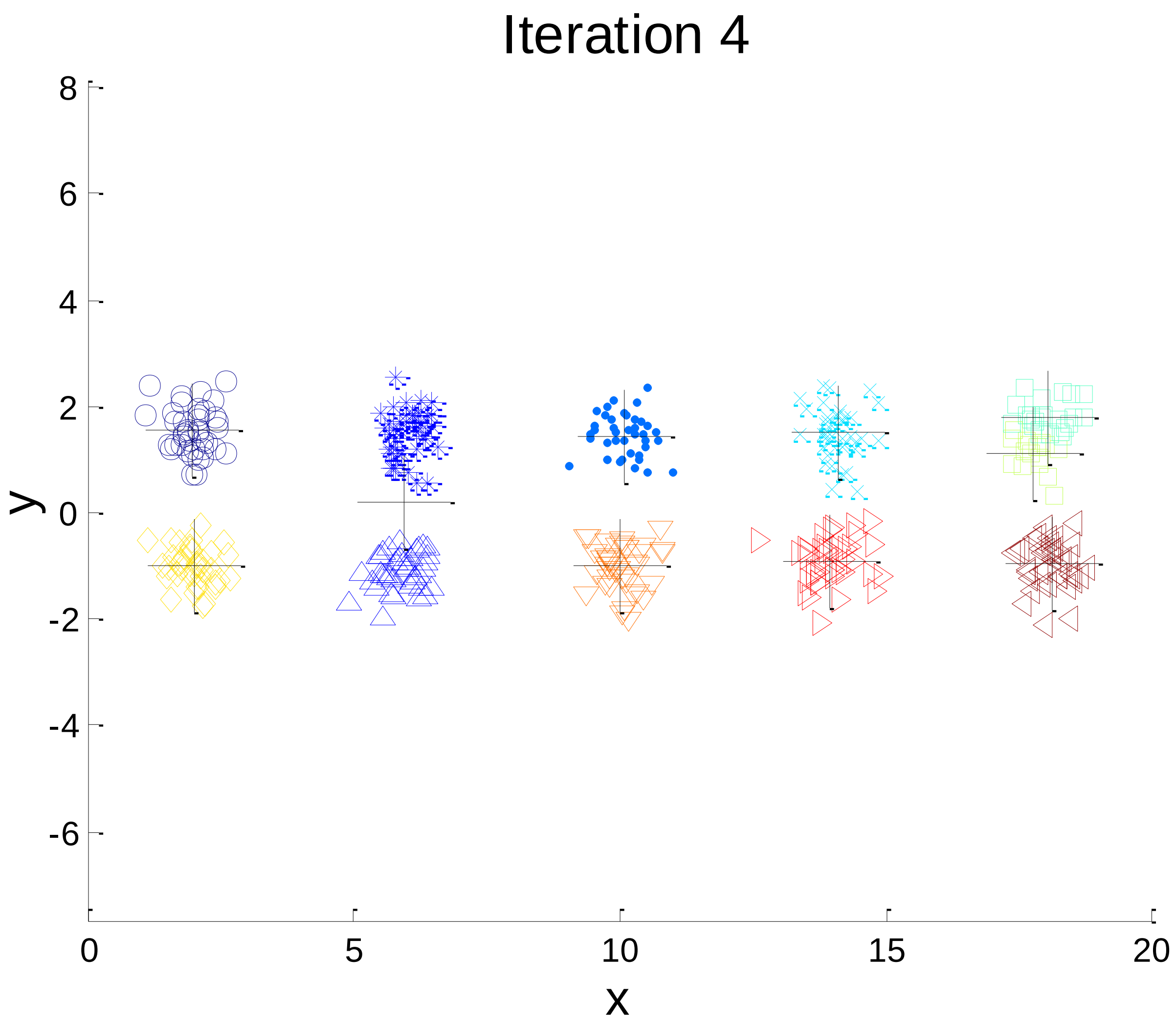
Starting with two initial centroids in one cluster of each pair of clusters

10 Clusters Example



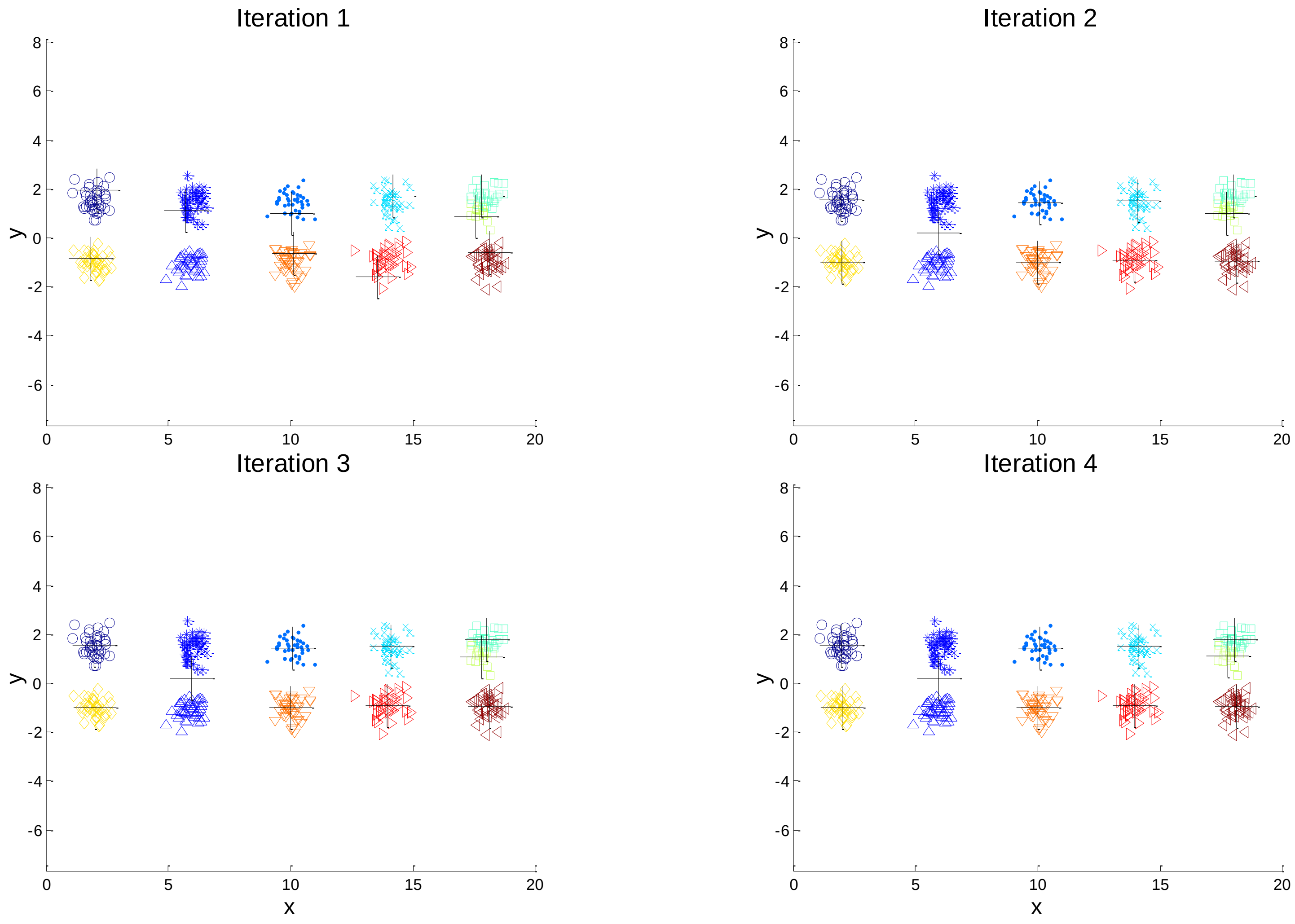
Starting with two initial centroids in one cluster of each pair of clusters

10 Clusters Example



Starting with some pairs of clusters having three initial centroids, while other have only one.

10 Clusters Example



Starting with some pairs of clusters having three initial centroids, while other have only one.

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

Postprocessing

Bisecting K-means

- Not as susceptible to initialization issues

Handling Empty Clusters

Basic K-means algorithm can yield empty clusters

Several strategies

Choose the point that contributes most to SSE	Choose a point from the cluster with the highest SSE	If there are several empty clusters, the above can be repeated several times.

Updating Centers Incrementally

In the basic K-means algorithm, centroids are updated after all points are assigned to a centroid

An alternative is to update the centroids after each assignment (incremental approach)

- Each assignment updates zero or two centroids
- More expensive
- Introduces an order dependency
- Never get an empty cluster
- Can use “weights” to change the impact

Pre-processing and Post-processing

Pre-processing

- Normalize the data
- Eliminate outliers

Post-processing

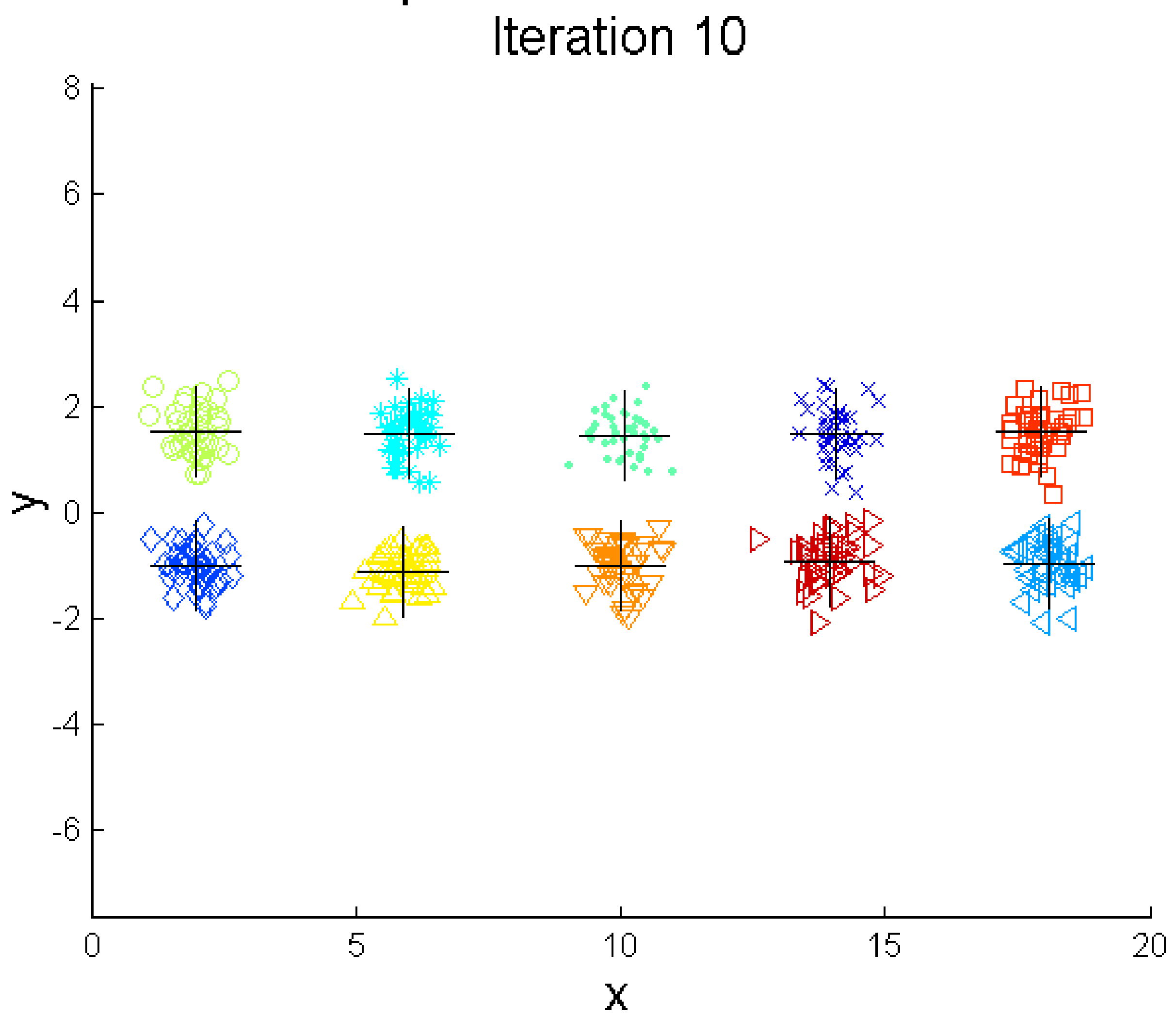
- Eliminate small clusters that may represent outliers
- Split ‘loose’ clusters, i.e., clusters with relatively high SSE
- Merge clusters that are ‘close’ and that have relatively low SSE
- Can use these steps during the clustering process
  - ISODATA

Bisecting K-means

- Bisecting K-means algorithm
  - Variant of K-means that can produce a partitional or a hierarchical clustering

```
Initialize the list of clusters to contain the cluster containing all points.
repeat
   Select a cluster from the list of clusters
   for i = 1 to number_of_iterations do
      Bisect the selected cluster using basic K-means
   end for
   Add the two clusters from the bisection with the lowest SSE to the list of clusters.
until Until the list of clusters contains K clusters
```

Bisecting K-means Example



Limitations of K-means

K-means has problems when clusters are of differing

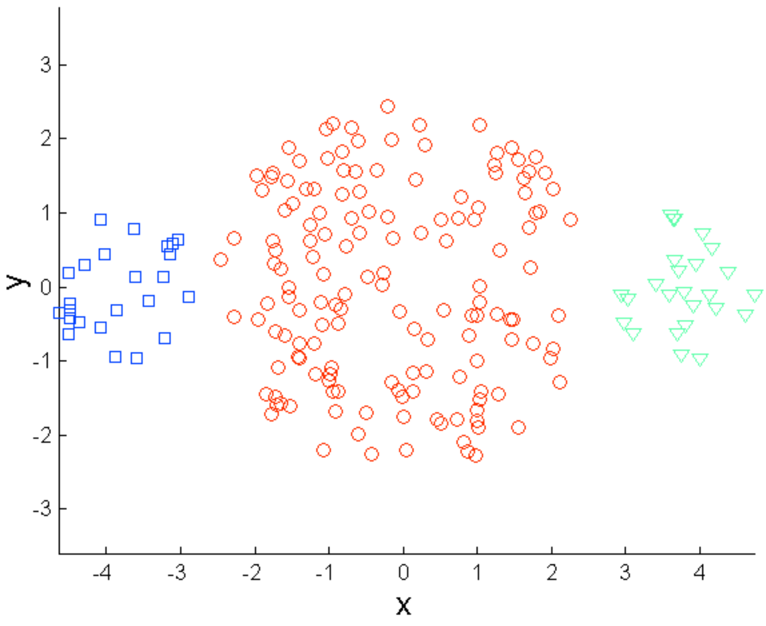
Sizes

Densities

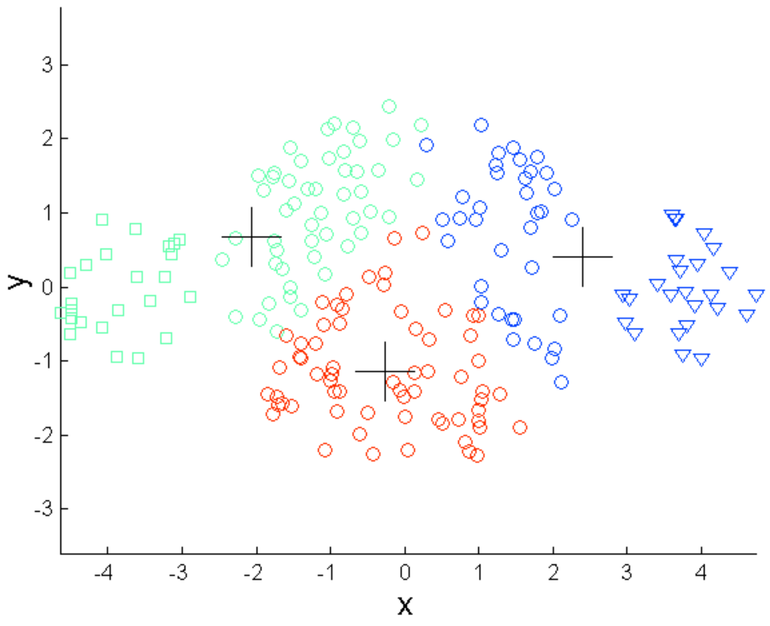
Non-globular shapes

K-means has problems when the data contains outliers.

Limitations of K-means: Differing Sizes

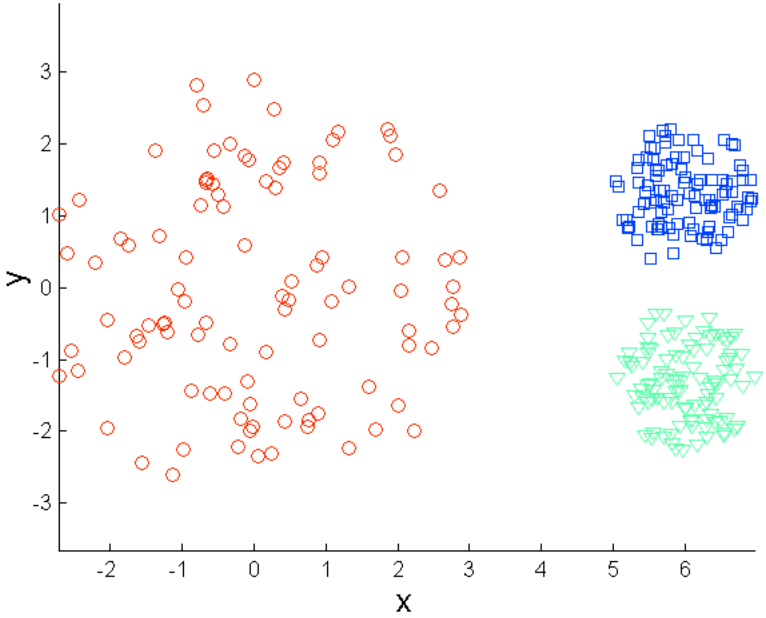


Original Points

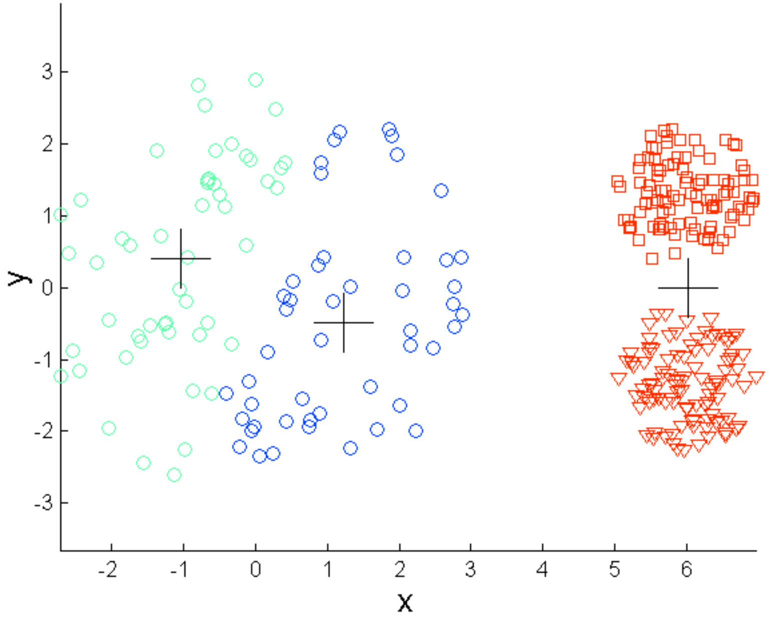


K-means (3 Clusters)

Limitations of K-means: Differing Density

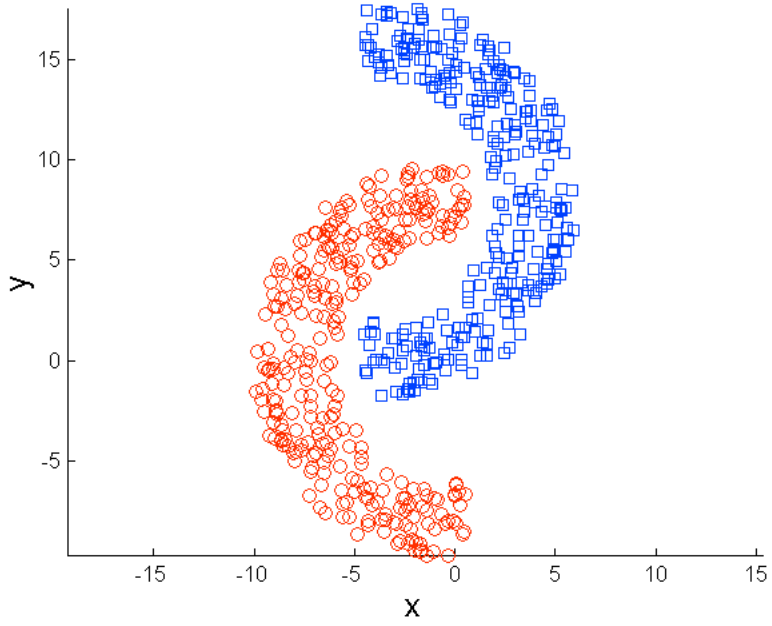


Original Points

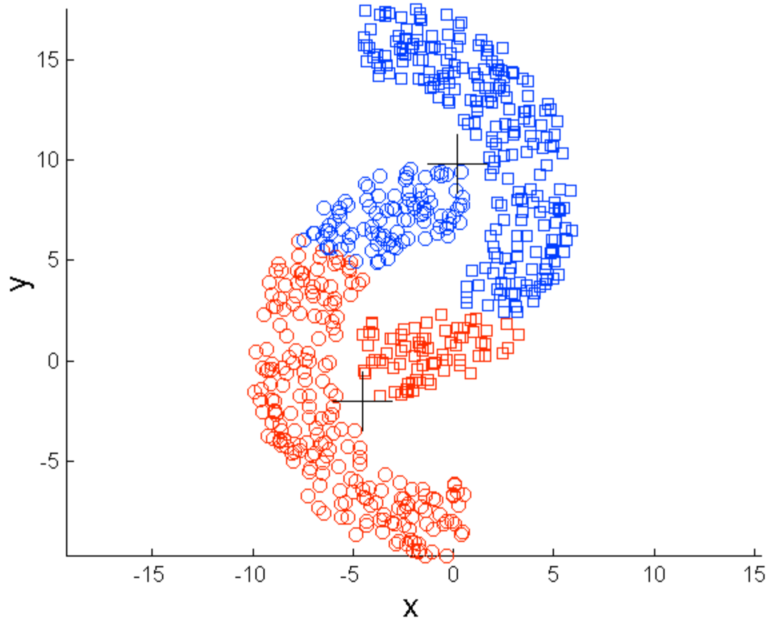


K-means (3 Clusters)

Limitations of K-means: Non-globular Shapes

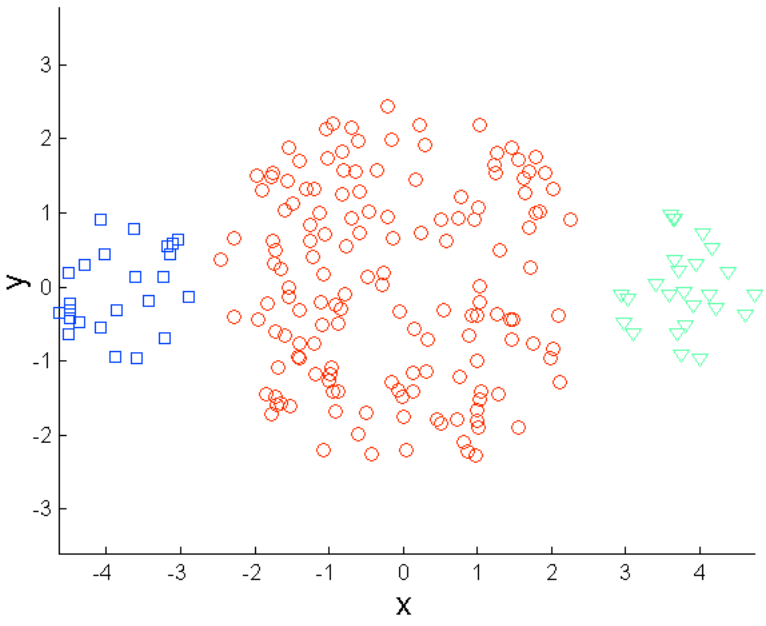


Original Points

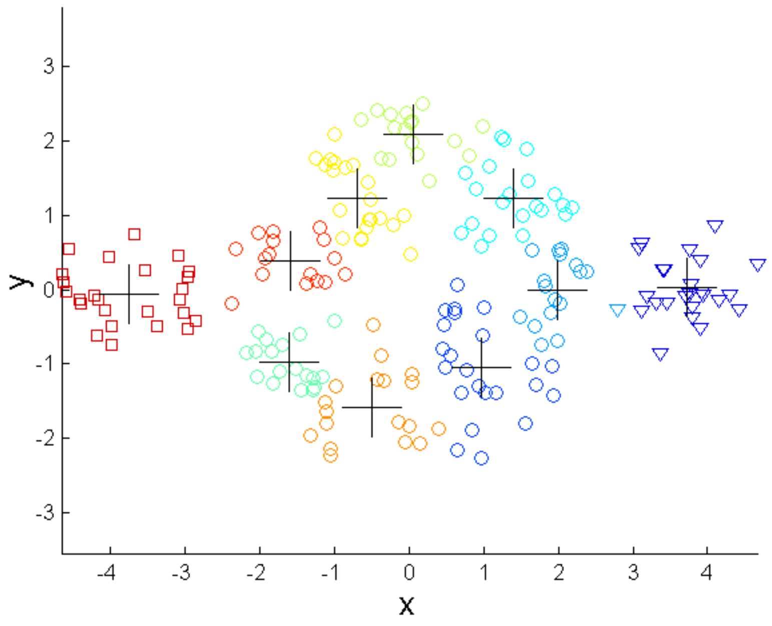


K-means (2 Clusters)

Overcoming K-means Limitations



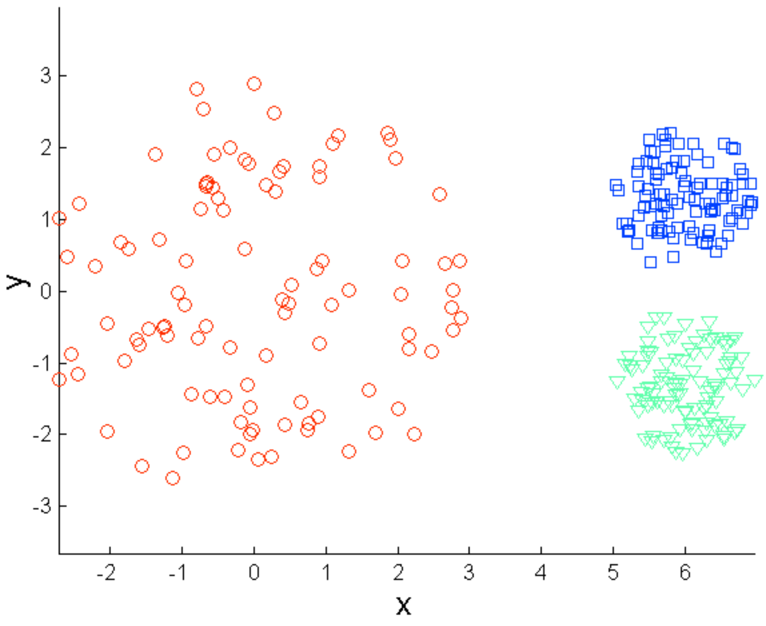
Original Points



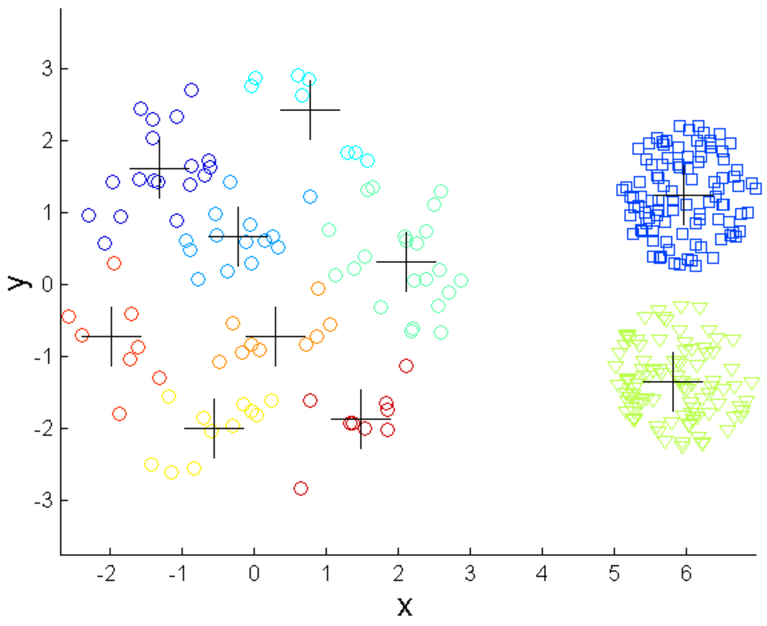
K-means Clusters

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

Overcoming K-means Limitations

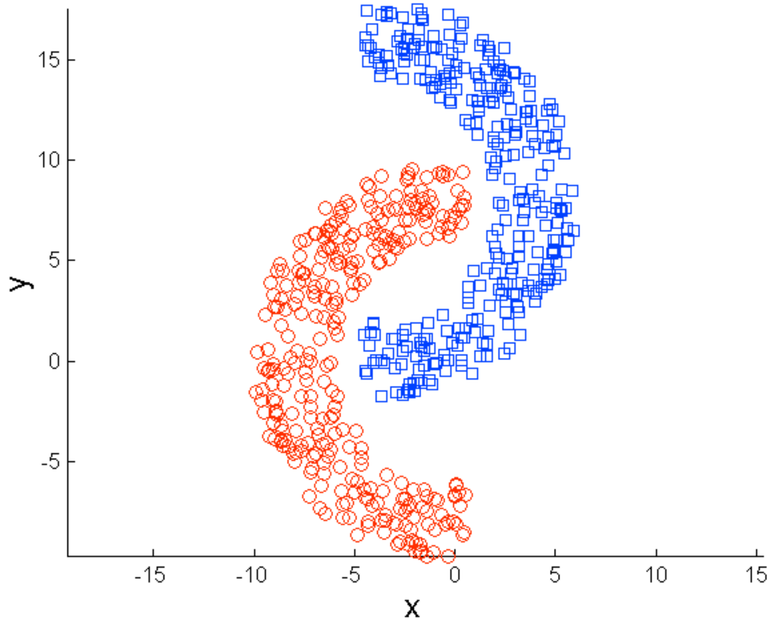


Original Points

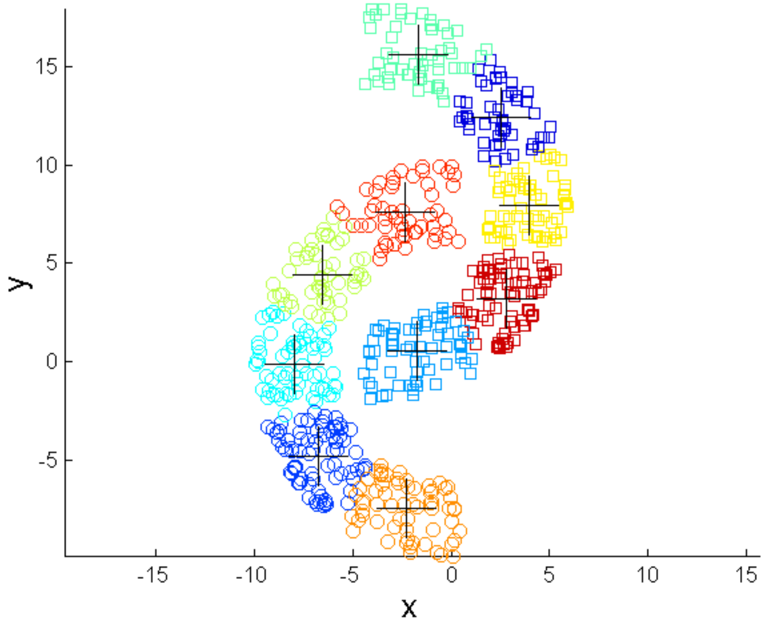


K-means Clusters

Overcoming K-means Limitations



Original Points



K-means Clusters

Hierarchical Clustering - Fun and Easy Machine Learning

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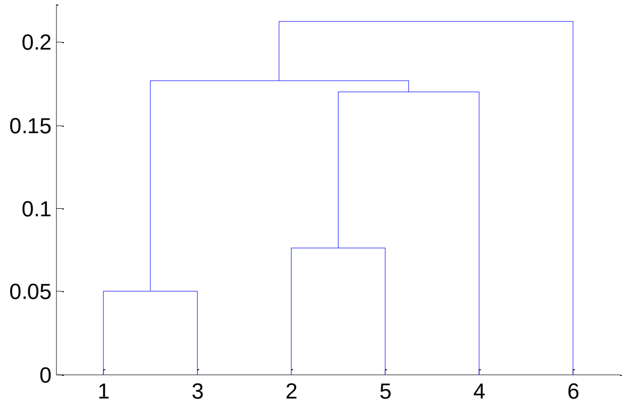
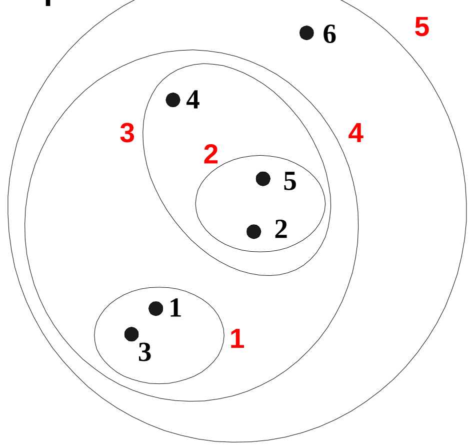
HIERARCHICAL CLUSTERING

HTTPS://YOUTU.BE/EUQY3HL38CW?SI=JKRYWEX84QVFJATY

Hierarchical Clustering

- Produces a set of nested clusters organized as a hierarchical tree
- Can be visualized as a dendrogram
  - 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

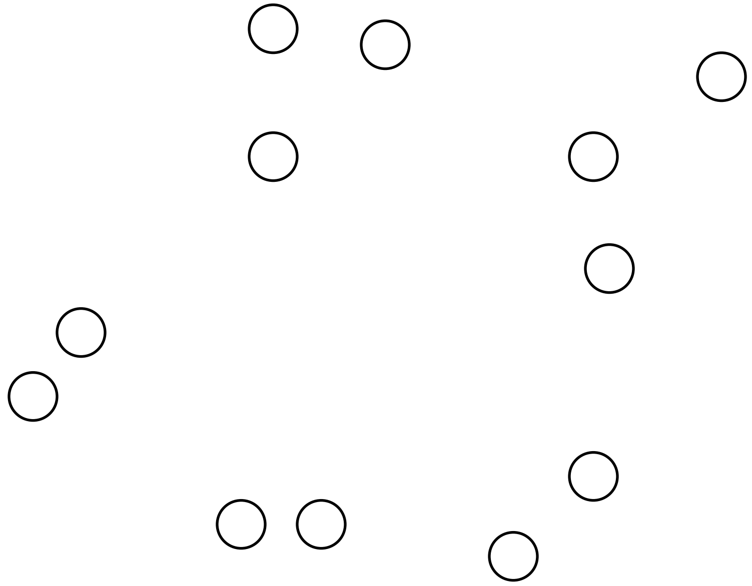
- Compute the proximity matrix
- Let each data point be a cluster
- **Repeat**
  - Merge the two closest clusters
  - Update the proximity matrix
- **Until** only a single cluster remains

Key operation is the computation of the proximity of two clusters

- Different approaches to defining the distance between clusters distinguish the different algorithms

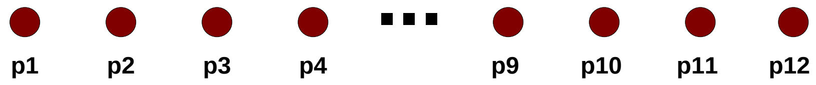
Starting Situation

- Start with clusters of individual points and a proximity matrix



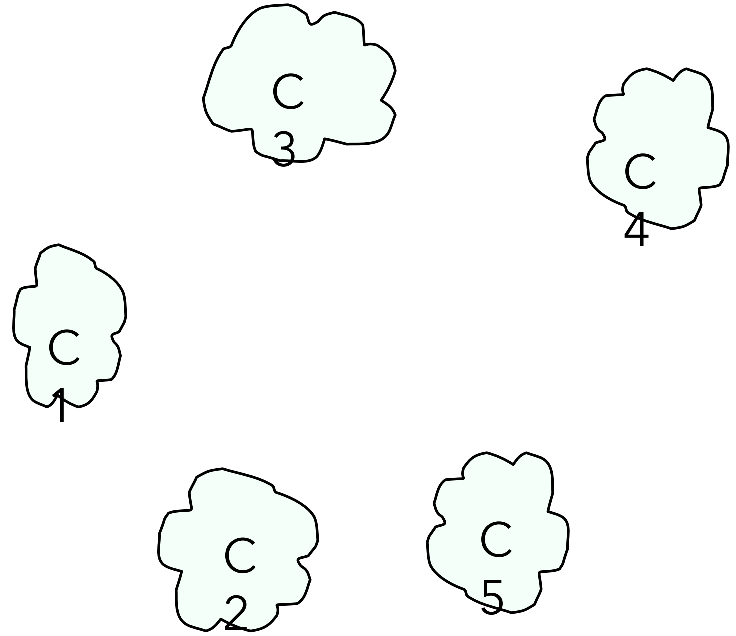
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix



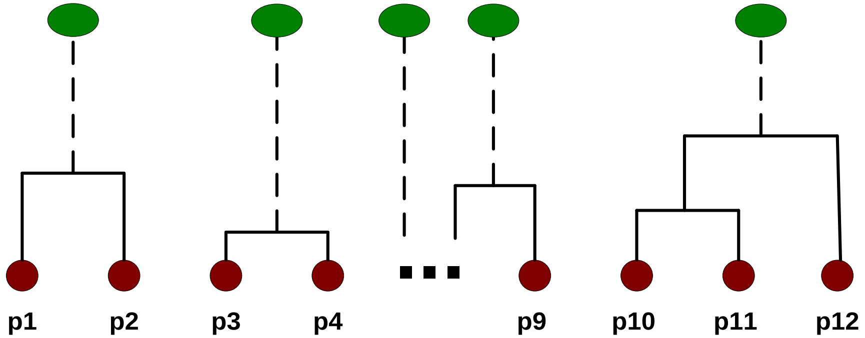
Intermediate Situation

- After some merging steps, we have some clusters



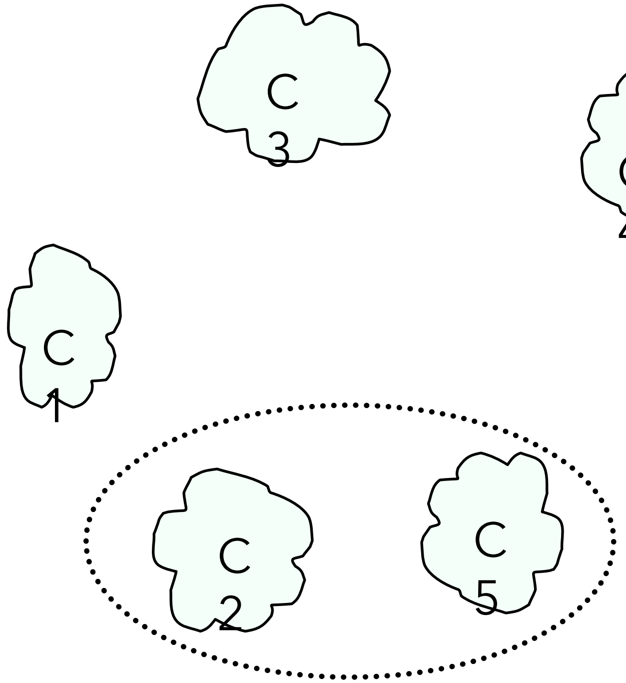
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

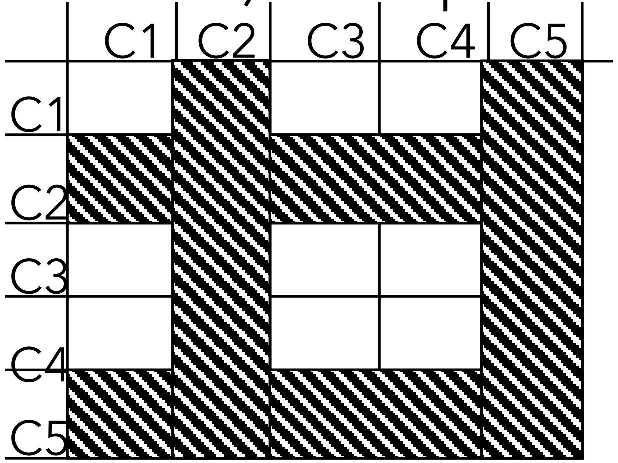
Proximity Matrix



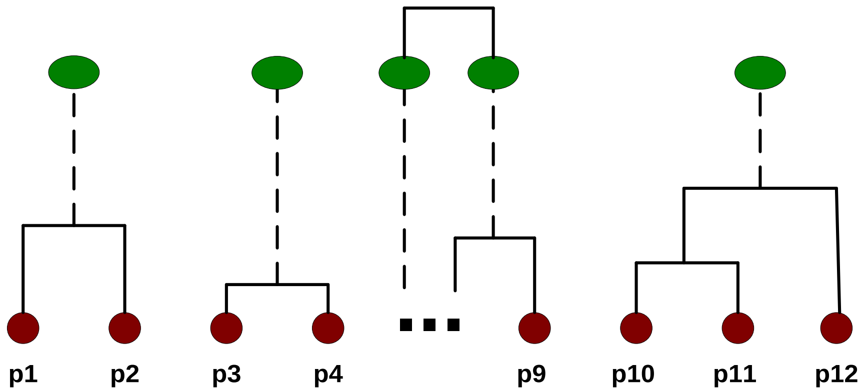
Intermediate Situation

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



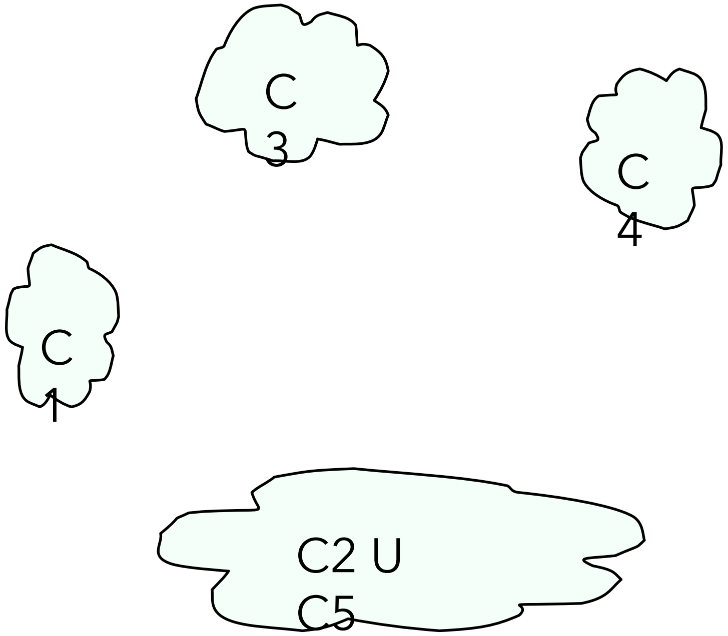


Proximity Matrix



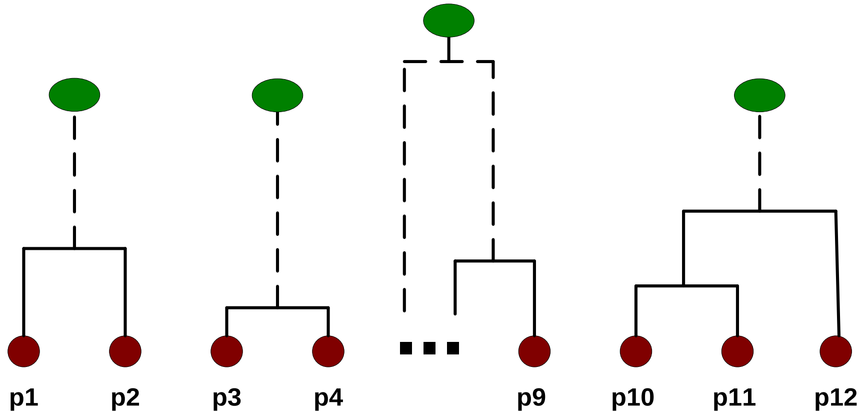
After Merging

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

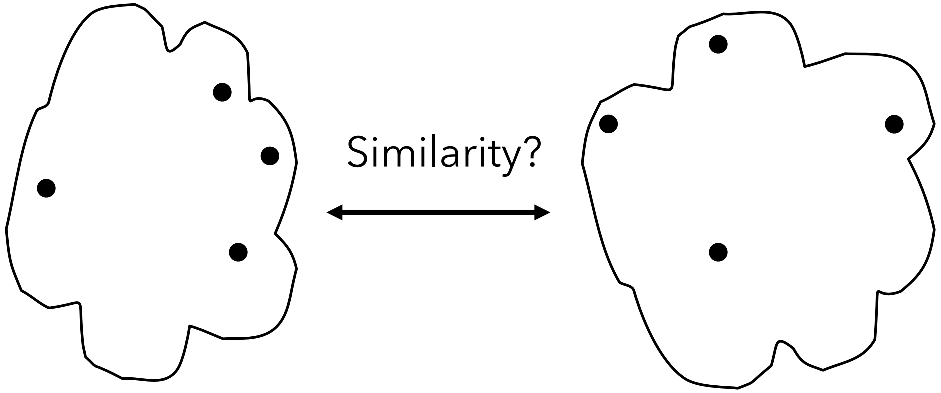


	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		

Proximity Matrix



How to Define Inter-Cluster Similarity

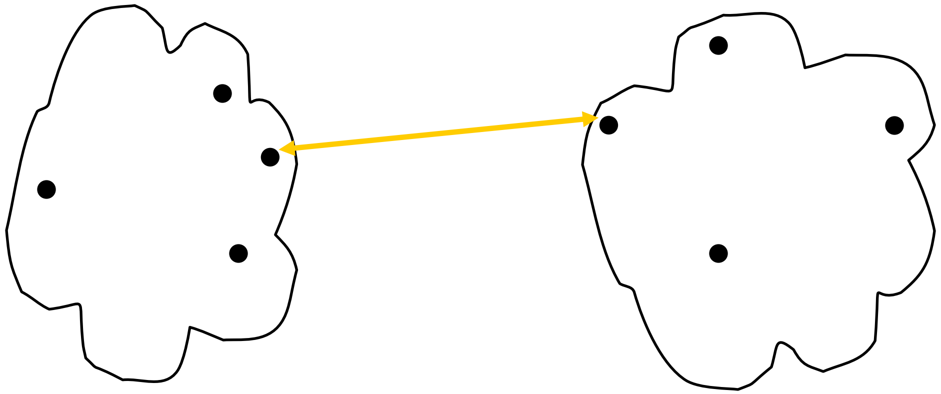


	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

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

How to Define Inter-Cluster Similarity



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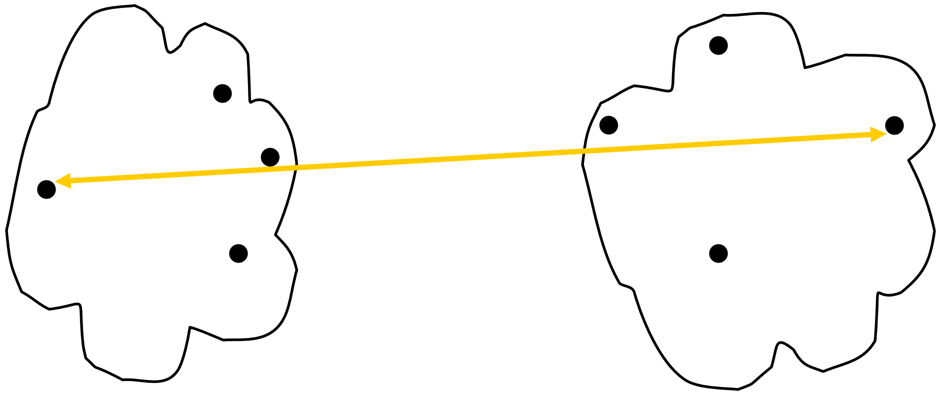

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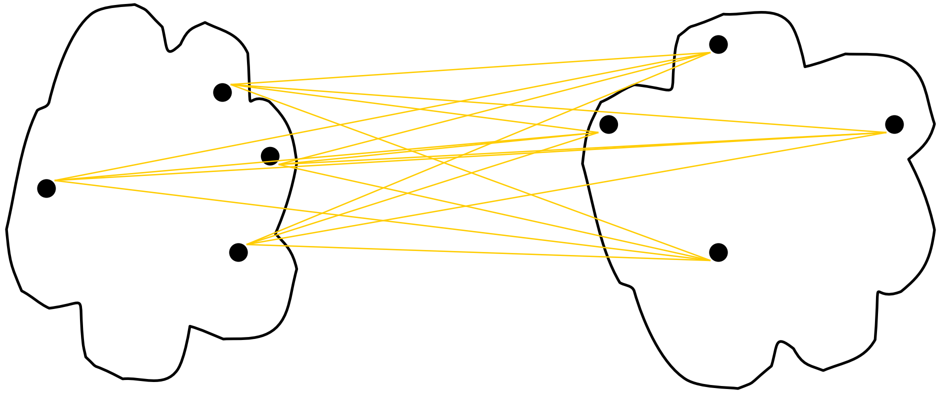

	p1	p2	p3	p4	p5	. . .
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p2						
p3						
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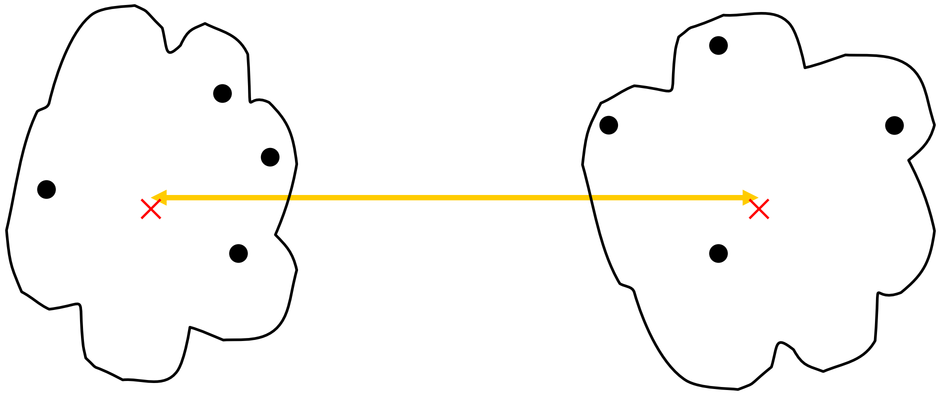
How to Define Inter-Cluster Similarity



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

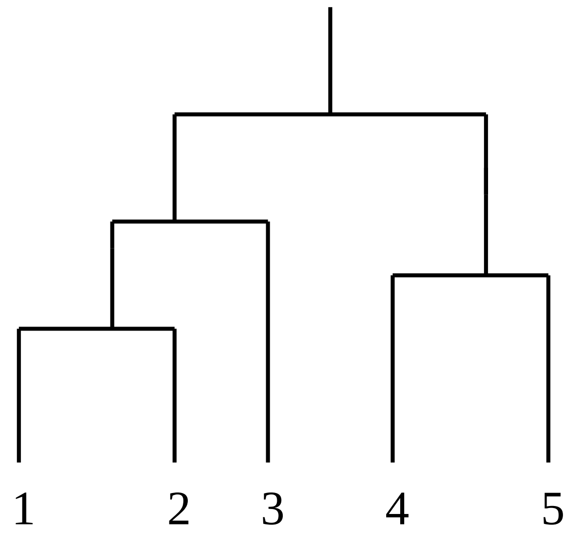
Proximity Matrix

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

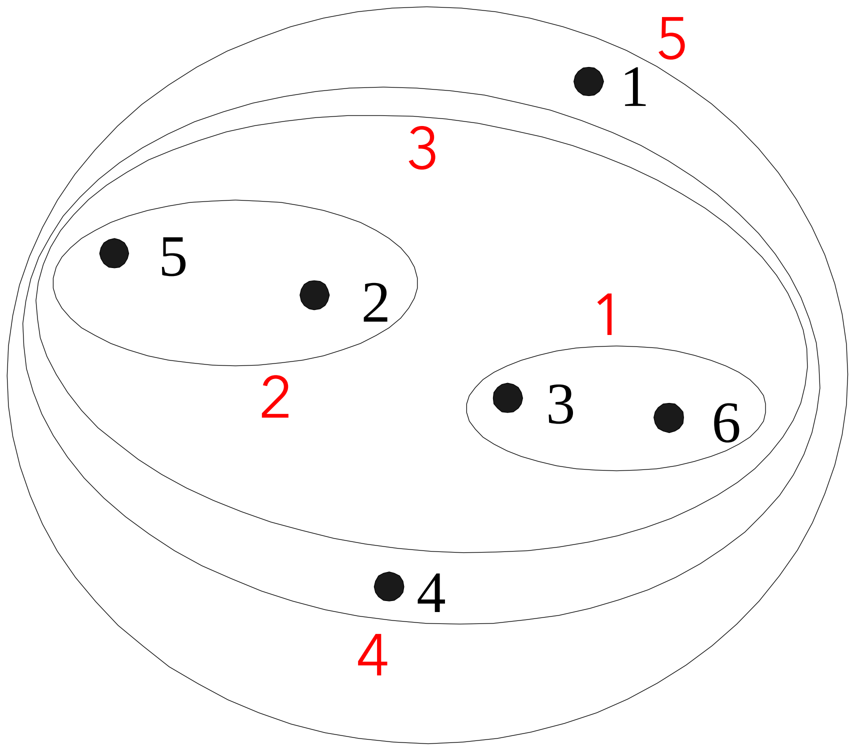
Cluster Similarity: MIN or Single Link

- 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.

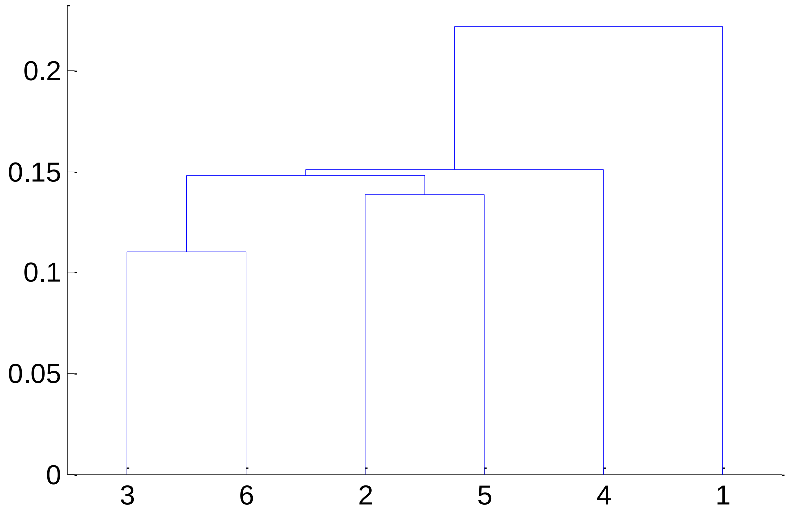
	I1	I2	I3	I4	I5
I1	1.00	0.90	0.10	0.65	0.20
I2	0.90	1.00	0.70	0.60	0.50
I3	0.10	0.70	1.00	0.40	0.30
I4	0.65	0.60	0.40	1.00	0.80
I5	0.20	0.50	0.30	0.80	1.00



Hierarchical Clustering: MIN

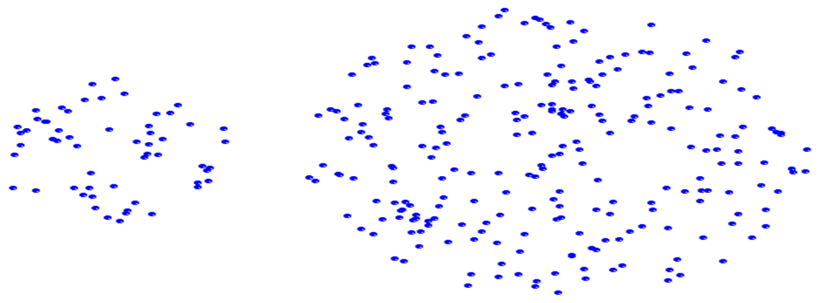


Nested Clusters

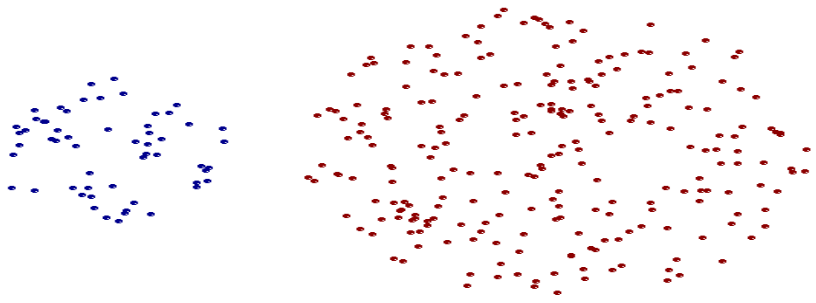


Dendrogram

Strength of MIN



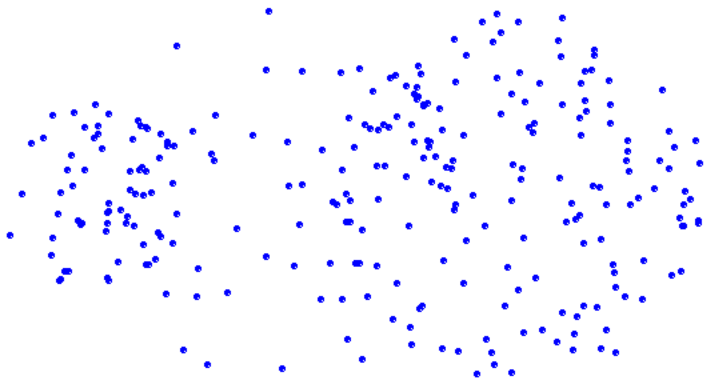
Original Points



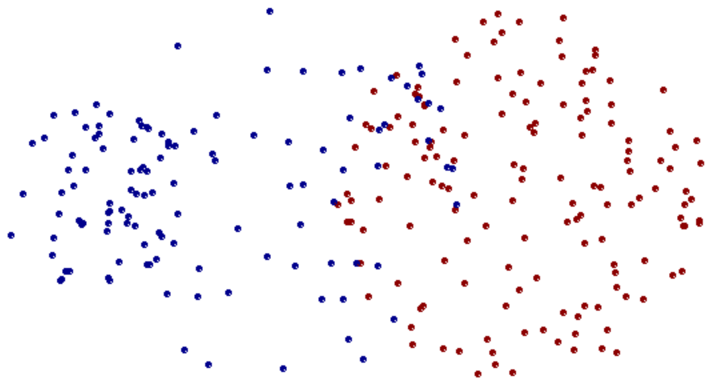
Two Clusters

- Can handle non-elliptical shapes

Limitations of MIN



Original Points



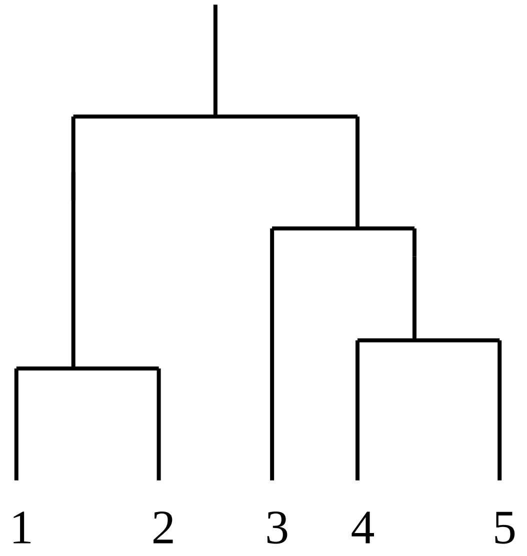
Two Clusters

- Sensitive to noise and outliers

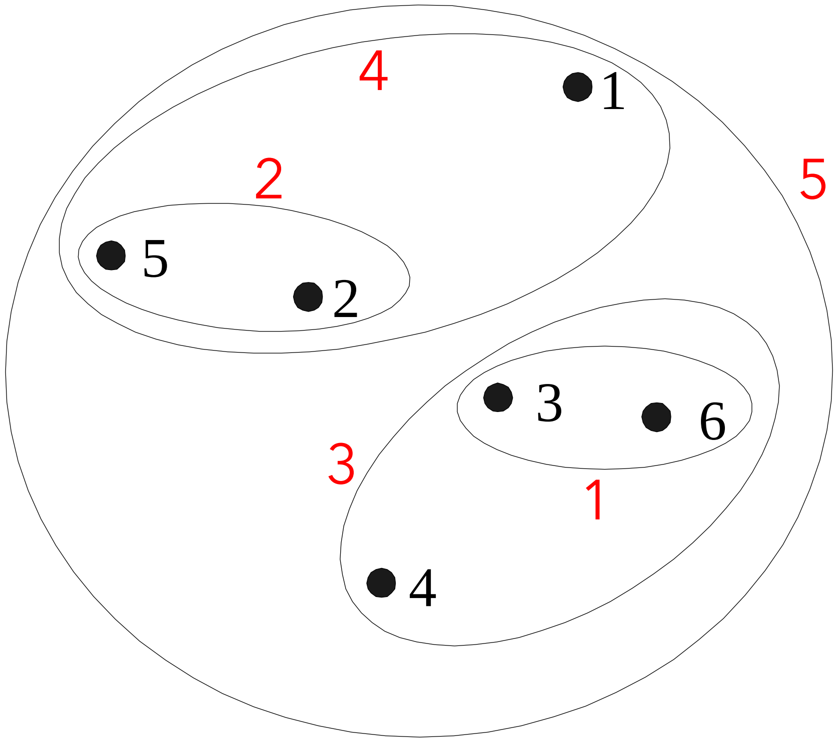
Cluster Similarity: MAX or Complete Linkage

- 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

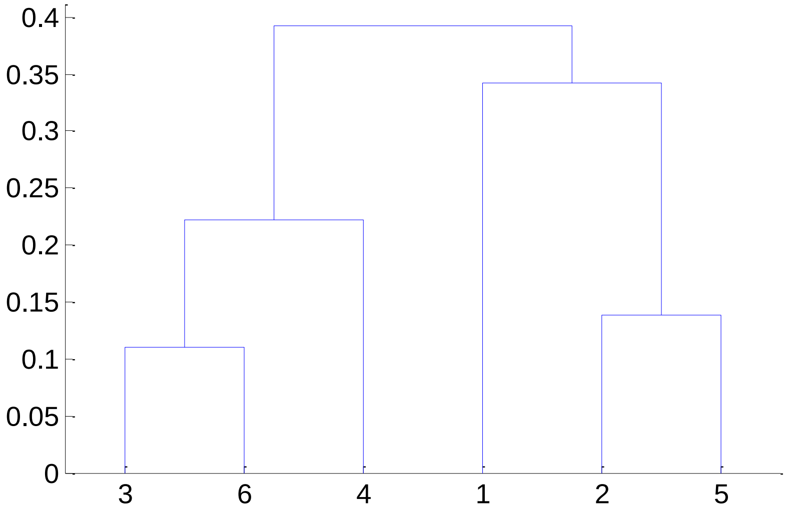
	I1	I2	I3	I4	I5
I1	1.00	0.90	0.10	0.65	0.20
I2	0.90	1.00	0.70	0.60	0.50
I3	0.10	0.70	1.00	0.40	0.30
I4	0.65	0.60	0.40	1.00	0.80
I5	0.20	0.50	0.30	0.80	1.00



Hierarchical Clustering: MAX

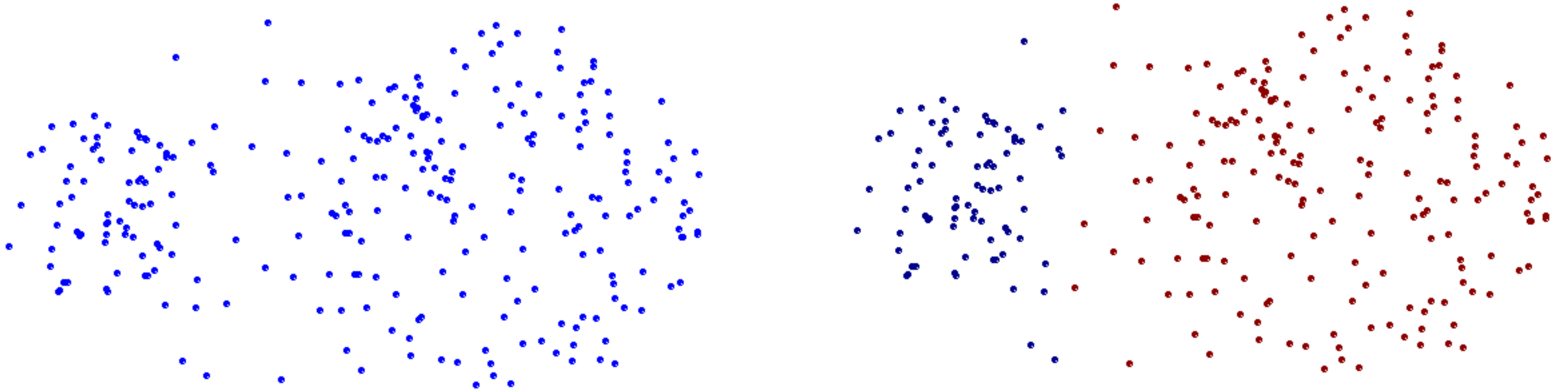


Nested Clusters



Dendrogram

Strength of MAX

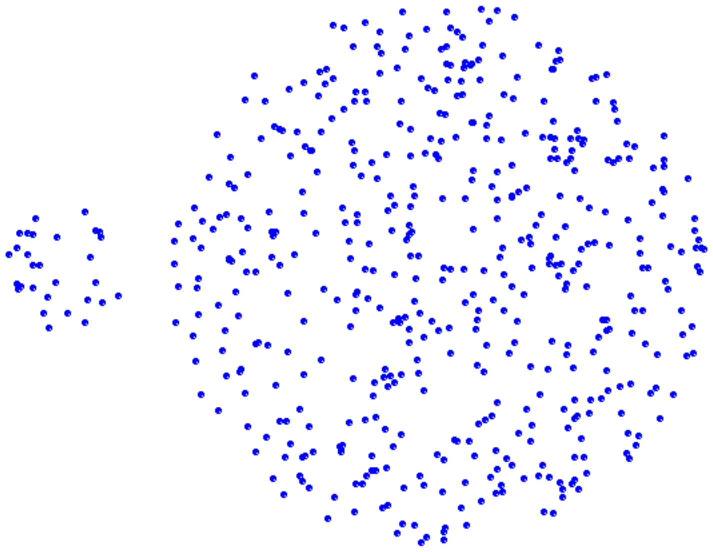


Original Points

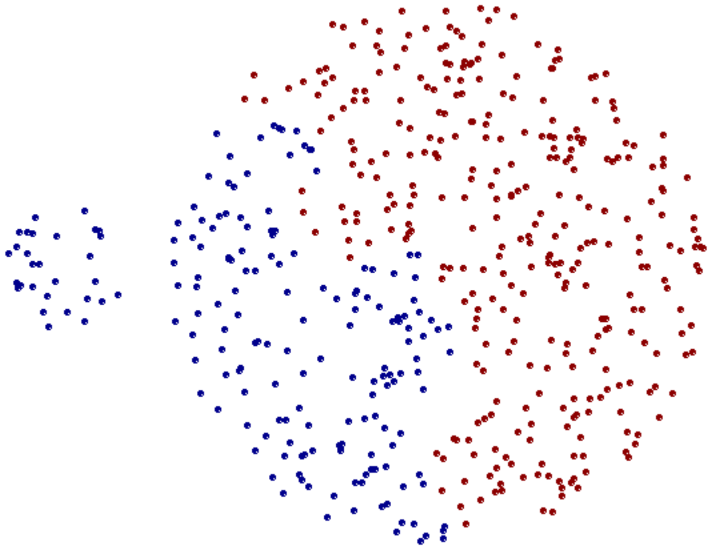
Two Clusters

- Less susceptible to noise and outliers

Limitations of MAX



Original Points



Two Clusters

- Tends to break large clusters
- Biased towards globular clusters

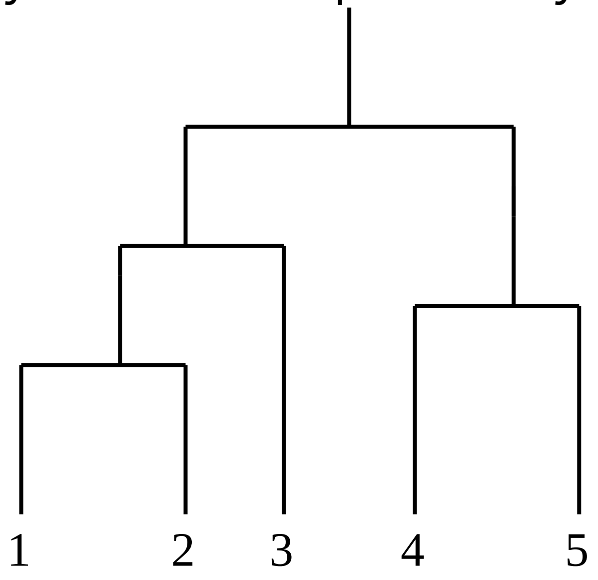
Cluster Similarity: Group Average

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

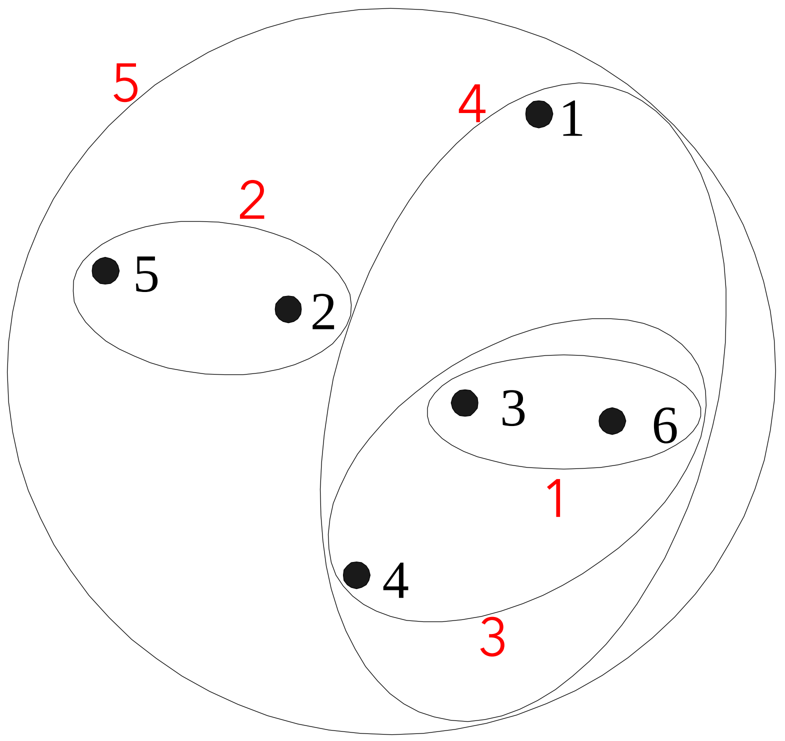
$$\mathbf{proximity}(\mathbf{Cluster}_i,\mathbf{Cluster}_j)=\frac{\sum\limits_{\substack{p_i\in \mathrm{Cluster}_i\\ p_j\in \mathrm{Cluster}_j}}\mathbf{proximity}(p_i,p_j)}{|\mathbf{Cluster}_i|*|\mathbf{Cluster}_j|}$$

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

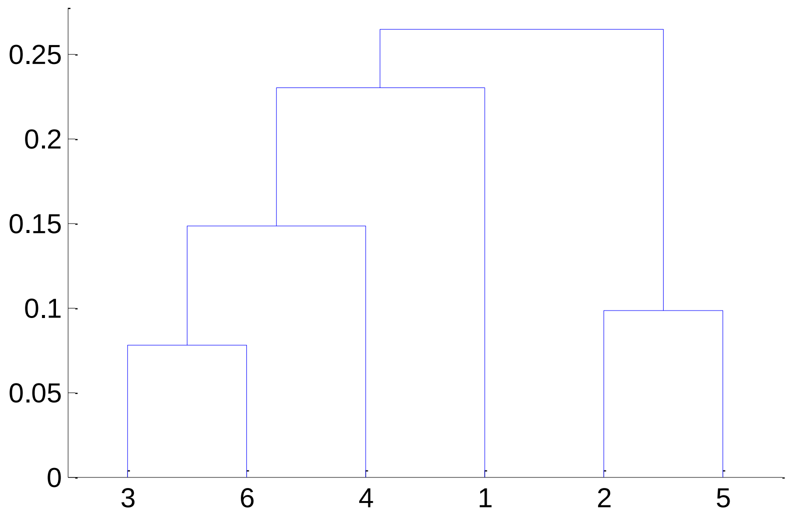
	I1	I2	I3	I4	I5
I1	1.00	0.90	0.10	0.65	0.20
I2	0.90	1.00	0.70	0.60	0.50
I3	0.10	0.70	1.00	0.40	0.30
I4	0.65	0.60	0.40	1.00	0.80
I5	0.20	0.50	0.30	0.80	1.00



Hierarchical Clustering: Group Average



Nested Clusters



Dendrogram

Hierarchical Clustering: Group Average

Compromise between Single and Complete Link

Strengths

- Less susceptible to noise and outliers

Limitations

- Biased towards globular clusters

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

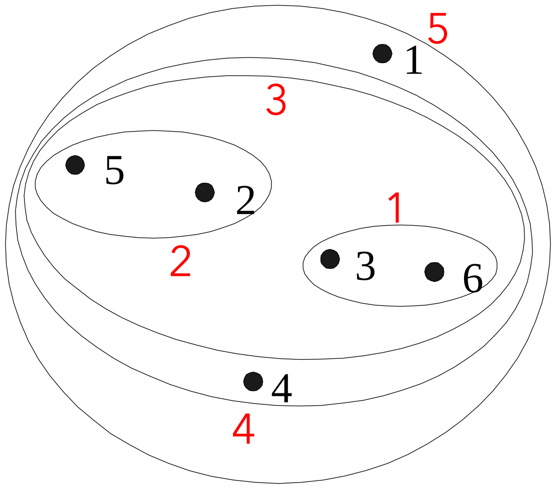
Less susceptible to noise and outliers

Biased towards globular clusters

Hierarchical analogue of K-means

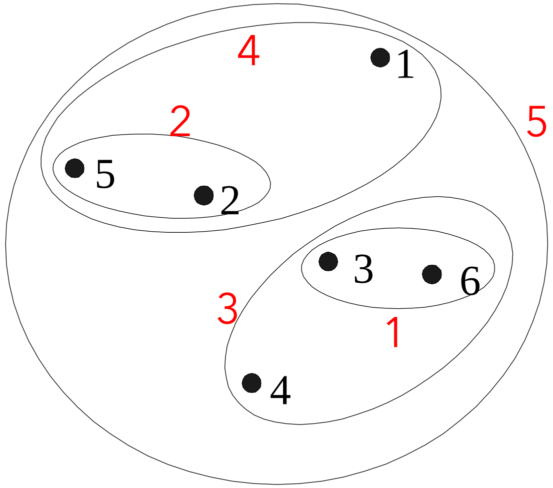
- Can be used to initialize K-means

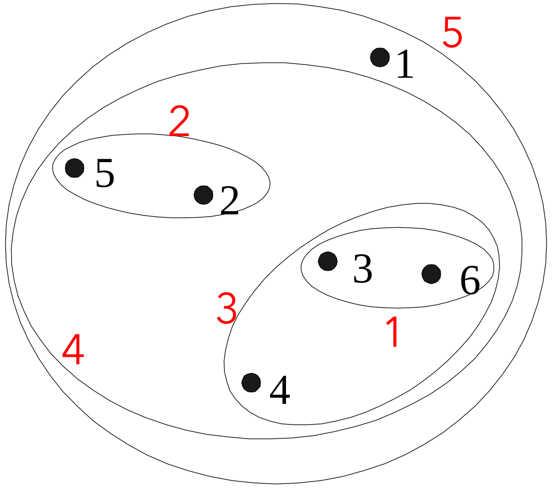
Hierarchical Clustering: Comparison



MIN

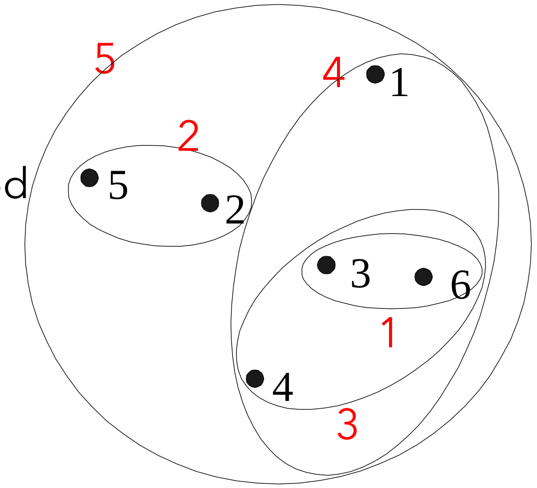
MAX





Group Average

Ward's Method



Hierarchical Clustering: Time and Space requirements

$O(N^2)$ space since it uses the proximity matrix.

- N is the number of points.

$O(N^3)$ time in many cases

- There are N steps and at each step the size, N^2, proximity matrix must be updated and searched
- Complexity can be reduced to $O(N^2 \log(N))$ time for some approaches

Hierarchical Clustering: Problems and Limitations

Once a decision is made to combine two clusters, it cannot be undone

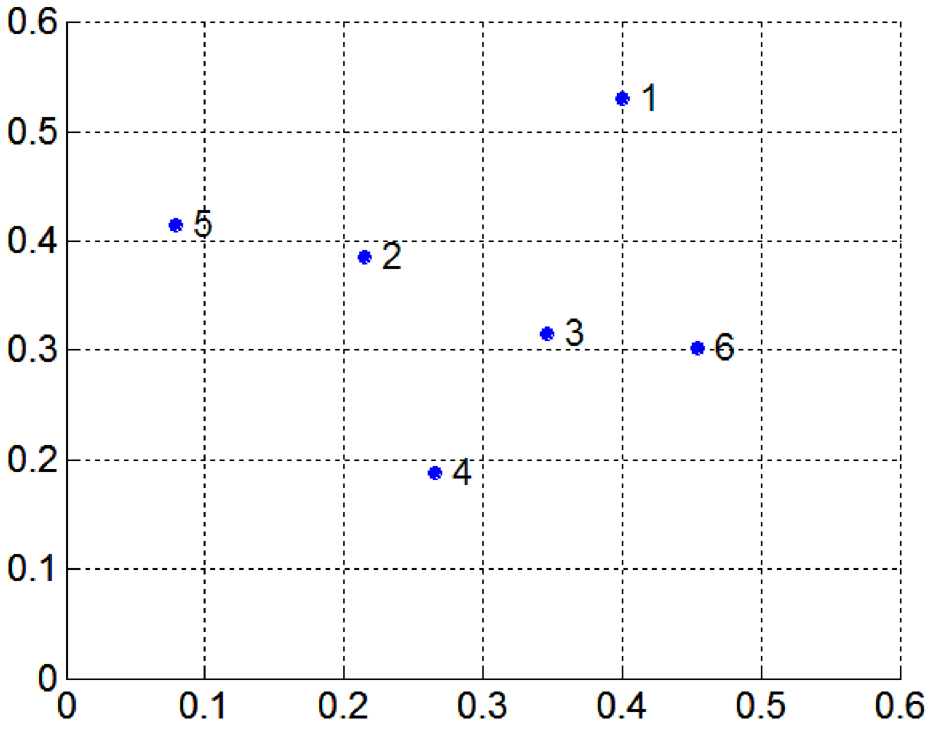
No objective function is directly minimized

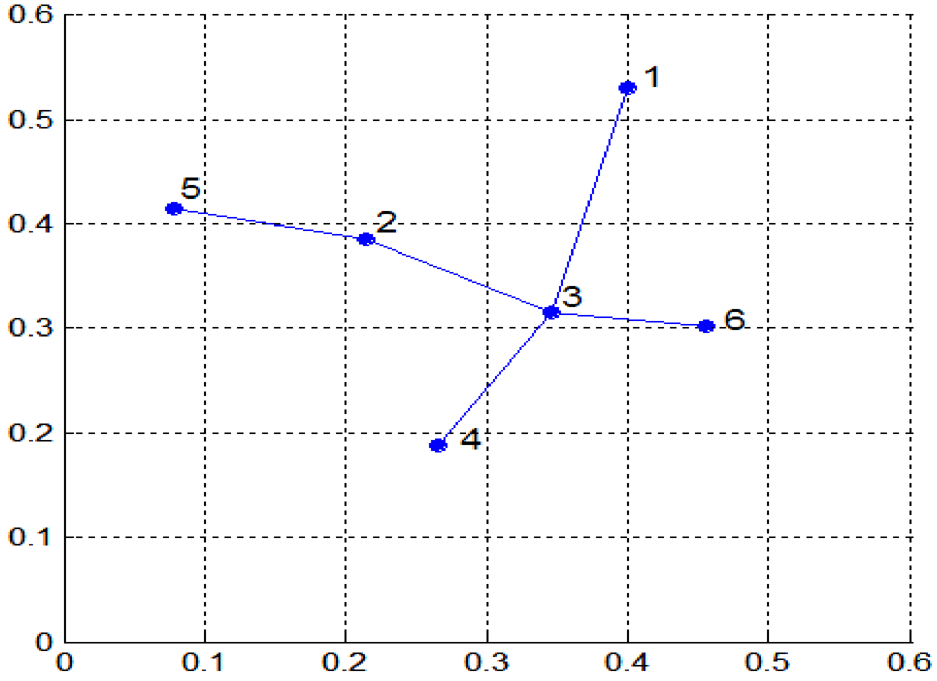
Different schemes have problems with one or more of the following:

- Sensitivity to noise and outliers
- Difficulty handling different sized clusters and convex shapes
- Breaking large clusters

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





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 - a density-based algorithm

Density = number of points within a specified radius (Eps)

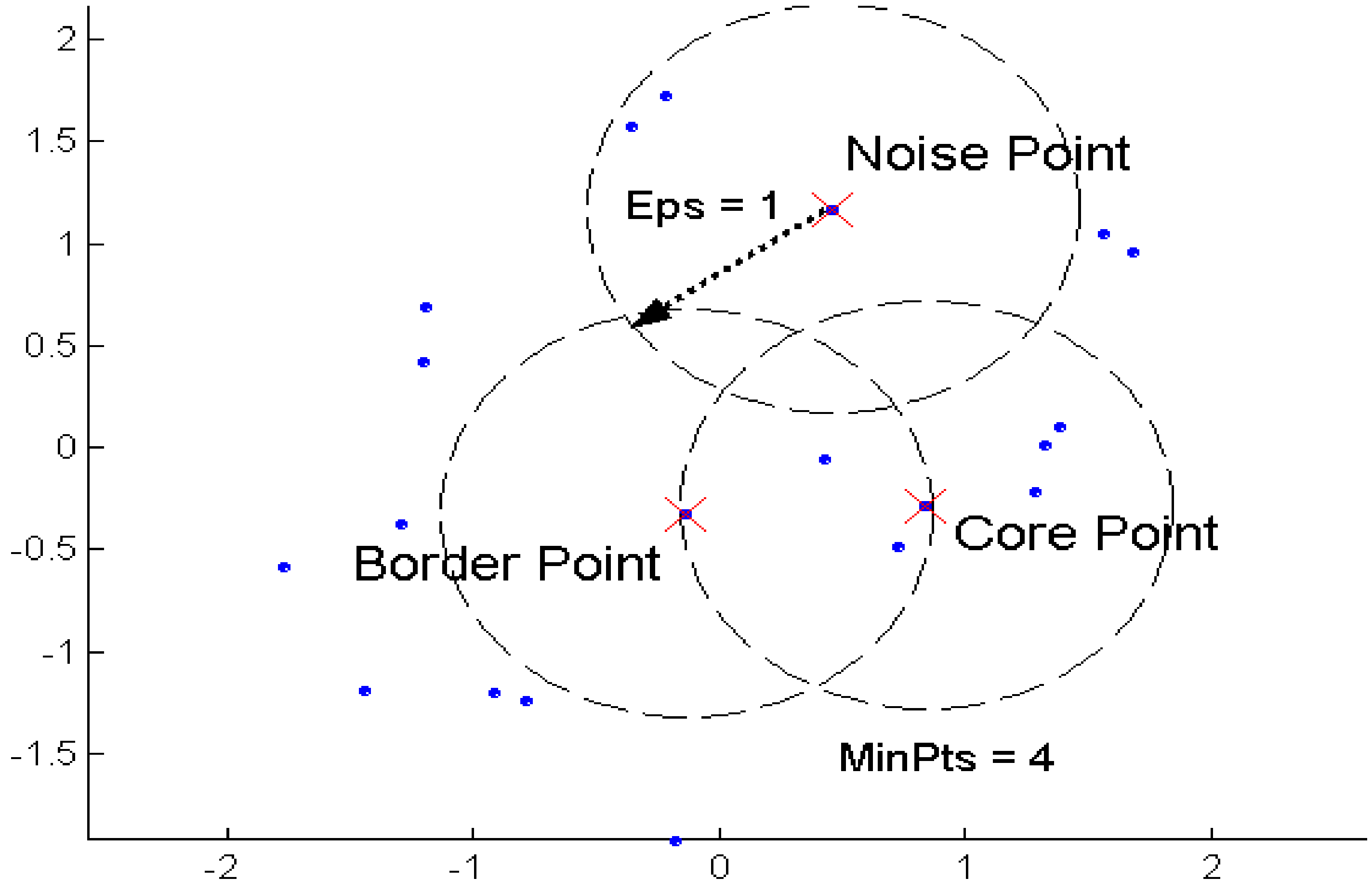
A point is a core point if it has more than a specified number of points (MinPts) within Eps

- 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



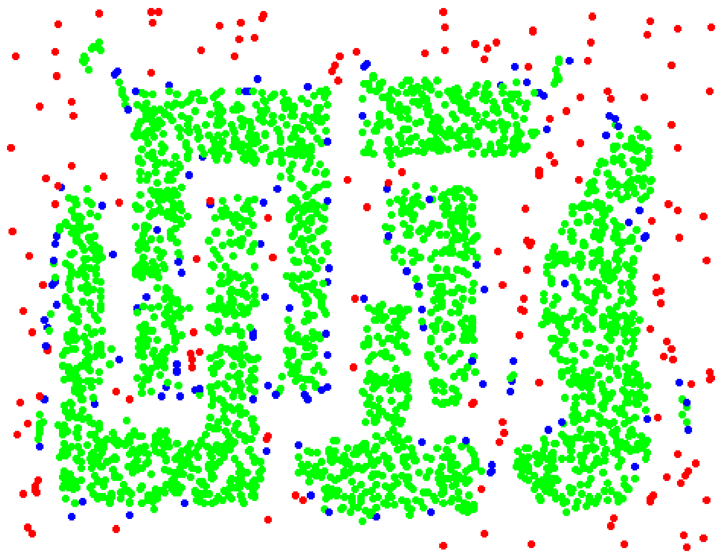
DBSCAN Algorithm

- 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

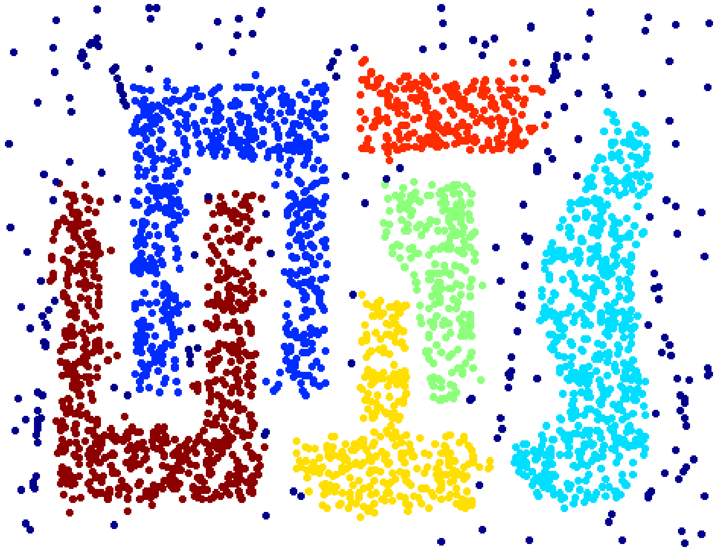


Point types: core, border and noise

Eps = 10, MinPts = 4

When DBSCAN Works Well

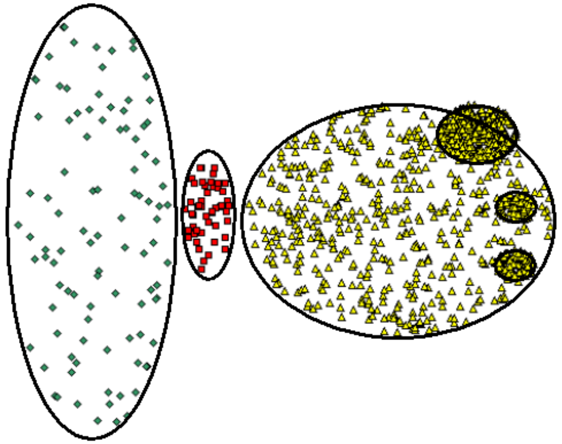
Original Points



Clusters

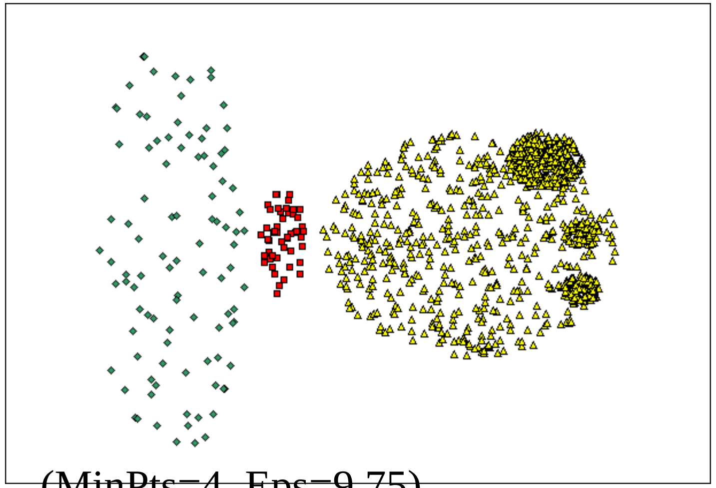
- Resistant to Noise
- Can handle clusters of different shapes and sizes

When DBSCAN Does NOT Work Well

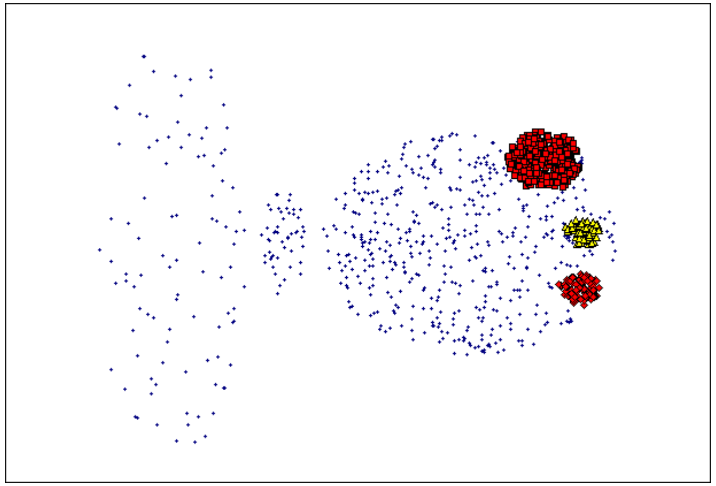


Original Points

- Varying densities
- High-dimensional data



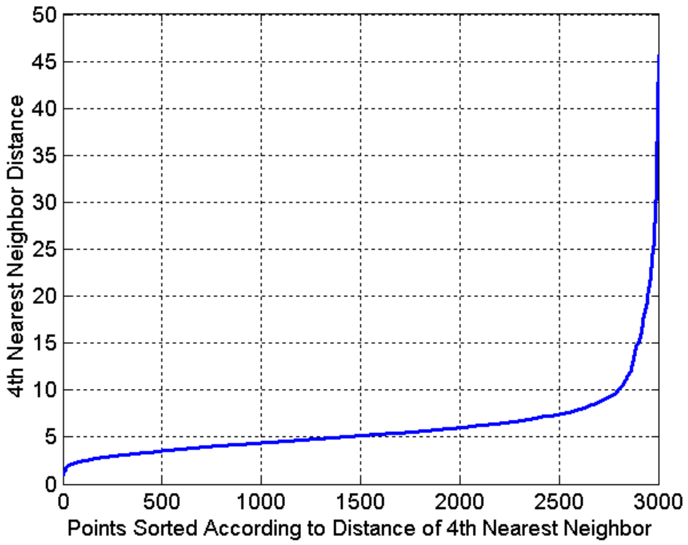
(MinPts=4, Eps=9.75).



(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

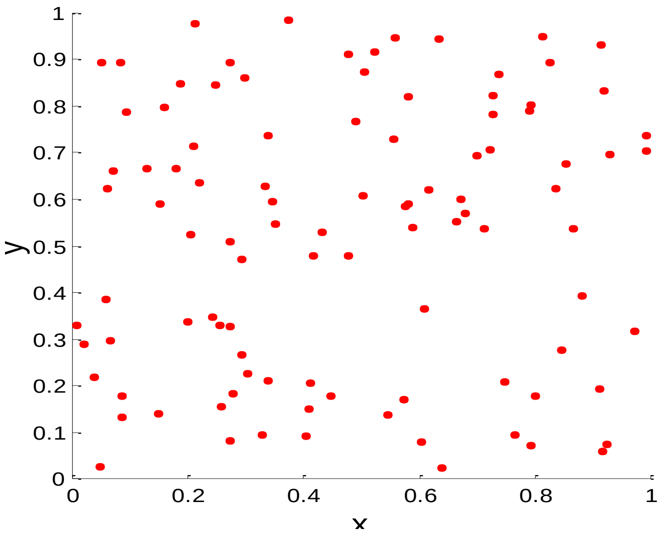
To compare clustering algorithms

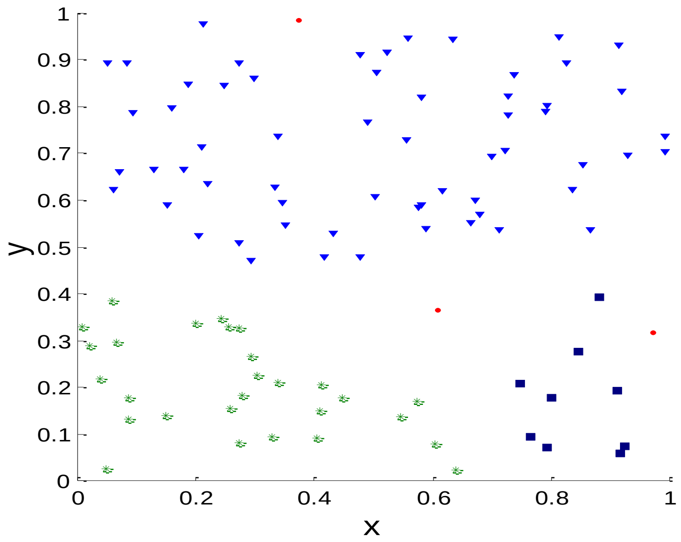
To compare two sets of clusters

To compare two clusters

Clusters found in Random Data

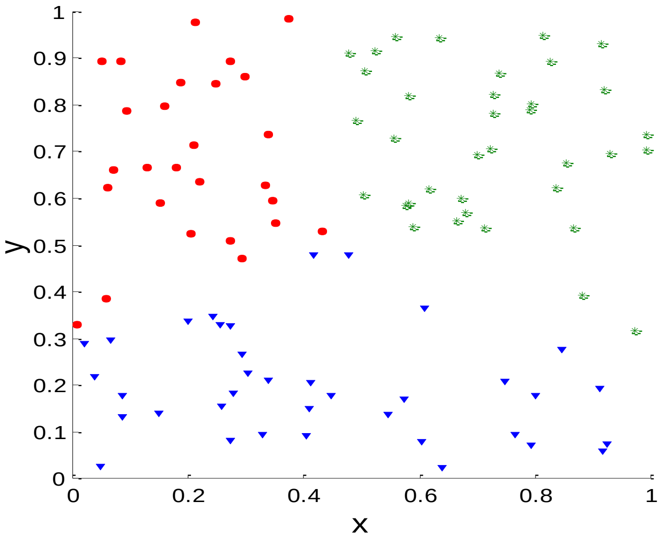
Random Points

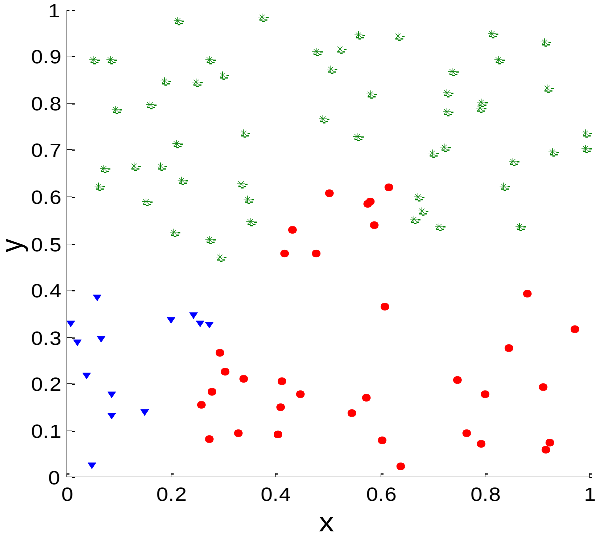




DBSCAN

K-means





Complete Link

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

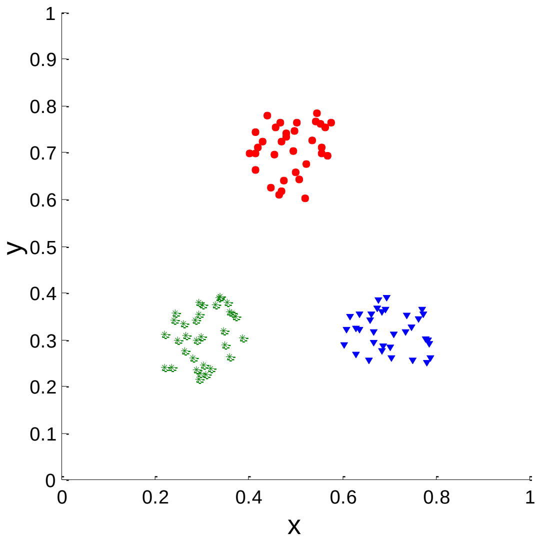
However, sometimes criterion is the general strategy and index is the numerical measure that implements the criterion.

Measuring Cluster Validity Via Correlation

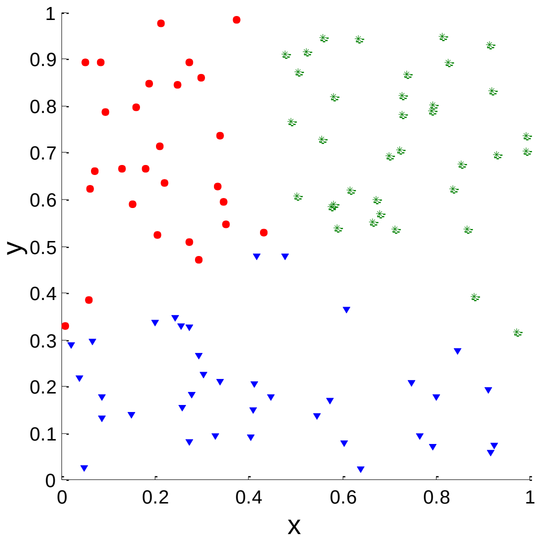
- Two matrices
  - Proximity Matrix
  - "Incidence" Matrix
    - One row and one column for each data point
    - An entry is 1 if the associated pair of points belong to the same cluster
    - An entry is 0 if the associated pair of points belongs to different clusters
- Compute the correlation between 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

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



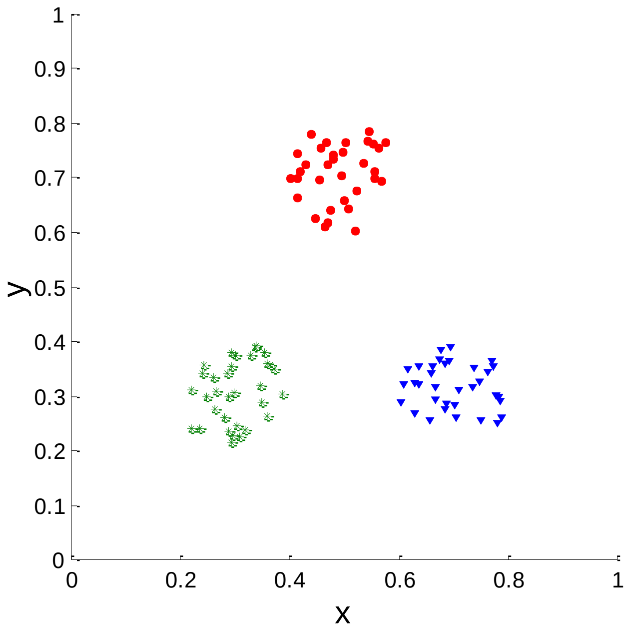
Corr = -0.9235

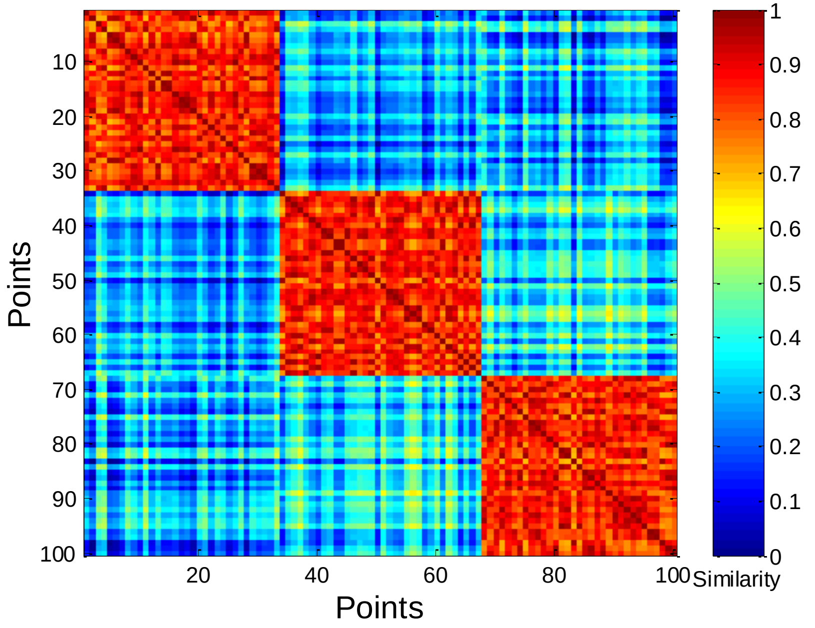


Corr = -0.5810

Using Similarity Matrix for Cluster Validation

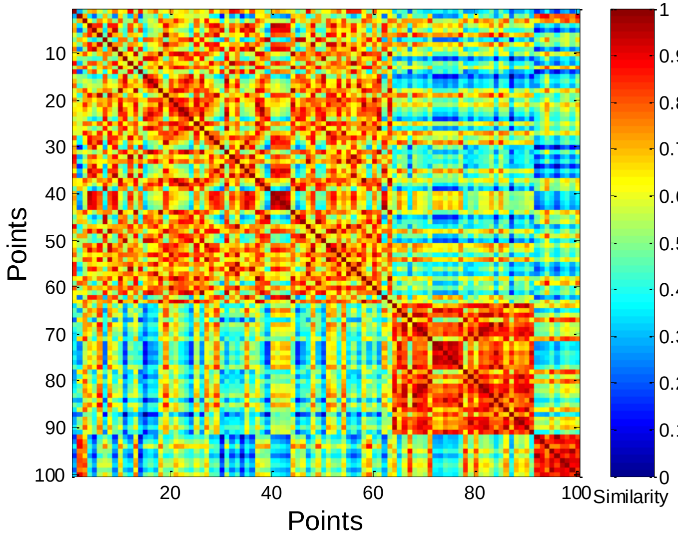
- Order the similarity matrix with respect to cluster labels and inspect visually.

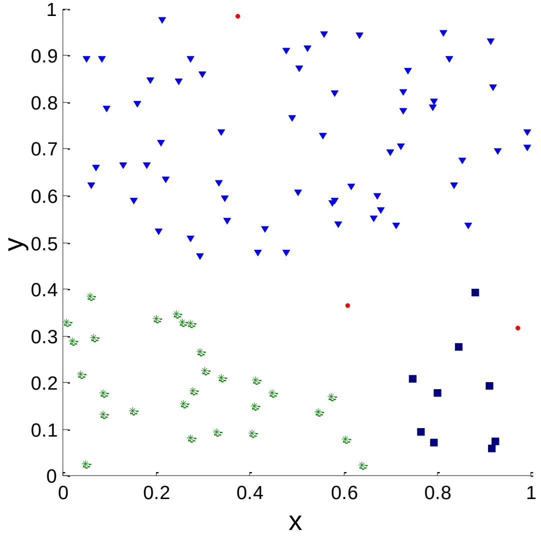




Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp

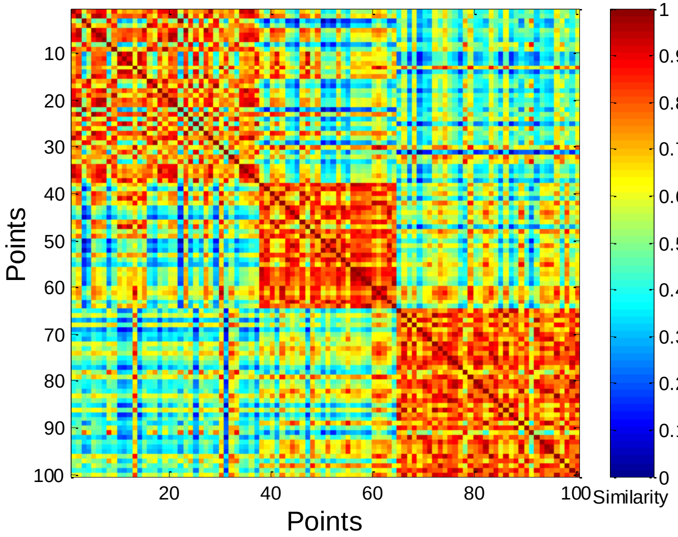


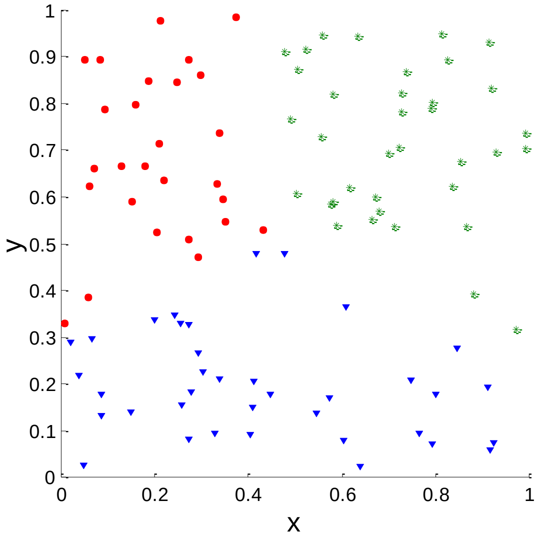


DBSCAN

Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp

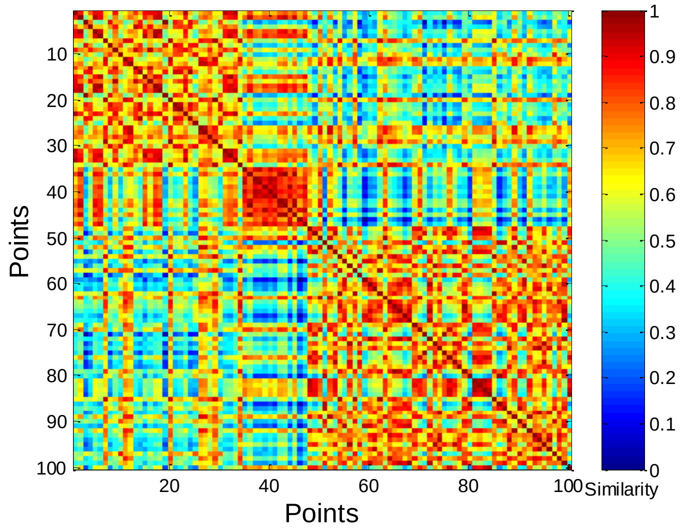


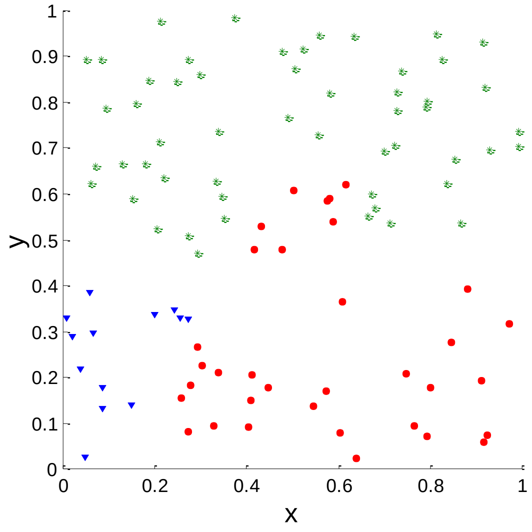


K-means

Using Similarity Matrix for Cluster Validation

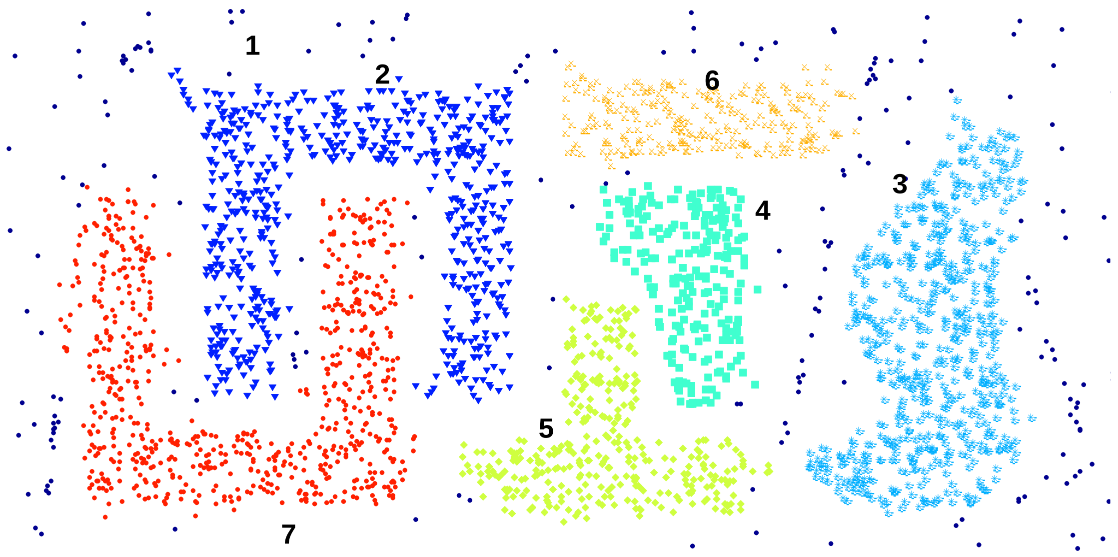
Clusters in random data are not so crisp

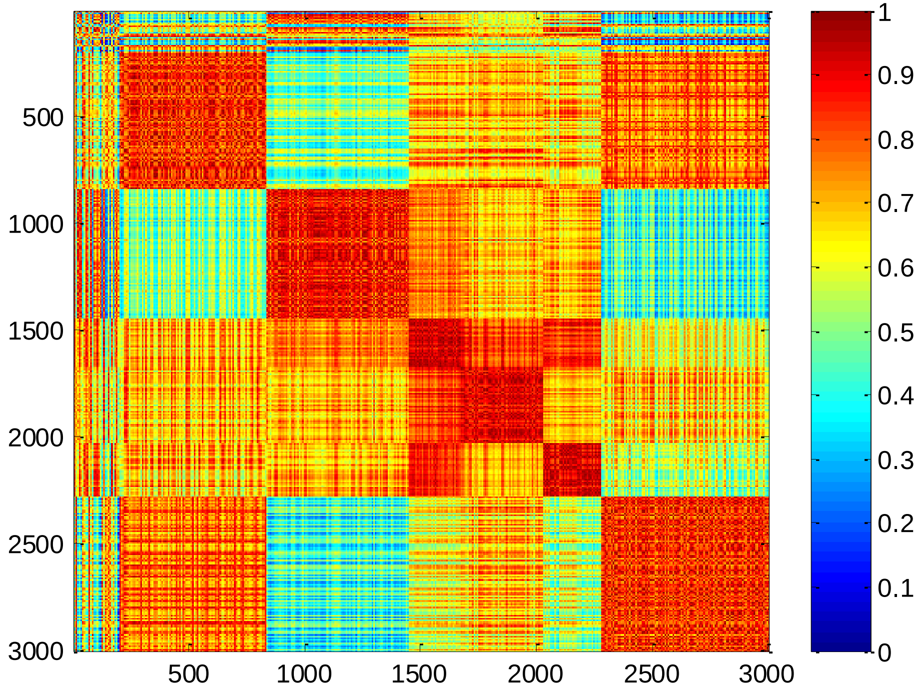




Complete Link

Using Similarity Matrix for Cluster Validation

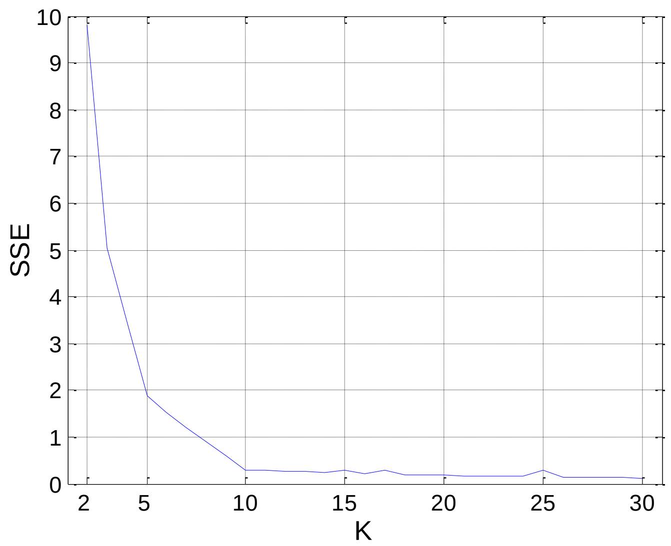


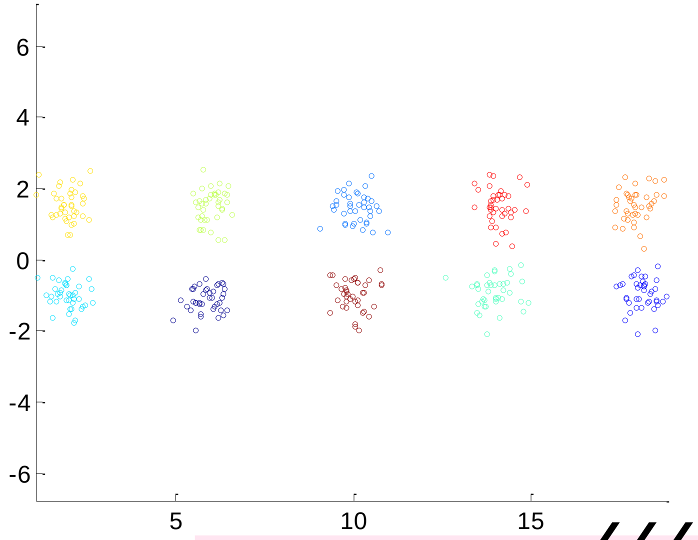


DBSCAN

Internal Measures: SSE

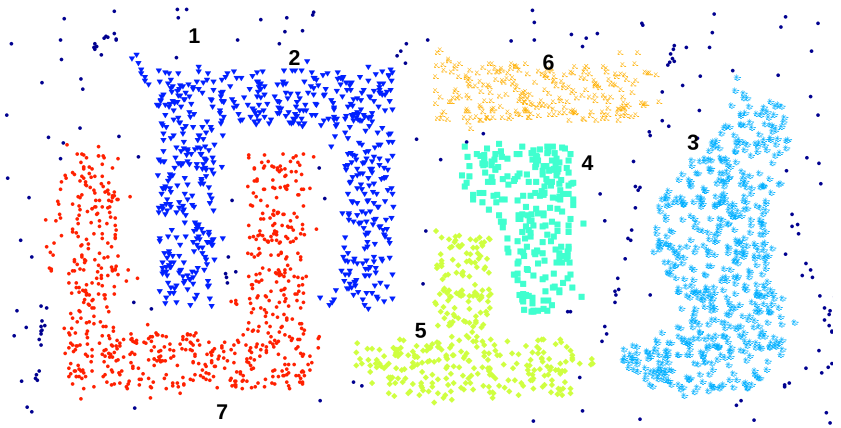
- Clusters in more complicated figures aren't well separated
- Internal Index: Used to measure the goodness of a clustering structure without respect to external information
  - SSE
- SSE is good for comparing two clusterings or two clusters (average SSE).
- Can also be used to estimate the number of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

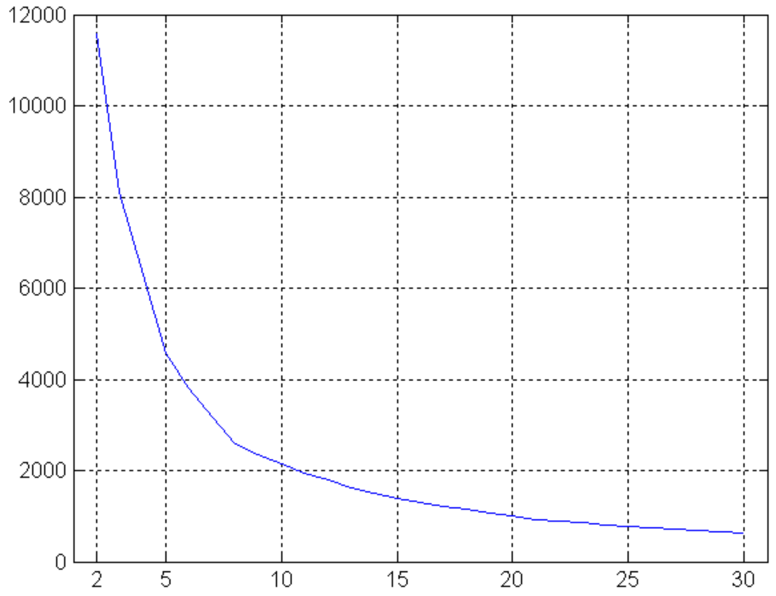




Internal Measures: SSE

- SSE curve for a more complicated data set





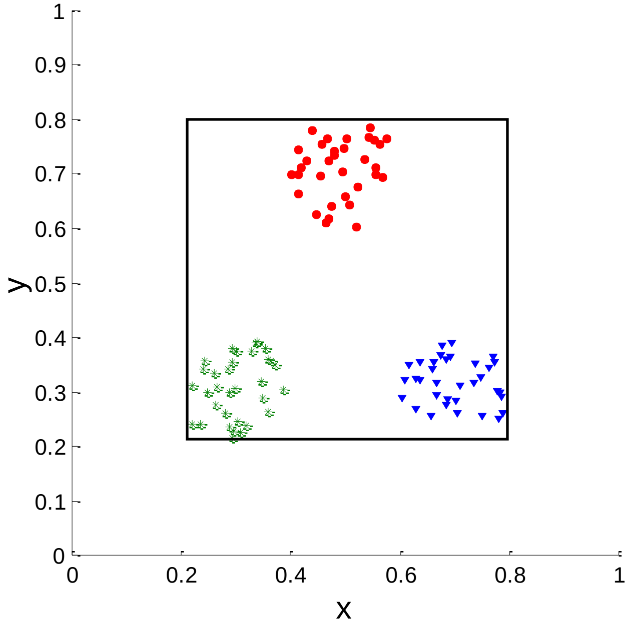
SSE of clusters found using K-means

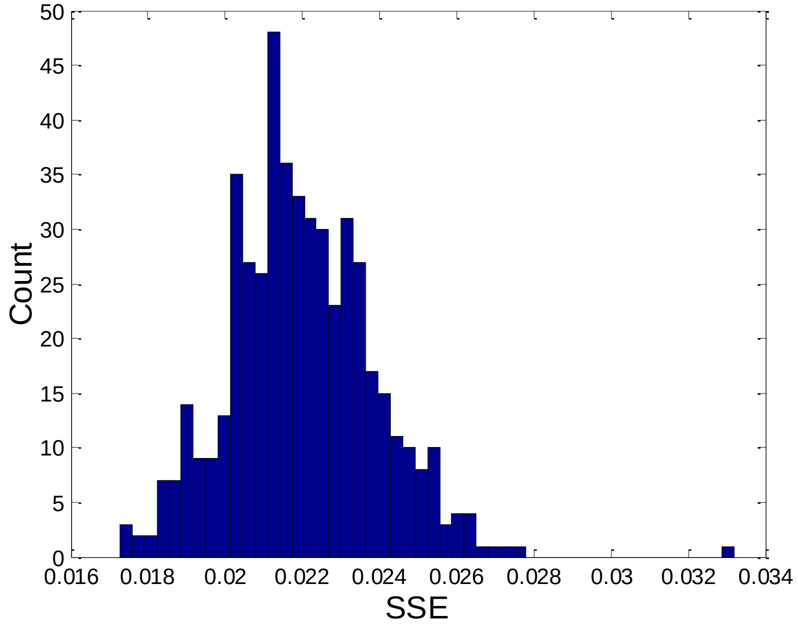
Framework for Cluster Validity

- 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

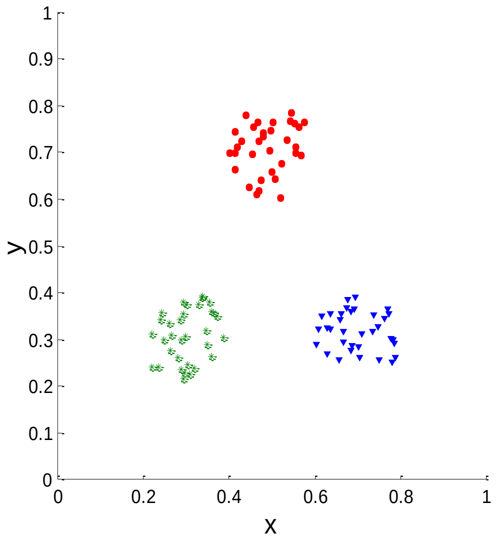
- Example
  - Compare SSE of 0.005 against three clusters in random data
  - Histogram shows SSE of three clusters in 500 sets of random data points of size 100 distributed over the range 0.2 – 0.8 for x and y values

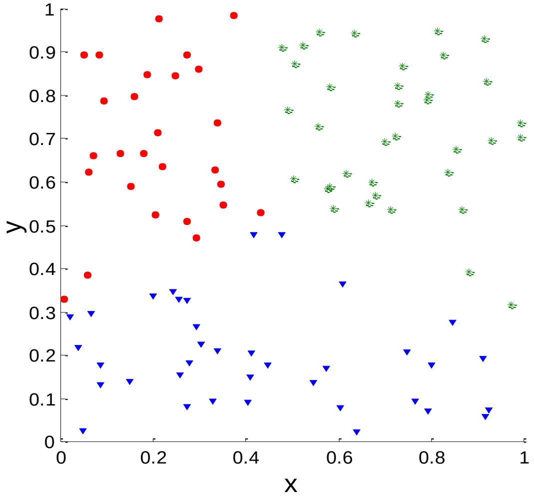


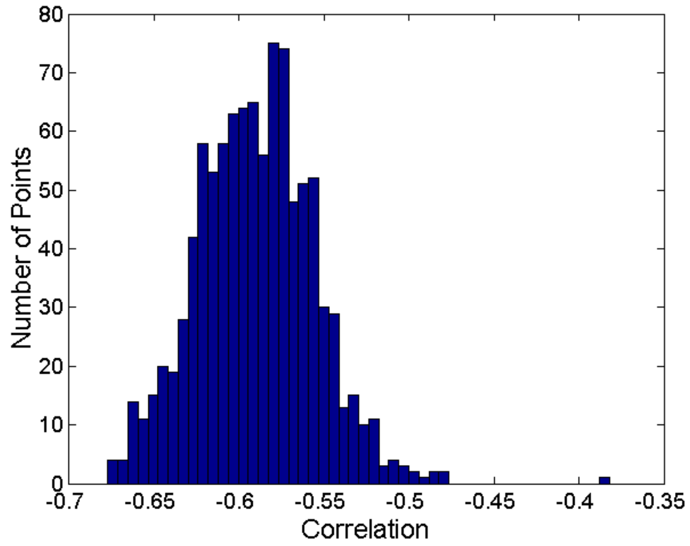


Statistical Framework for Correlation

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







Corr = -0.9235

Corr = -0.5810

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)

$$\boldsymbol{WSS} = \sum_{\boldsymbol{i}} \sum_{\boldsymbol{x} \in \boldsymbol{C}_{\boldsymbol{i}}} (\boldsymbol{x} - \boldsymbol{m}_{\boldsymbol{i}})^2$$

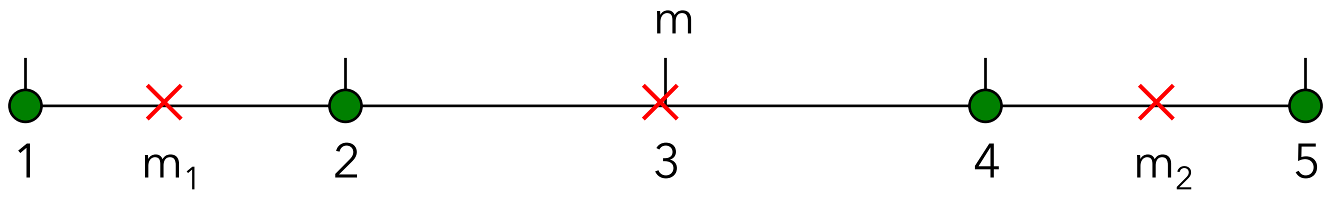
  - Separation is measured by the between cluster sum of squares

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

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

Internal Measures: Cohesion and Separation

- Example: SSE
  - BSS + WSS = 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:

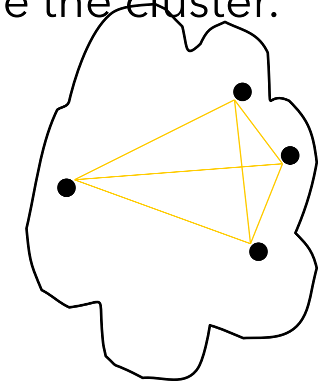
$$WSS = (1-1.5)^2 + (2-1.5)^2 + (4-4.5)^2 + (5-4.5)^2 = 1$$

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

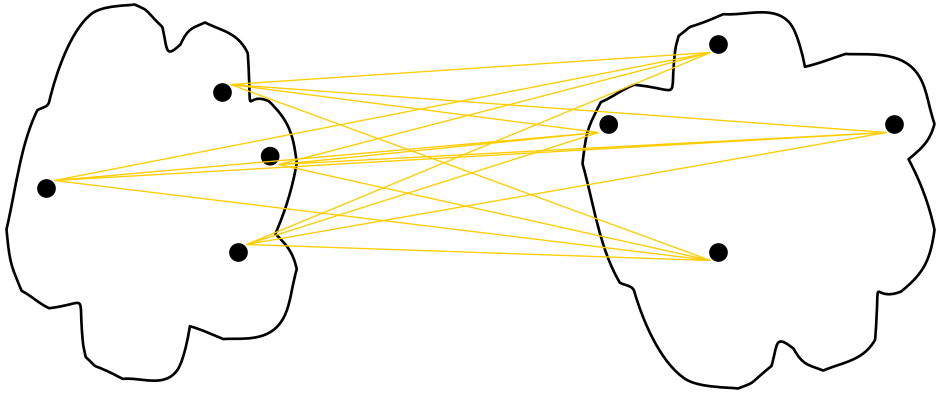
$$Total = 1 + 9 = 10$$

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

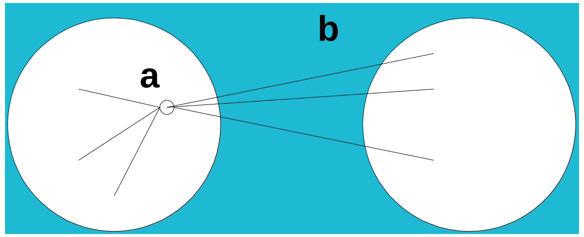


separation

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

    $s = 1 - a/b$ if $a < b$, (or $s = b/a - 1$ if $a \geq b$, 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

External Measures of Cluster Validity: Entropy and Purity

Table 5.9. K-means Clustering Results for LA Document Data Set

Cluster	Entertainment	Financial	Foreign	Metro	National	Sports	Entropy	Purity
1	3	5	40	506	96	27	1.2270	0.7474
2	4	7	280	29	39	2	1.1472	0.7756
3	1	1	1	7	4	671	0.1813	0.9796
4	10	162	3	119	73	2	1.7487	0.4390
5	331	22	5	70	13	23	1.3976	0.7134
6	5	358	12	212	48	13	1.5523	0.5525
Total	354	555	341	943	273	738	1.1450	0.7203

entropy For each cluster, the class distribution of the data is calculated first, i.e., for cluster j we compute p_{ij}, the 'probability' that a member of cluster j belongs to class i as follows: $p_{ij} = m_{ij}/m_j$, where m_j is the number of values in cluster j and m_{ij} is the number of values of class i in cluster j. Then using this class distribution, the entropy of each cluster j is calculated using the standard formula $e_j = \sum_{i=1}^{L} p_{ij} \log_2 p_{ij}$, where the L is the number of classes. The total entropy for a set of clusters is calculated as the sum of the entropies of each cluster weighted by the size of each cluster, i.e., $e = \sum_{i=1}^{K} \frac{m_i}{m} e_j$, where m_j is the size of cluster j, K is the number of clusters, and m is the total number of data points.

purity Using the terminology derived for entropy, the purity of cluster j, is given by $purity_j = \max p_{ij}$ and the overall purity of a clustering by $purity = \sum_{i=1}^{K} \frac{m_i}{m} purity_j$.

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