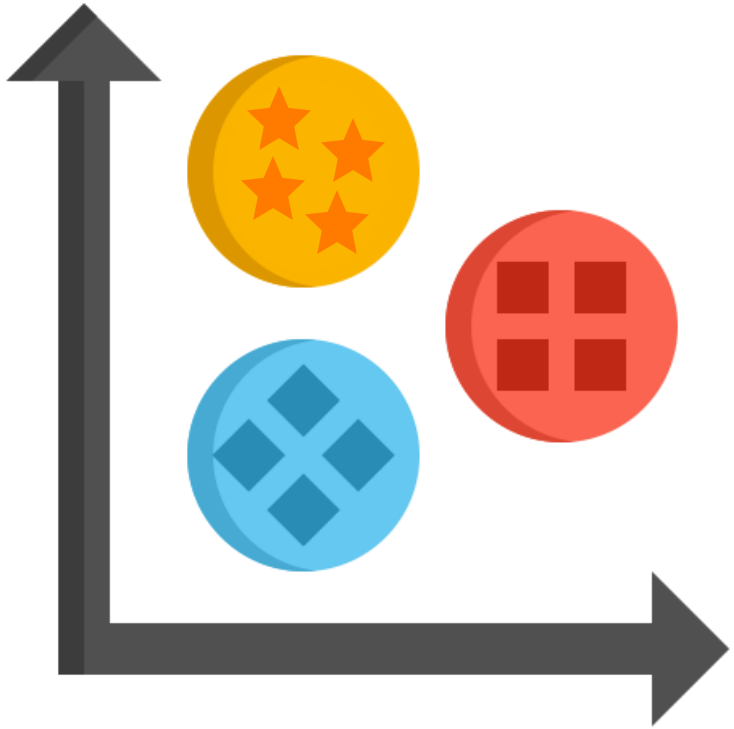
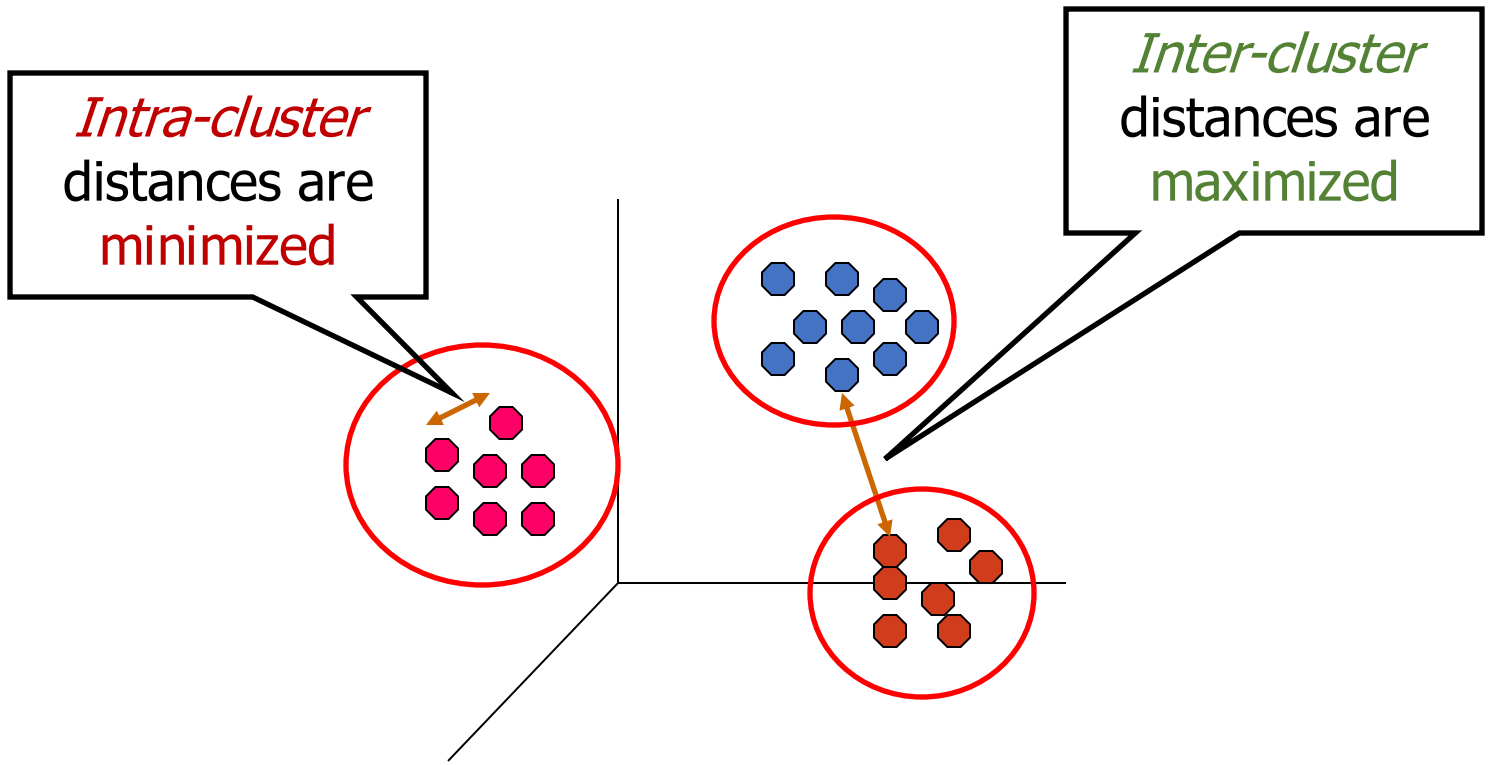
UNIVERSITÀ DEL SALENTO

Clustering



What is Cluster Analysis?

Given a set of objects, place them in groups such that the objects in **a group** are **similar** (or related) to one another and **different** from (or unrelated to) the objects in **other groups**



Notion of a Cluster can be Ambiguous

How many clusters?

Six Clusters

Two Clusters

Four Clusters

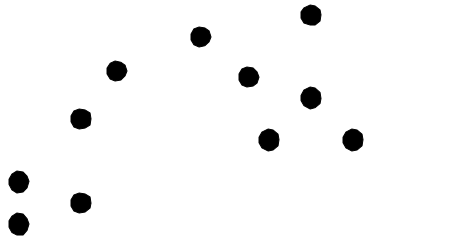
Types of Clusterings

A clustering is a set of clusters

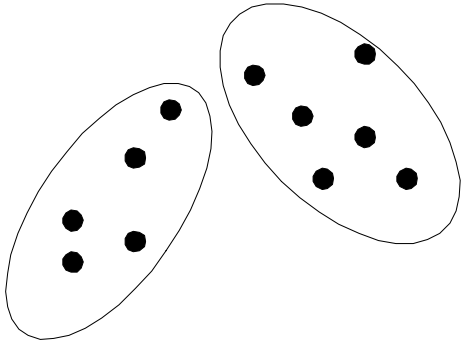
Important distinction between hierarchical and partitional sets of clusters

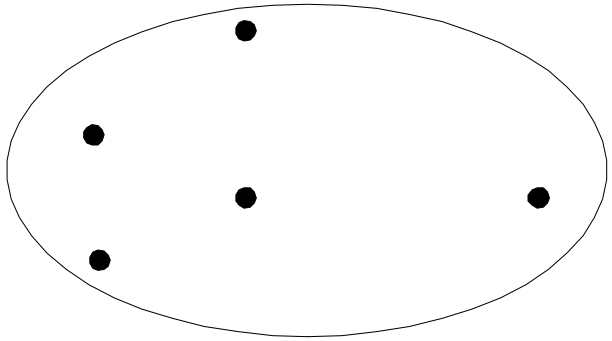
- **Partitional Clustering**: A division of data objects into non-overlapping subsets (clusters)
- **Hierarchical clustering**: A set of nested clusters organized as a hierarchical tree

Partitional Clustering



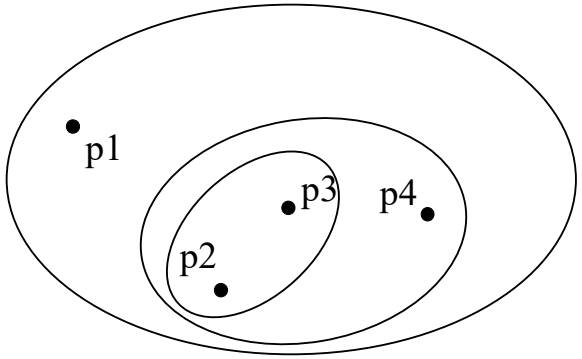
Original Points



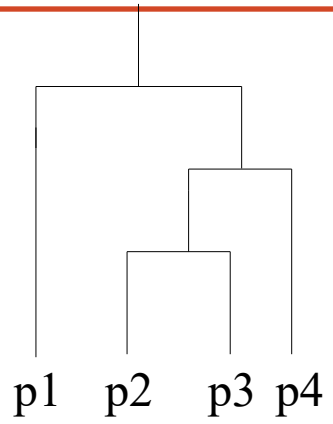


A Partitional Clustering

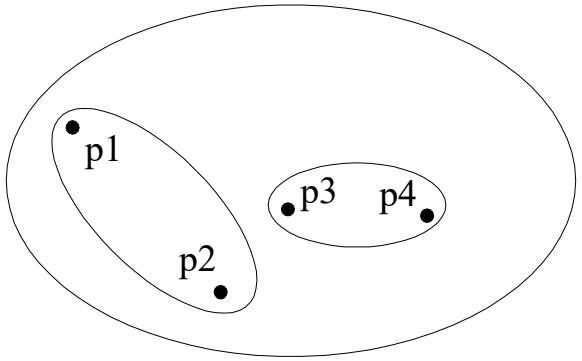
Hierarchical Clustering



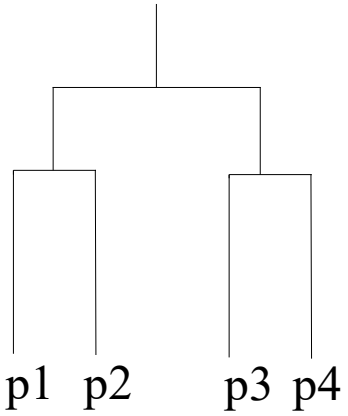
Traditional Hierarchical Clustering



Traditional Dendrogram



Non-traditional Hierarchical Clustering



Non-traditional Dendrogram

Other Distinctions Between Sets of Clusters

Exclusive versus **non-exclusive** versus **Fuzzy**

- **Overlapping** or non-exclusive clusterings, points may belong to multiple clusters:
  - Can belong to multiple classes or could be 'border' points
- **Fuzzy** clustering (one type of non-exclusive)
  - 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

Types of Clusters

a) Well-separated clusters

b) Prototype-based clusters

c) Contiguity-based clusters

d) Density-based clusters

e) Conceptual clusters

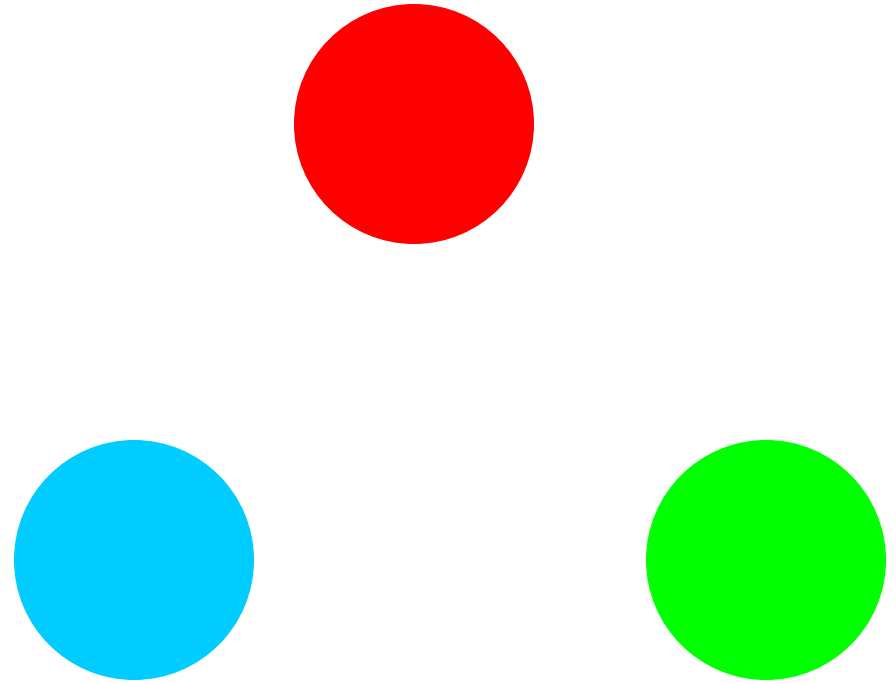
Types of Clusters: Well-Separated

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.

Clusters that are quite far from each other.

The distance between any two points in different groups is larger than the distance between any two points within a group.

Well-separated clusters do not need to be **globular**, but can have any shape.

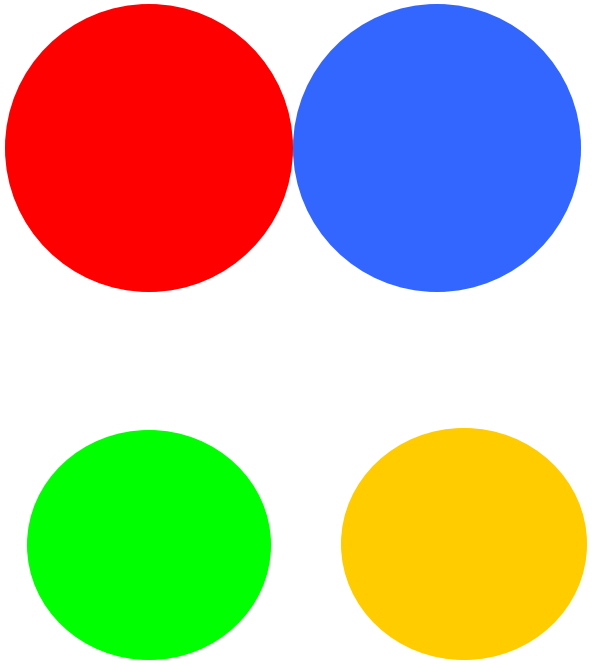


3 well-separated clusters

Types of Clusters: Prototype-Based

Prototype-based: A cluster is a set of objects such that an object in a cluster is closer (more similar) to the prototype or "**center**" of a cluster, than to the center of any other cluster

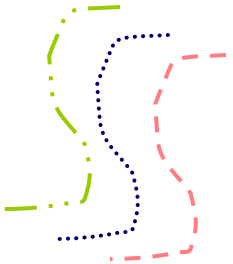
The center of a cluster is often a **centroid**, the average of all the points in the cluster, or a **medoid**, the most "representative" point of a cluster

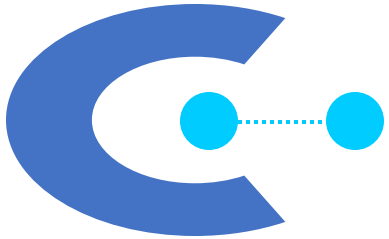


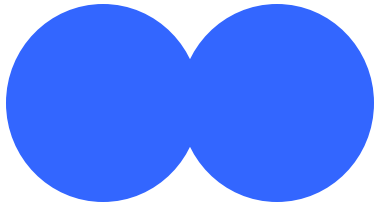
4 center-based clusters

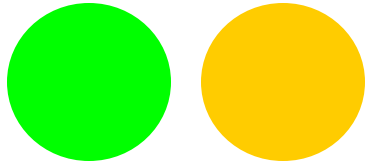
Types of Clusters: Contiguity-Based

Contiguous Cluster (Nearest neighbor or **Graph based**): 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.







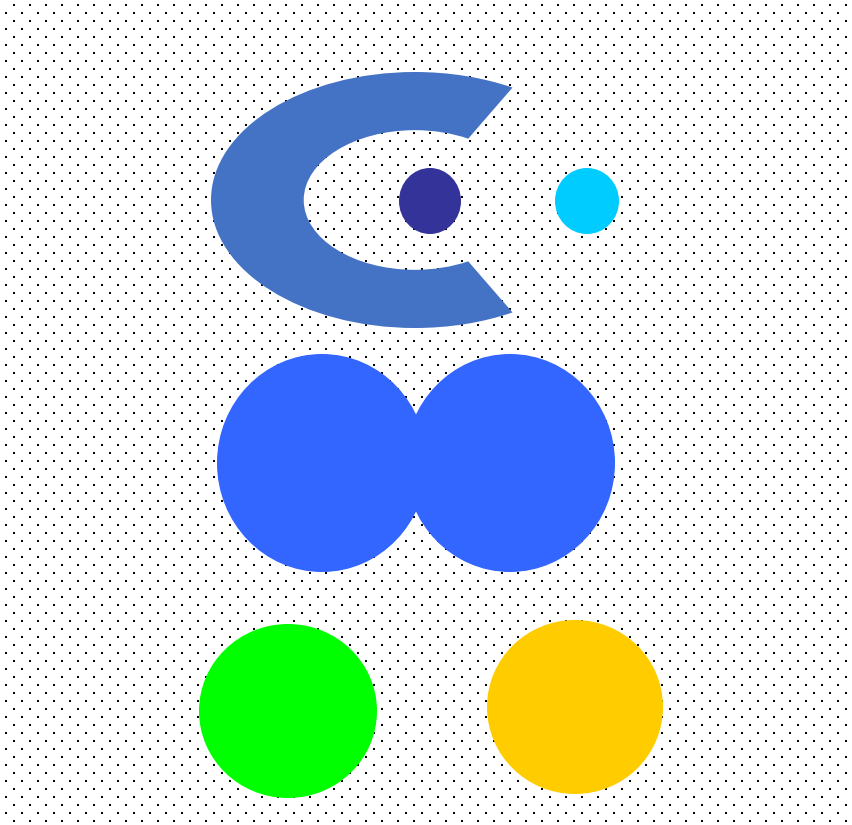


8 contiguous clusters

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.

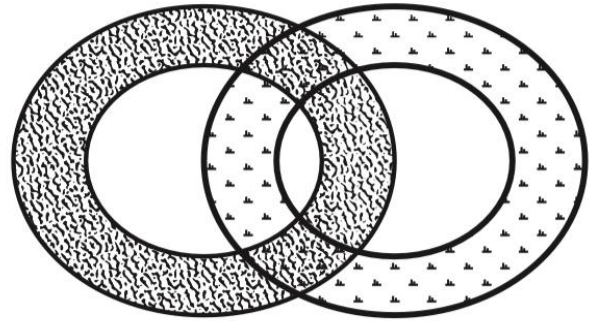


6 density-based clusters

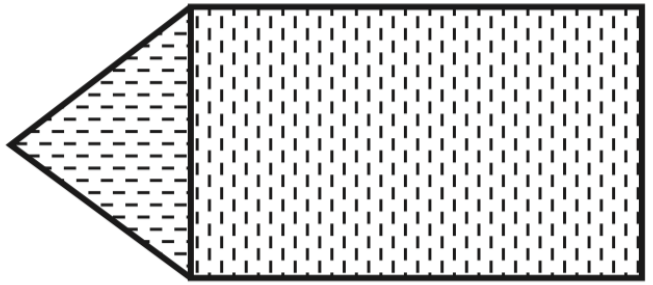
Types of Clusters: Conceptual cluster

Conceptual cluster: More generally, we can define a cluster as a set of objects that share some property.

This definition encompasses all the previous definitions of a cluster



New types of clusters --> clusters shown in figure: a triangular area is adjacent to a rectangular one



A clustering algorithm would need a very specific concept of a cluster to successfully detect these clusters.

Characteristics of the Input Data Are Important

Type of proximity or density measure

- Central to clustering
- Depends on data and application

Data characteristics that affect proximity and/or density are

- Dimensionality
- Sparseness
- Attribute type
- Special relationships in the data (autocorrelation)

Noise and Outliers

Clustering Algorithms

K-means

Hierarchical clustering

Density-based clustering

K-means Clustering

Partitional clustering approach

Number of clusters, **K**, must be specified

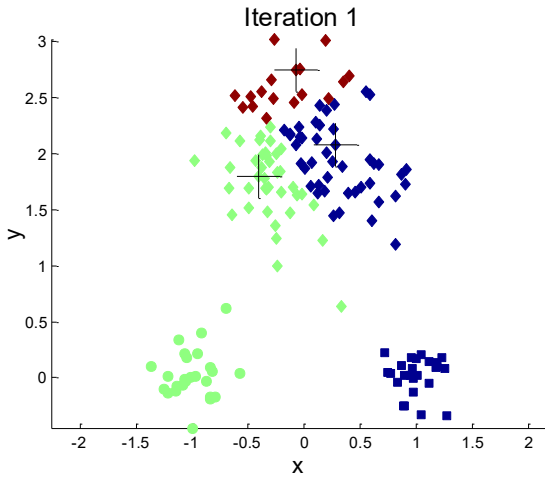
Each cluster is associated with a centroid (center point)

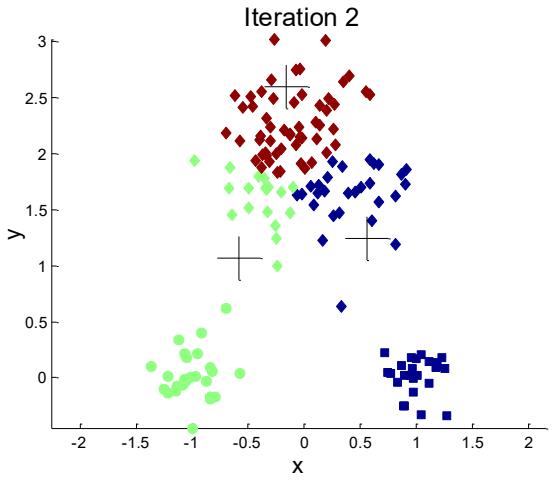
Each point is assigned to the cluster with the closest centroid

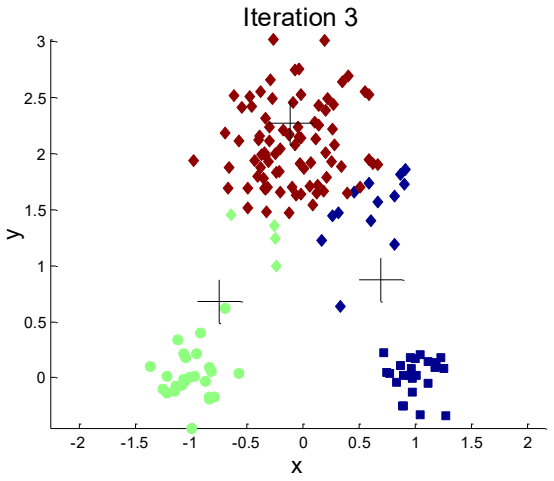
The basic algorithm is very simple

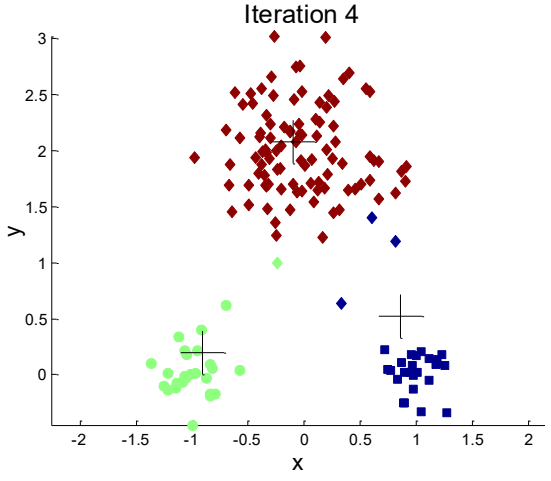
1: Select K points as the initial centroids.
2: **repeat**
3: Form K clusters by assigning all points to the closest centroid.
4: Recompute the centroid of each cluster.
5: **until** The centroids don't change

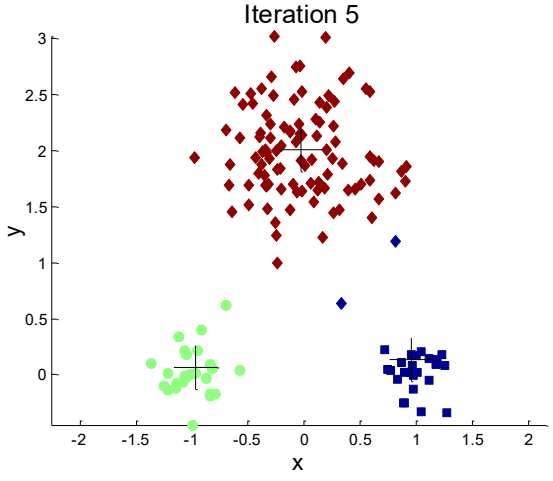
Example of K-means Clustering

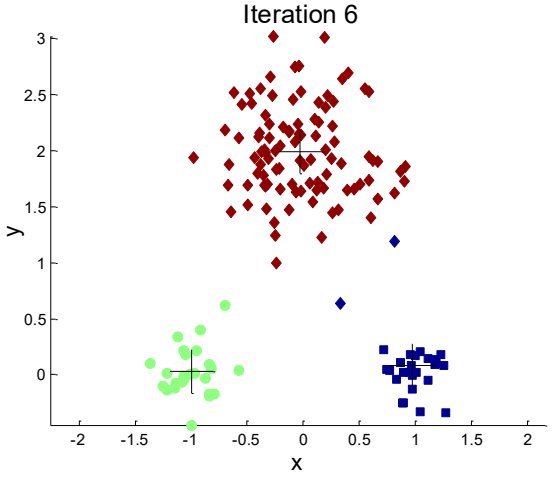












K-means Clustering – Details

Simple iterative algorithm.

- Choose initial centroids;
- repeat {assign each point to a nearest centroid; re-compute cluster centroids}
- until centroids stop changing.

Initial centroids are often chosen randomly.

- Clusters produced can vary from one run to another

The centroid is (typically) the mean of the points in the cluster, but other definitions are possible

K-means will converge for common proximity measures with appropriately defined centroid

Most of the convergence happens in the first few iterations.

- Often the stopping condition is changed to 'Until relatively few points change clusters'

K-means Objective Function

A common **objective function** (used with Euclidean distance measure) is

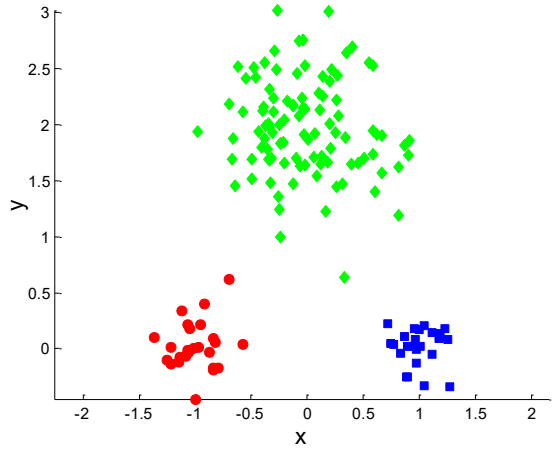
Sum of Squared Error **(SSE)**

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

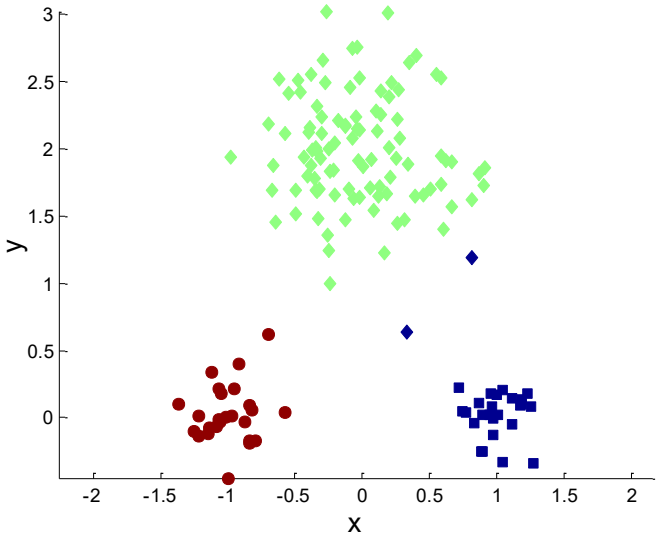
$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(m_i, x)$$

- x is a data point in cluster C_i and m_i is the centroid (mean) for cluster C_i
- SSE improves in each iteration of K-means until it reaches a local or global minima.

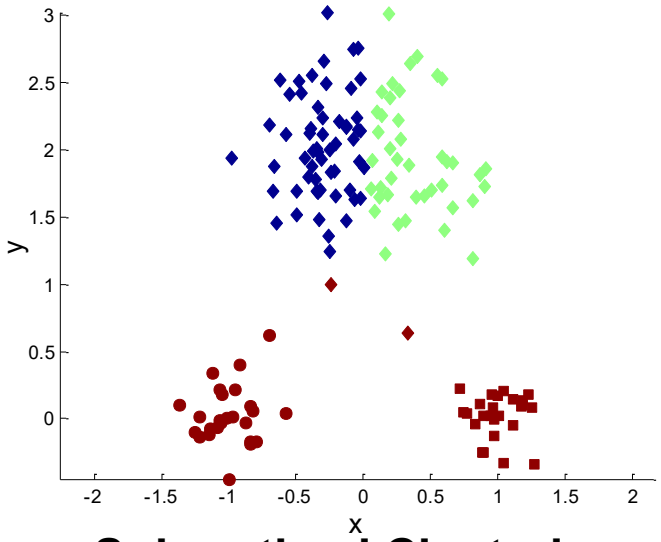
Two different K-means Clusterings



Original Points

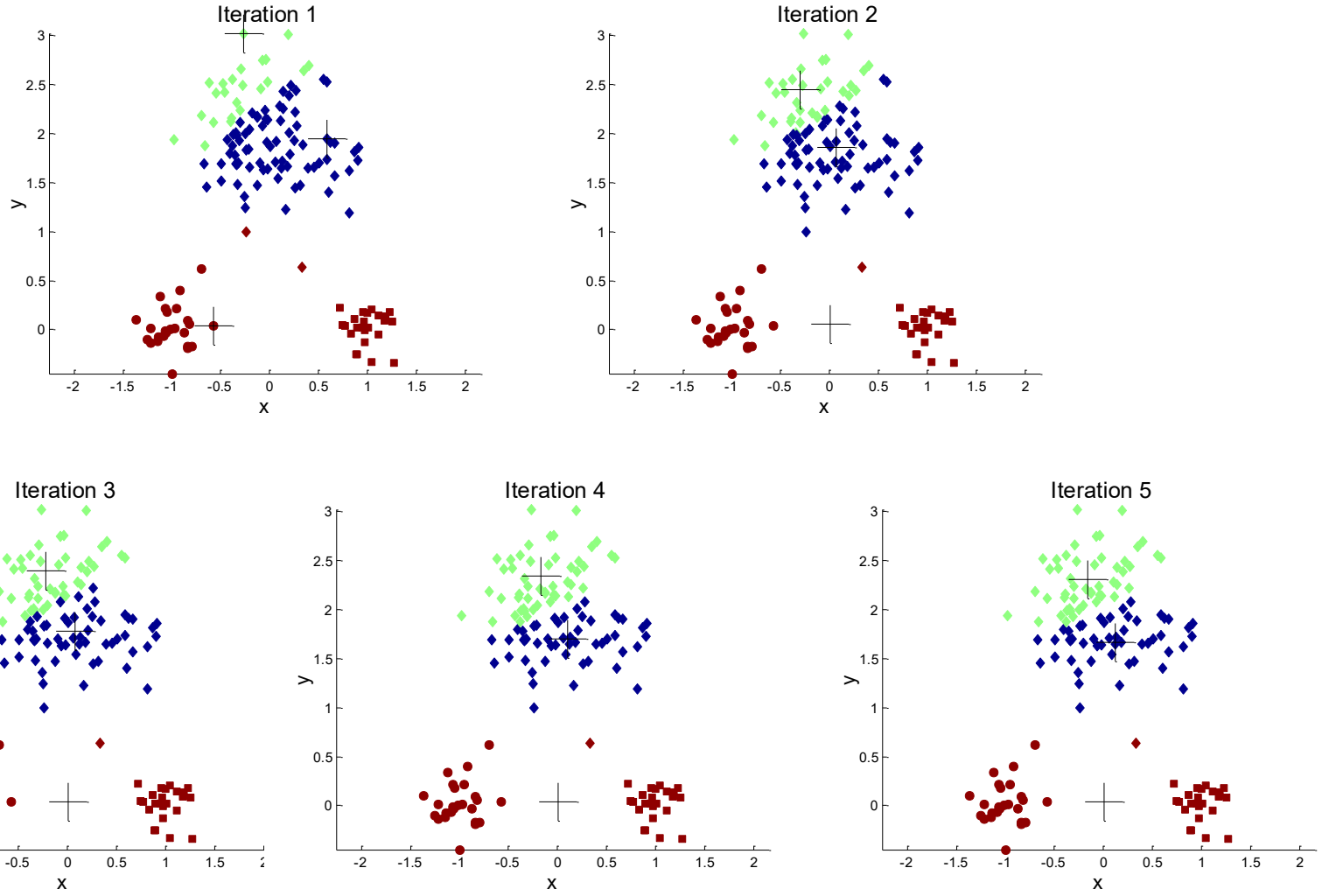


Optimal Clustering



Sub-optimal Clustering

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.

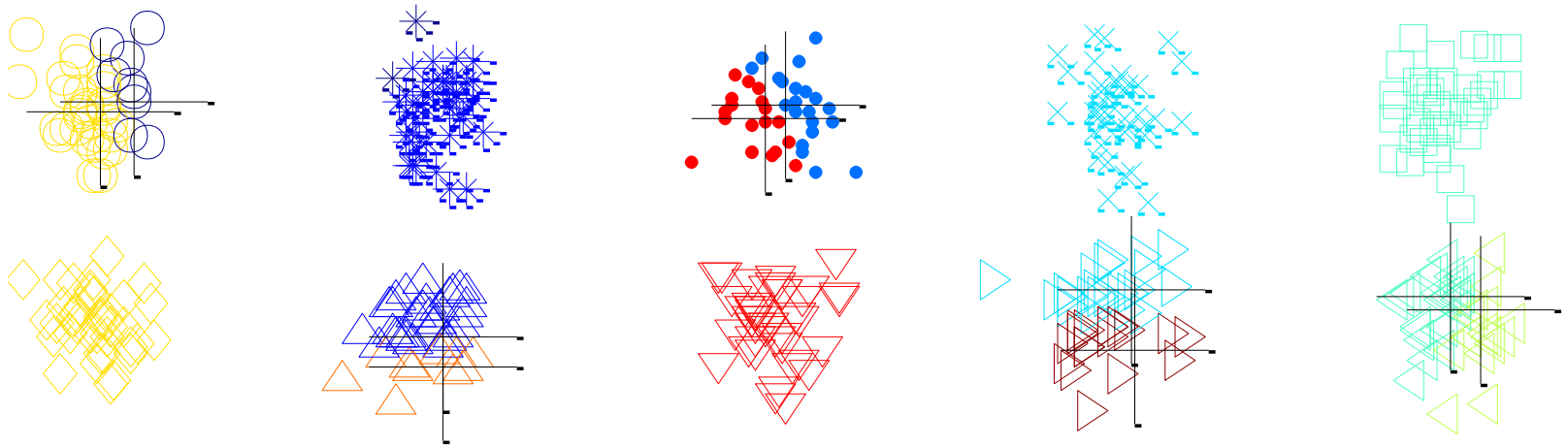
- Chance is relatively small when K is large
- If clusters are the same size, n, then

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

- 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

Limits in random initialization: 10 Clusters Example

The data consists of 5 pairs of clusters, where the clusters in each (top-bottom) pair are closer to each other than to the clusters in the other pair.



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

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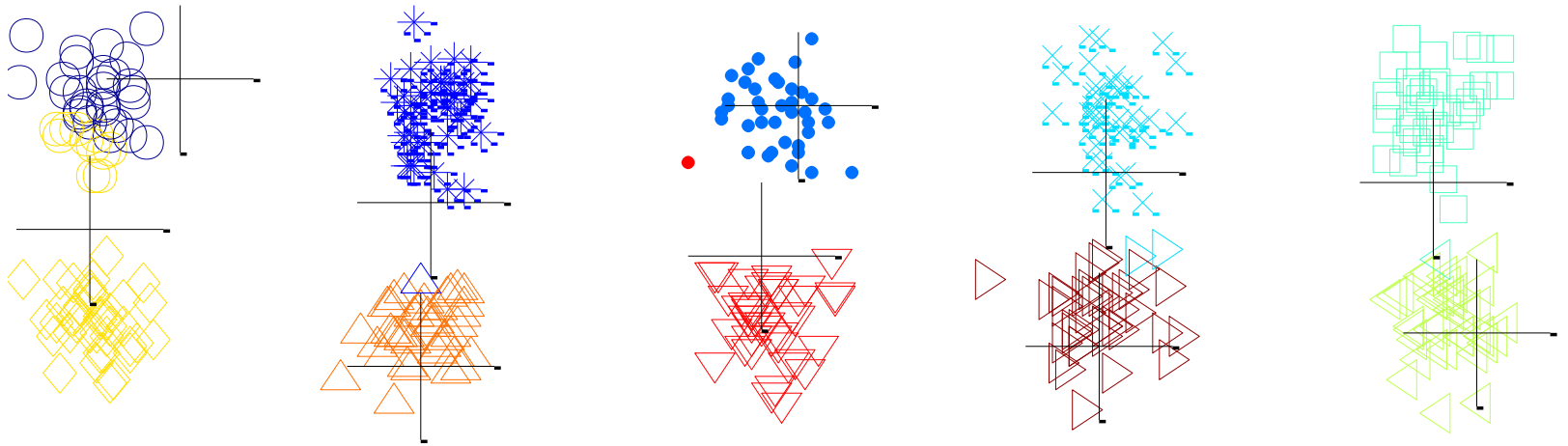

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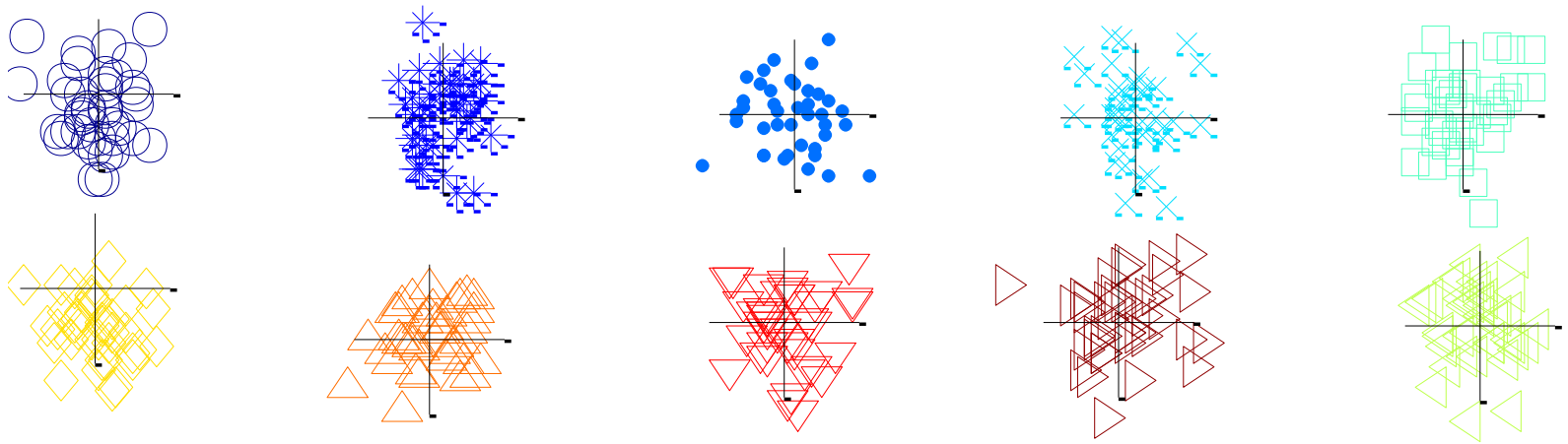

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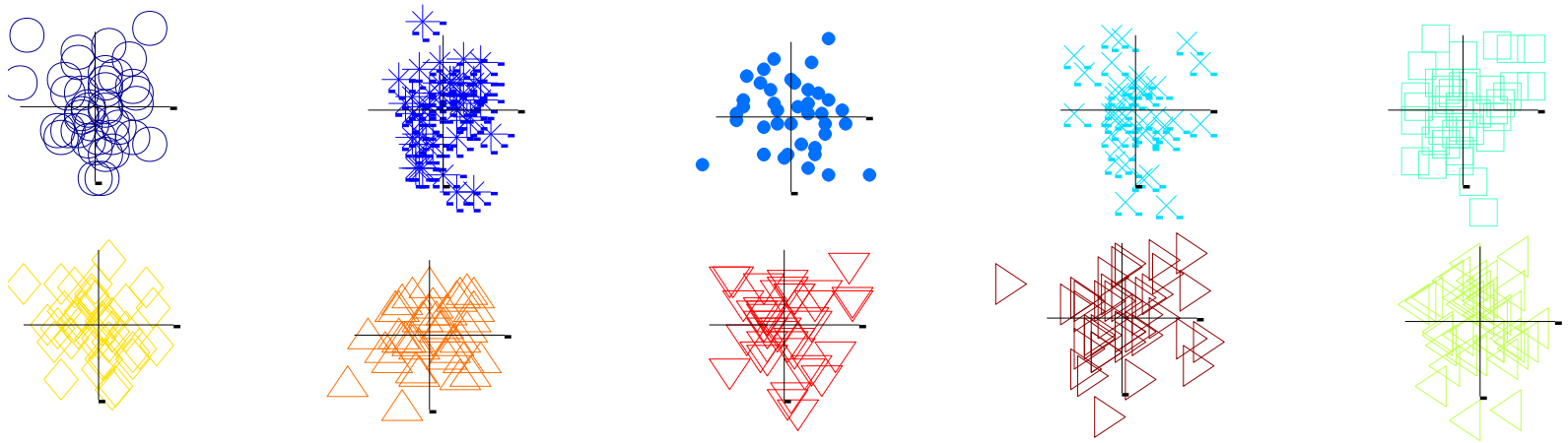

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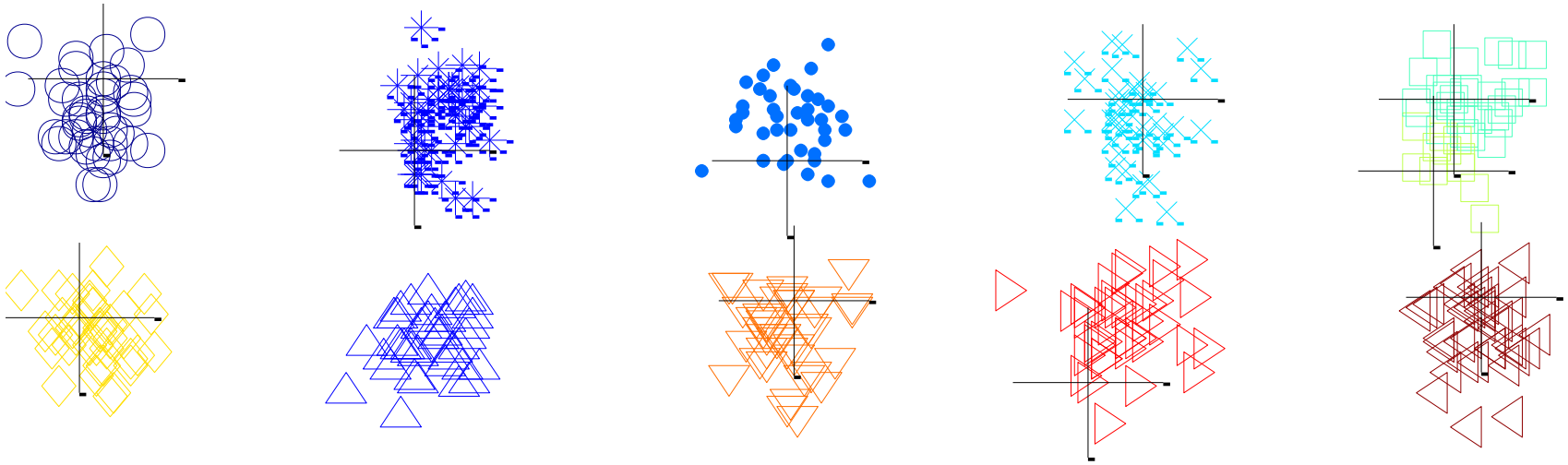

Starting with some pairs of clusters having three initial centroids, while other have only one.

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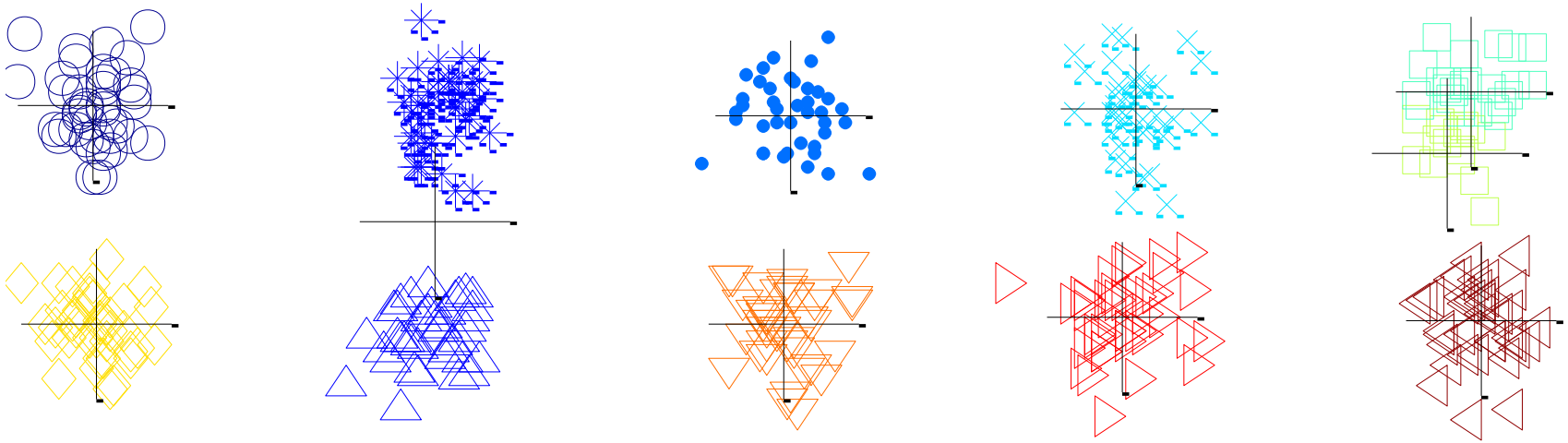

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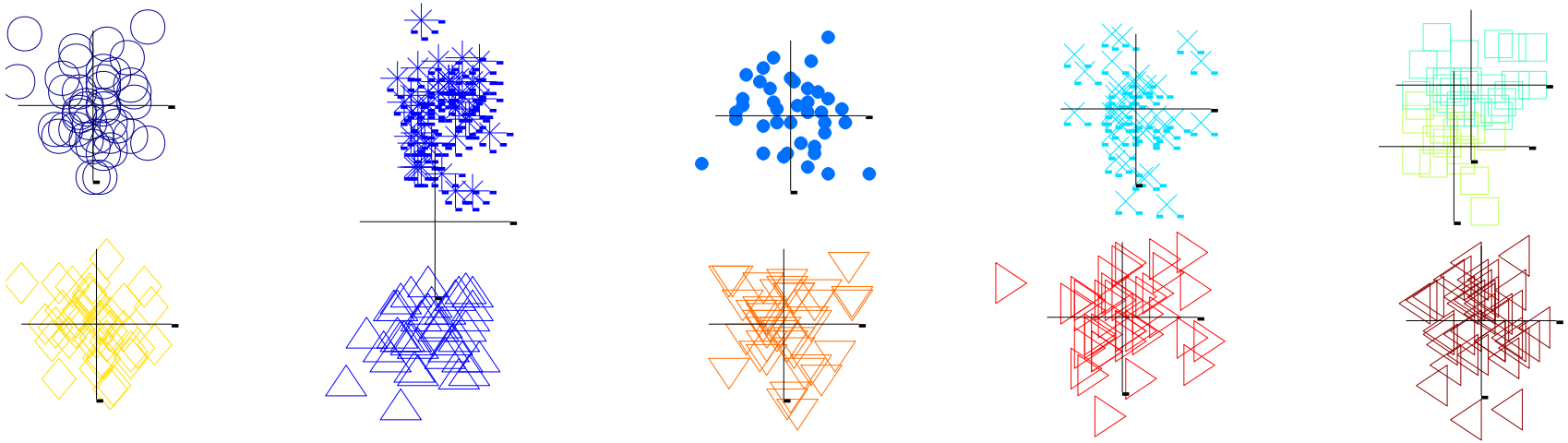

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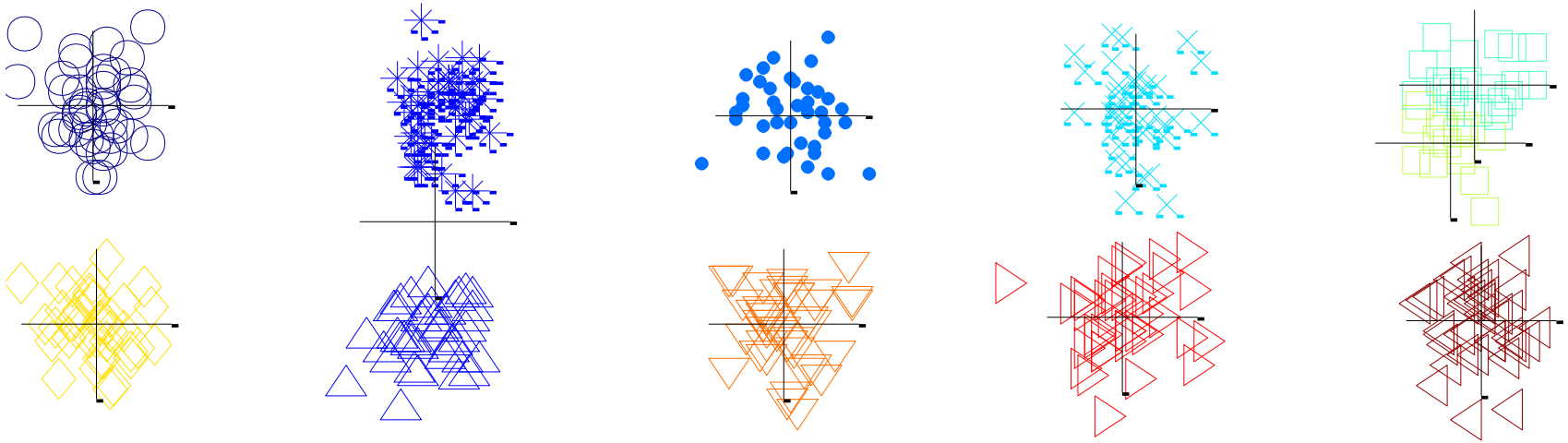


Starting with some pairs of clusters having three initial centroids, while other have only one.

Solutions to Initial Centroids Problem

Multiple runs

- Helps, but probability is not on your side

Use some strategy to select the k initial centroids and then select among these initial centroids

- Select most widely separated
    - K-means++ is a robust way of doing this selection
- Use hierarchical clustering to determine initial centroids

Bisecting K-means

- Not as susceptible to initialization issues

K-means++

This approach can be slower than random initialization, but very consistently produces better results in terms of SSE

To select a set of initial centroids, *C*, perform the following

1. Select an initial point at random to be the first centroid
2. For k – 1 steps
3. For each of the N points, x_i, $1 \leq i \leq N$, find the minimum squared distance to the currently selected centroids, C_1, ..., C_j, $1 \leq j < k$, i.e., $\min_j d^2(C_j, x_i)$
4. Randomly select a new centroid by choosing a point with probability proportional to $\frac{\min_j d^2(C_j, x_i)}{\sum_i \min_j d^2(C_j, x_i)}$ is
5. End For

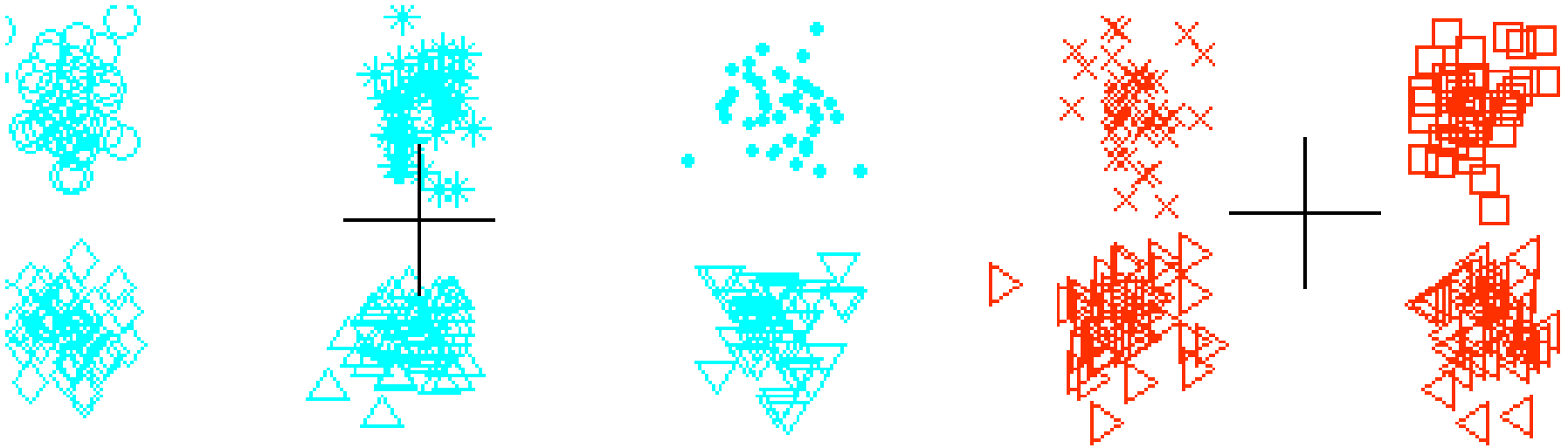
Bisecting K-means

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

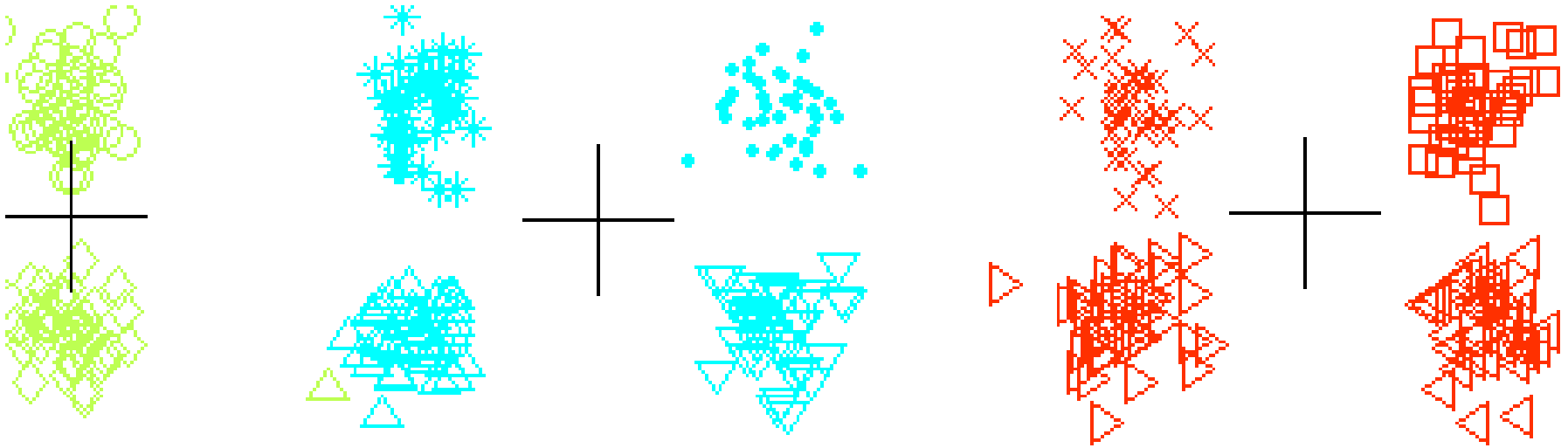
1: Initialize the list of clusters to contain the cluster containing all points.
2: **repeat**
3: Select a cluster from the list of clusters
4: **for** $i = 1$ to *number_of_iterations* **do**
5: Bisect the selected cluster using basic K-means
6: **end for**
7: Add the two clusters from the bisection with the lowest SSE to the list of clusters.
8: **until** Until the list of clusters contains K clusters

CLUTO: http://glaros.dtc.umn.edu/gkhome/cluto/cluto/overview

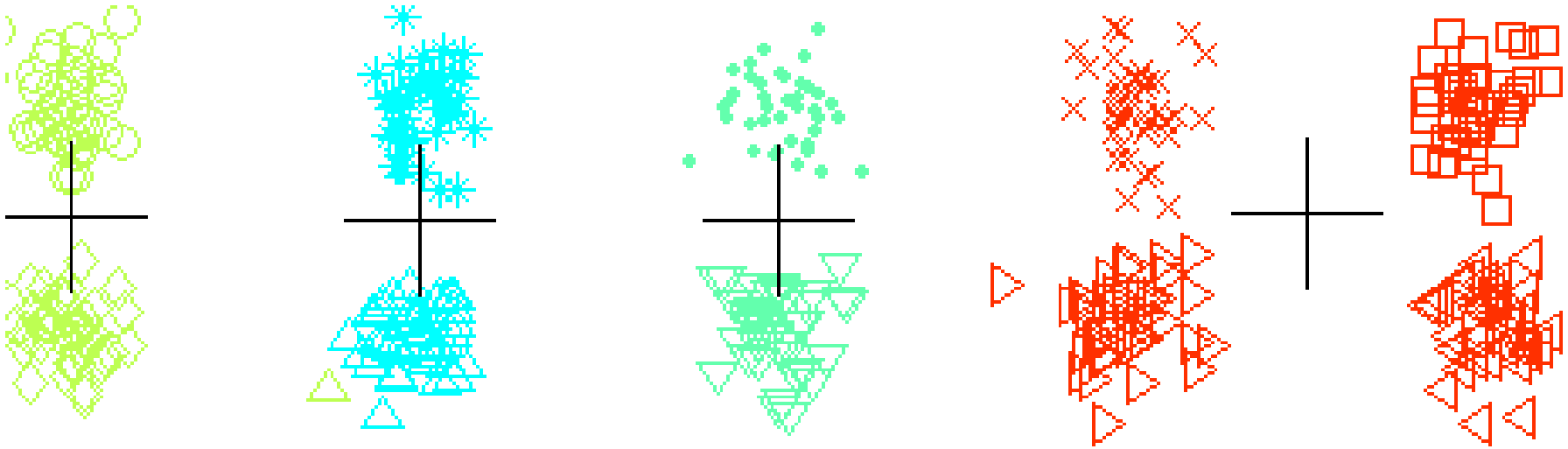
Bisecting K-means Example



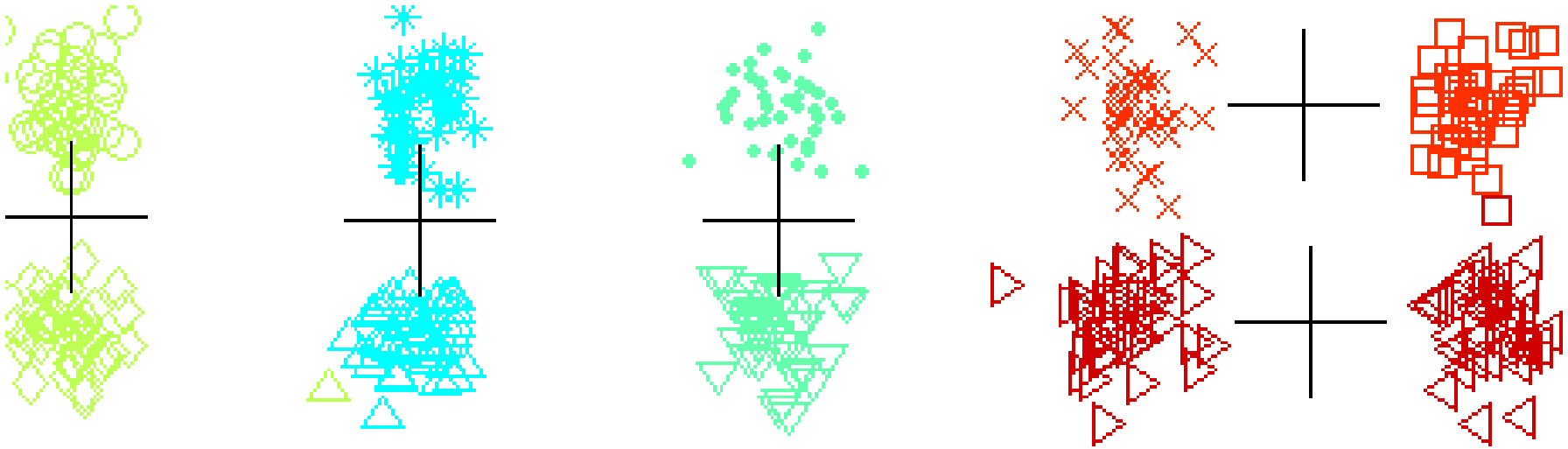
Bisecting K-means Example



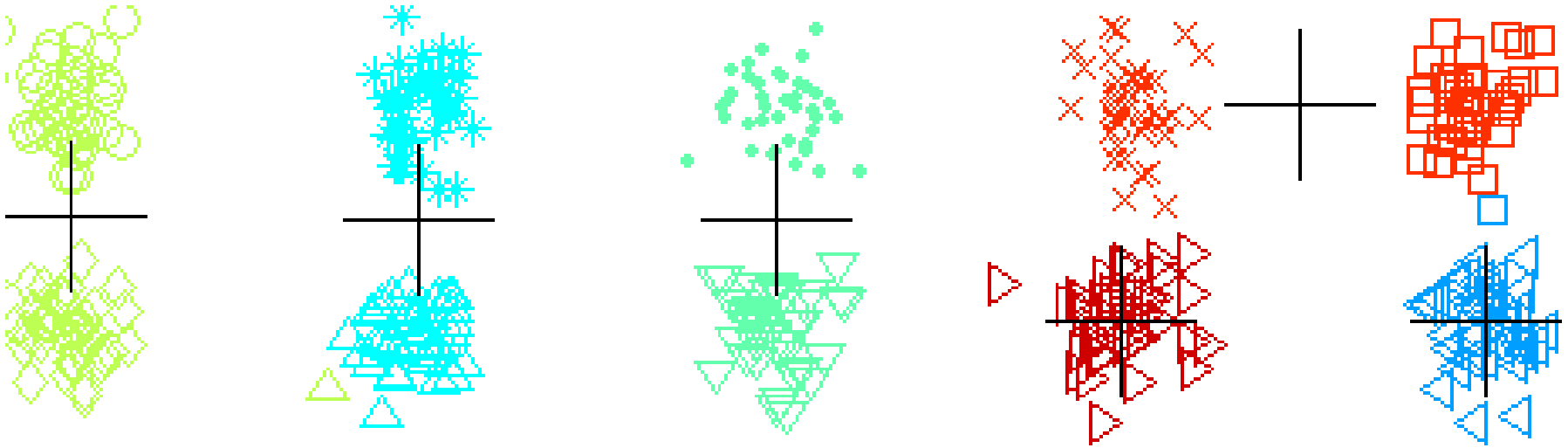
Bisecting K-means Example



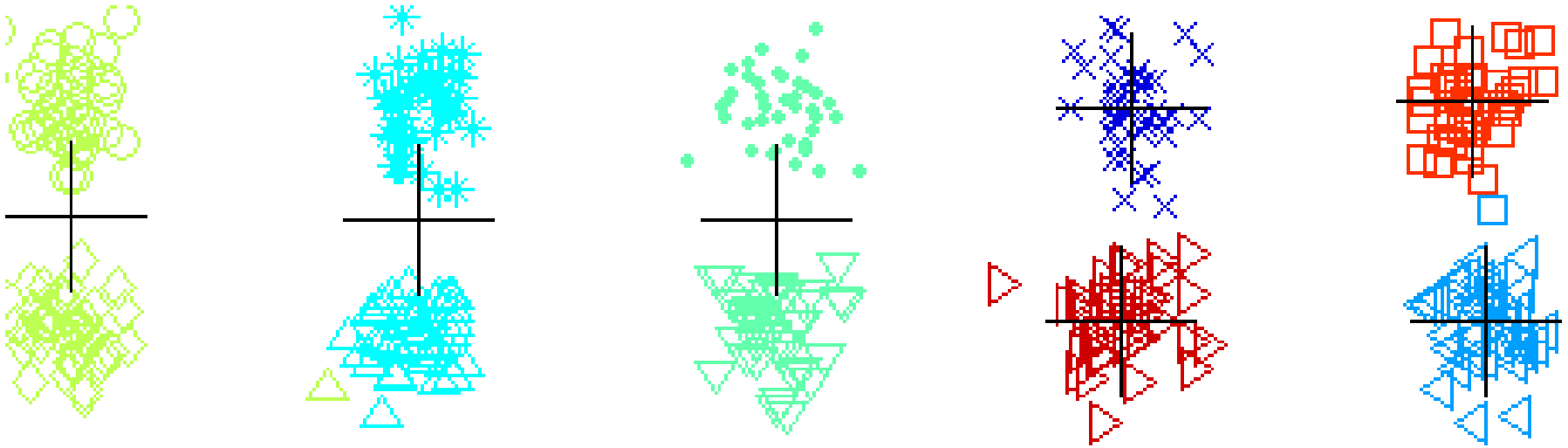
Bisecting K-means Example



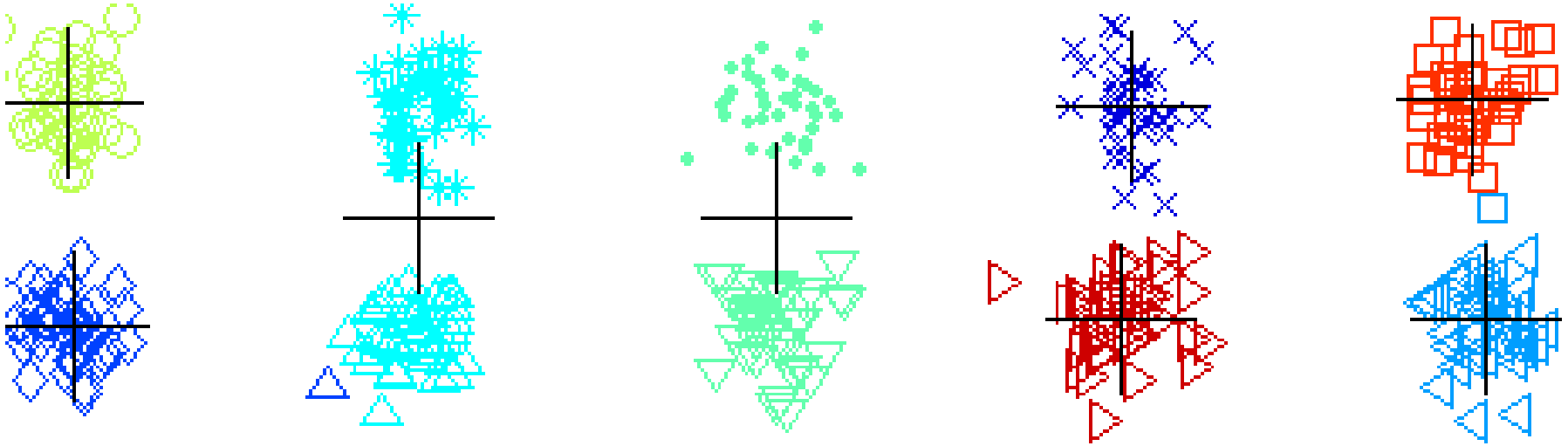
Bisecting K-means Example



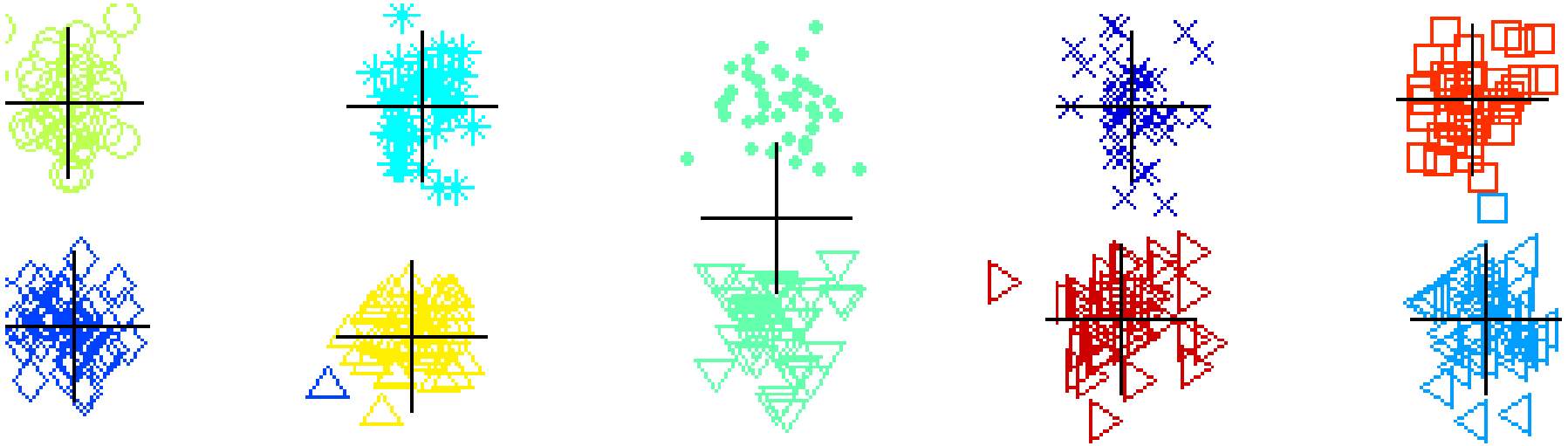
Bisecting K-means Example



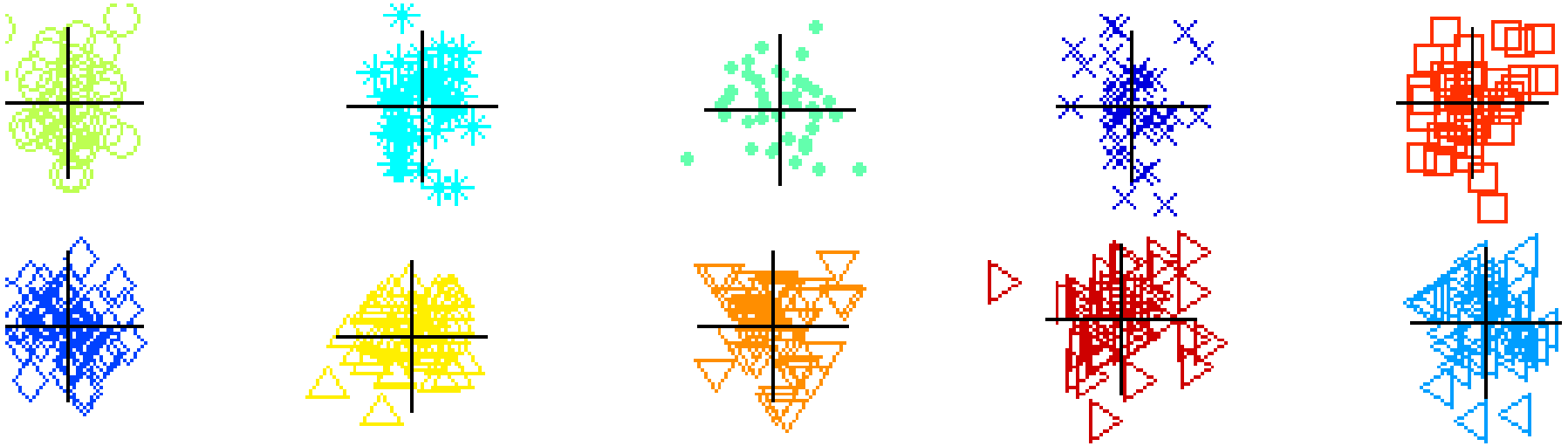
Bisecting K-means Example



Bisecting K-means Example



Bisecting K-means Example



Limitations of K-means

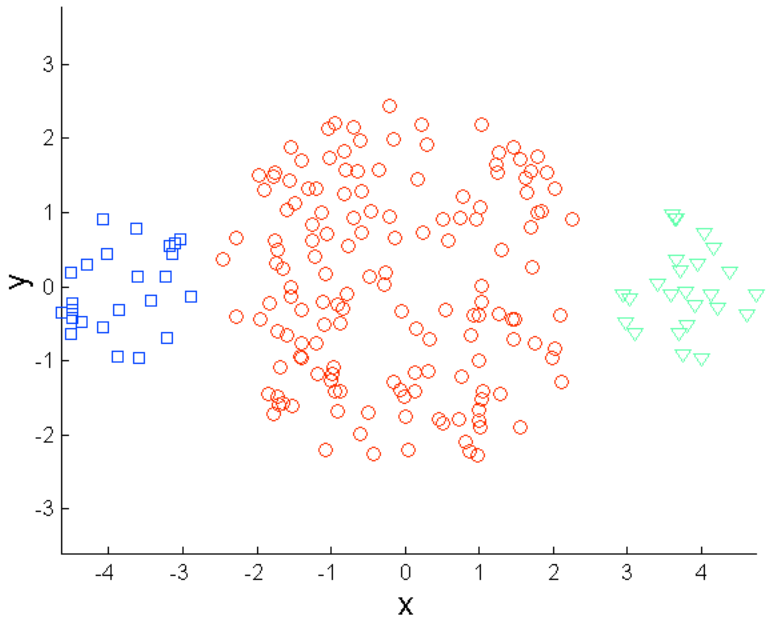
K-means has problems when clusters are of differing

- Sizes
- Densities
- Non-globular shapes

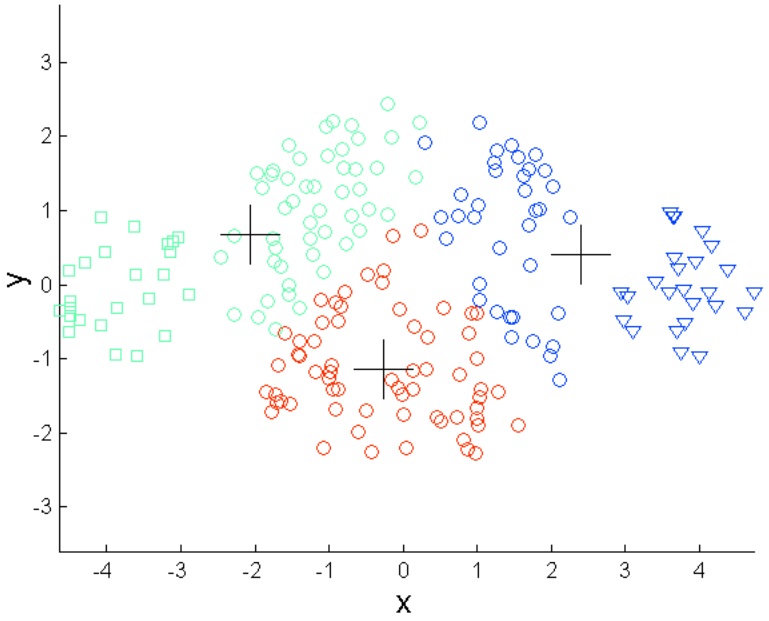
K-means has problems when the data contains outliers.

- One possible solution is to remove outliers before clustering

Limitations of K-means: Differing Sizes

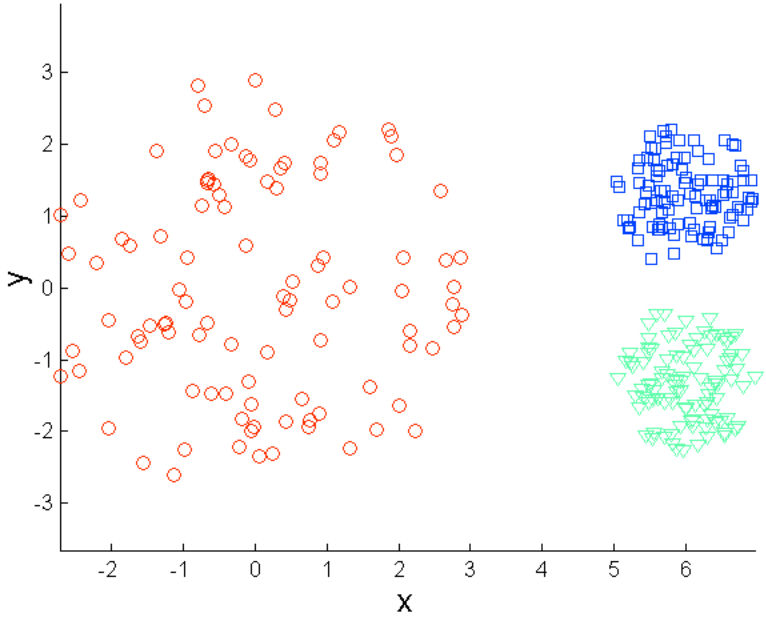


Original Points

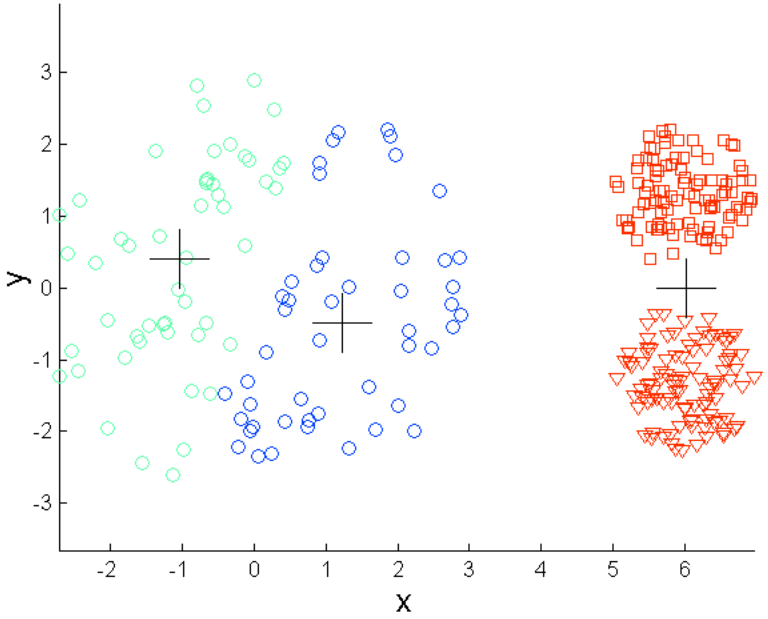


K-means (3 Clusters)

Limitations of K-means: Differing Density

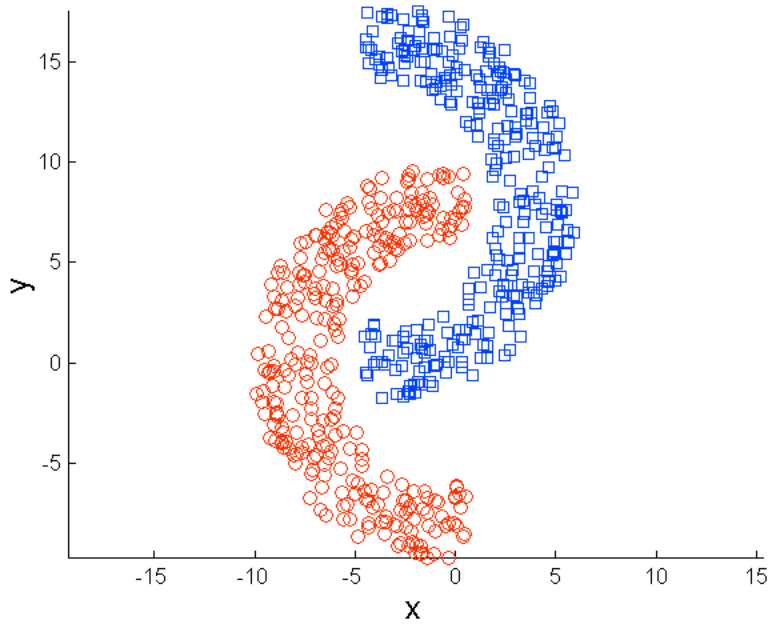


Original Points

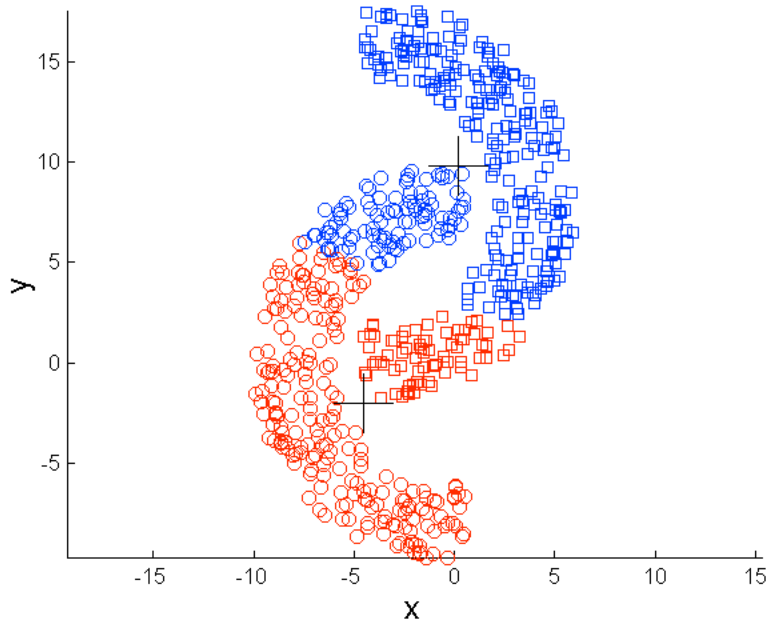


K-means (3 Clusters)

Limitations of K-means: Non-globular Shapes



Original Points

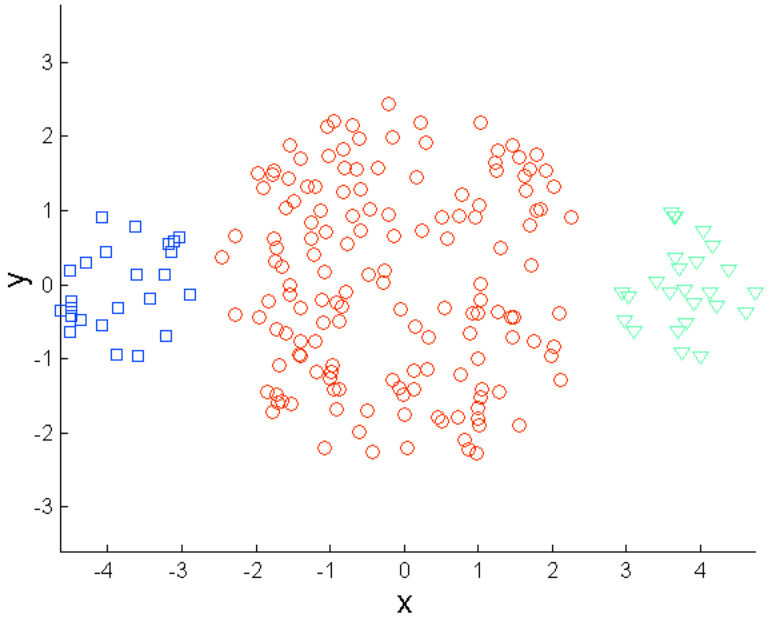


K-means (2 Clusters)

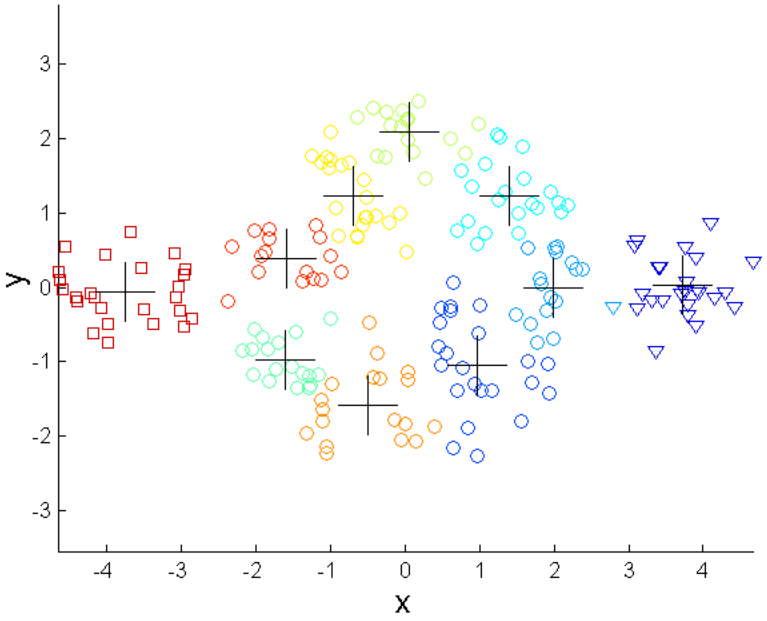
Overcoming K-means Limitations

One solution is to find a **large number of clusters** such that each of them represents a part of a natural cluster.

Small clusters need to be put together in a **post-processing** step.



Original Points



K-means Clusters

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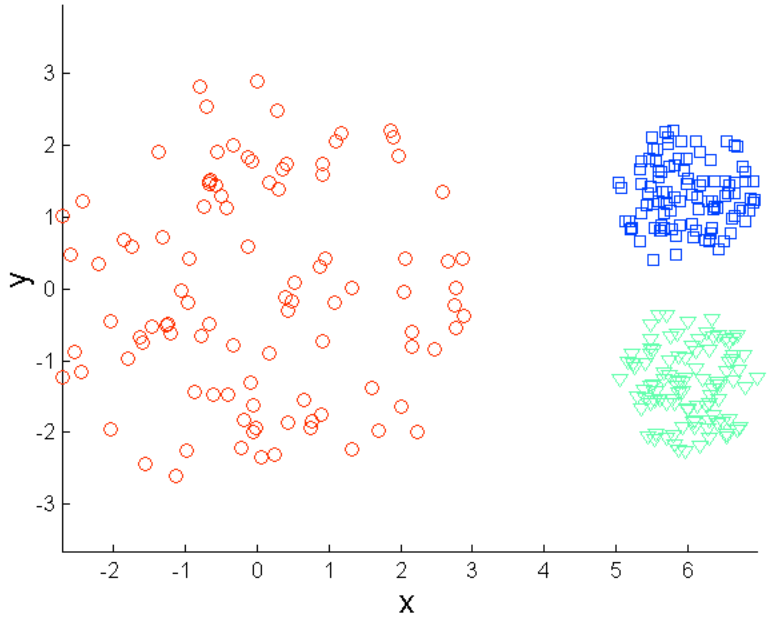
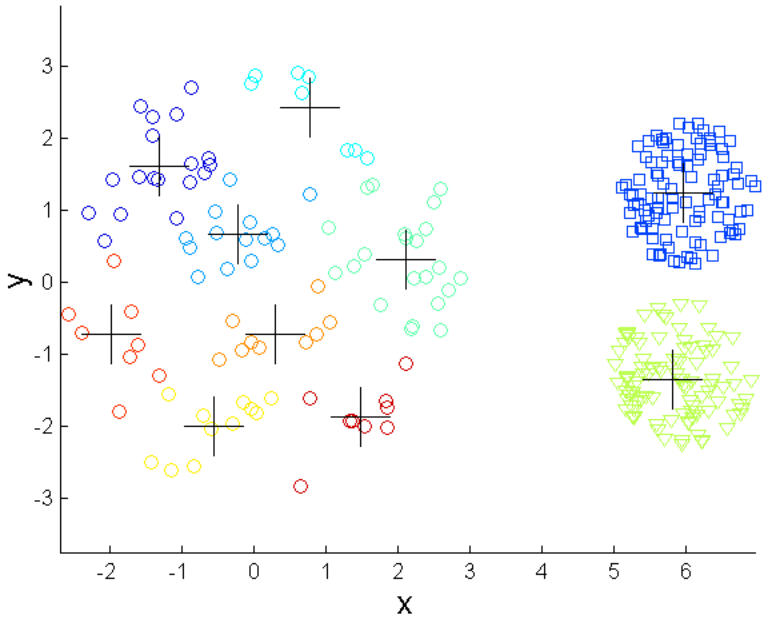


Original Points



K-means Clusters

Overcoming K-means Limitations

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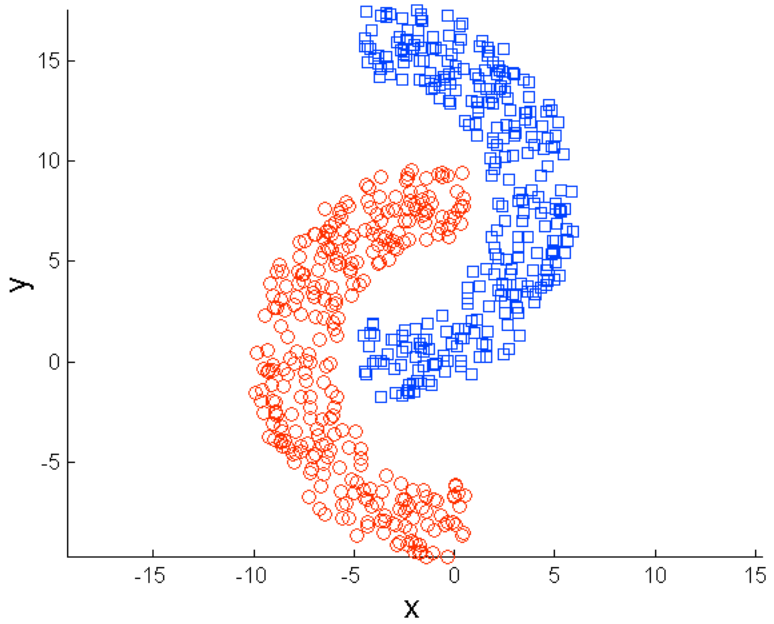
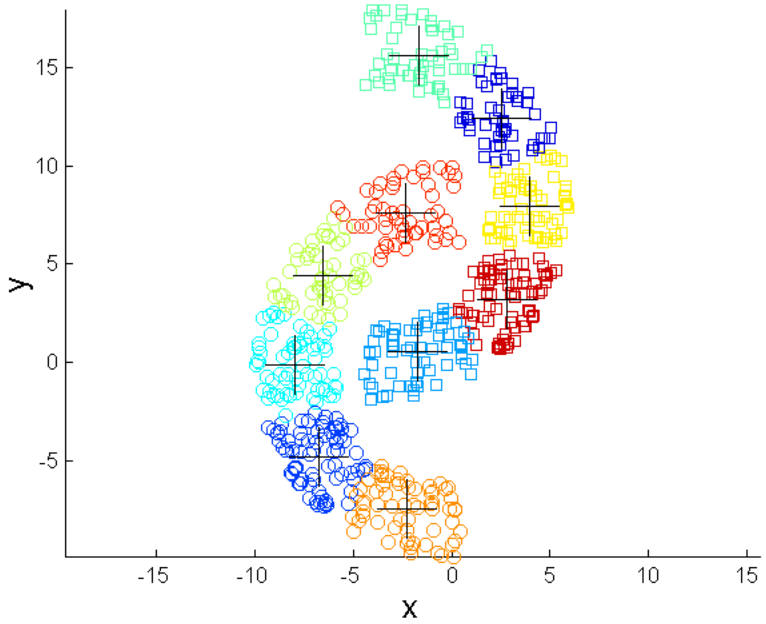


Original Points

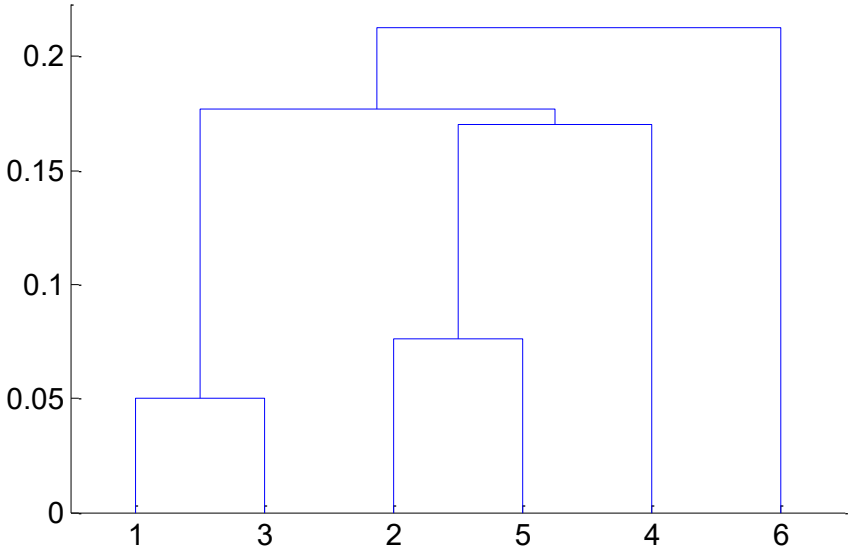


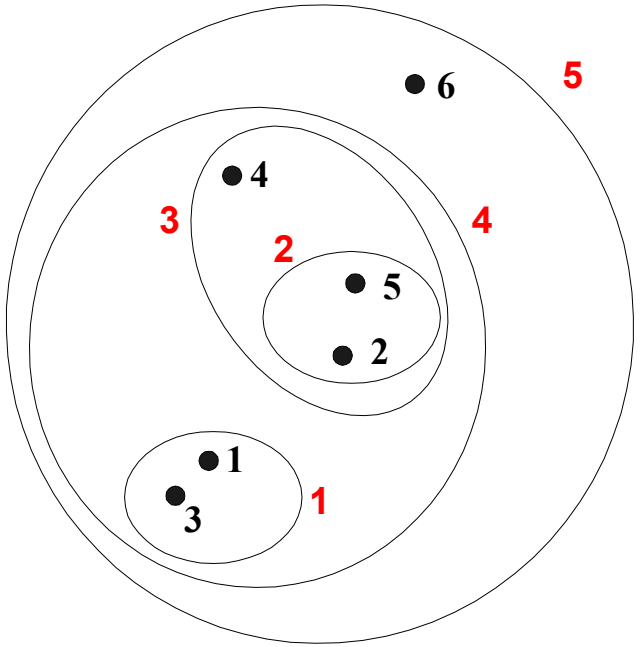
K-means Clusters

Hierarchical Clustering

Produces a set of nested clusters organized as a hierarchical tree (**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 dendrogram 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 an individual 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

Key Idea: Successively merge closest cluster

Basic algorithm

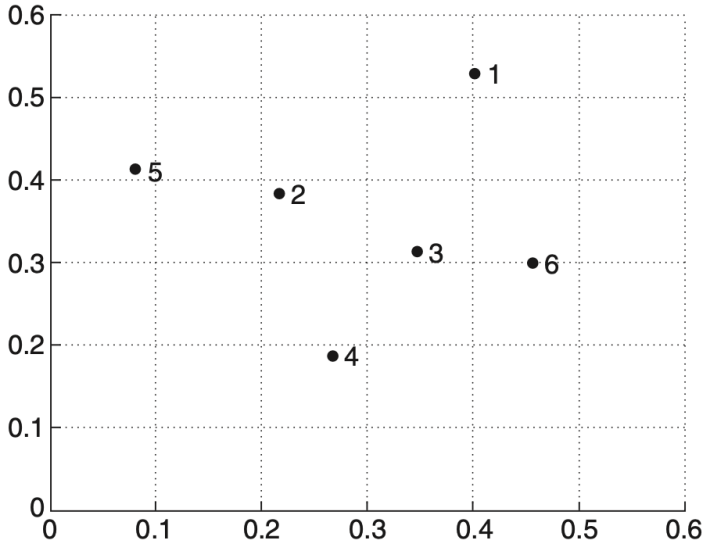
1. Compute the proximity matrix
2. Let each data point be a cluster
3. **Repeat**
4. Merge the two closest clusters
5. Update the proximity matrix
6. **Until** only a single cluster remains

Key operation is the computation of the proximity of two clusters

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

Proximity matrix

Start with clusters of individual points and a proximity matrix

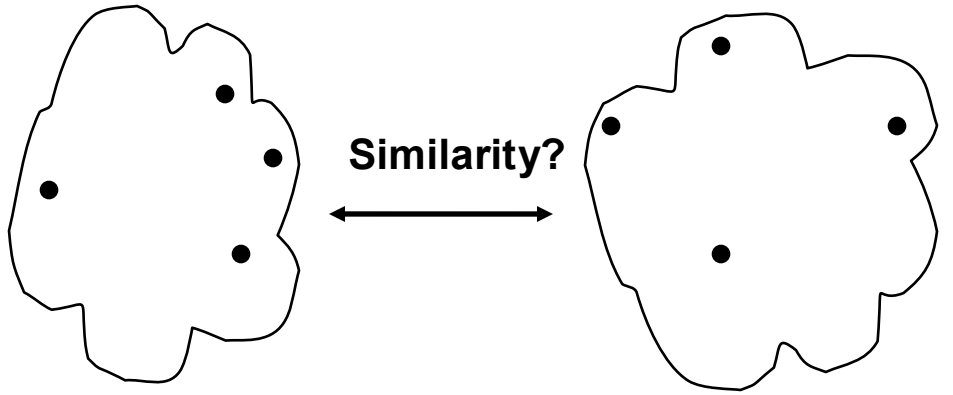


Point	x Coordinate	y Coordinate
p1	0.4005	0.5306
p2	0.2148	0.3854
p3	0.3457	0.3156
p4	0.2652	0.1875
p5	0.0789	0.4139
p6	0.4548	0.3022

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

Type of similarity

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



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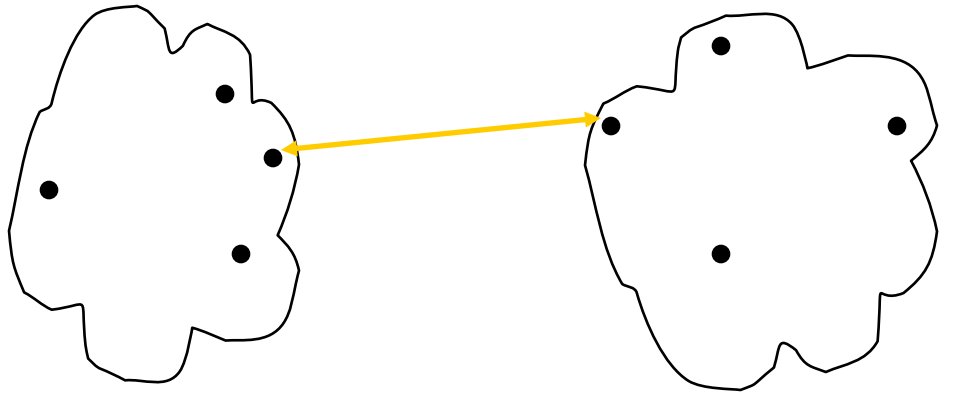

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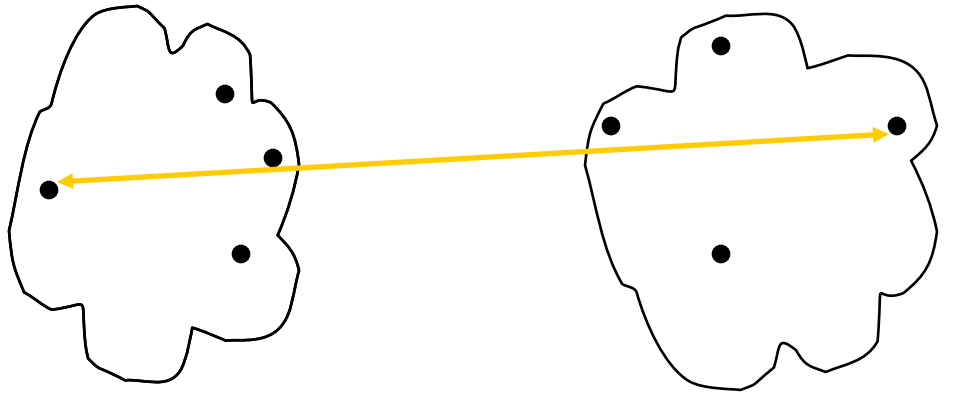

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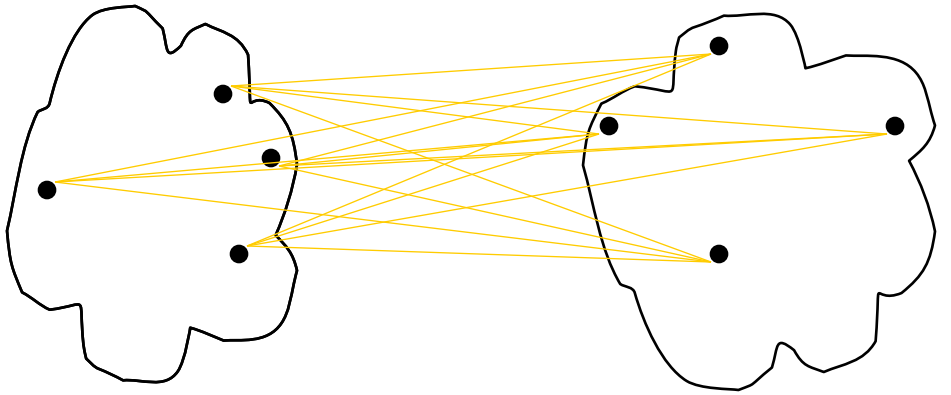

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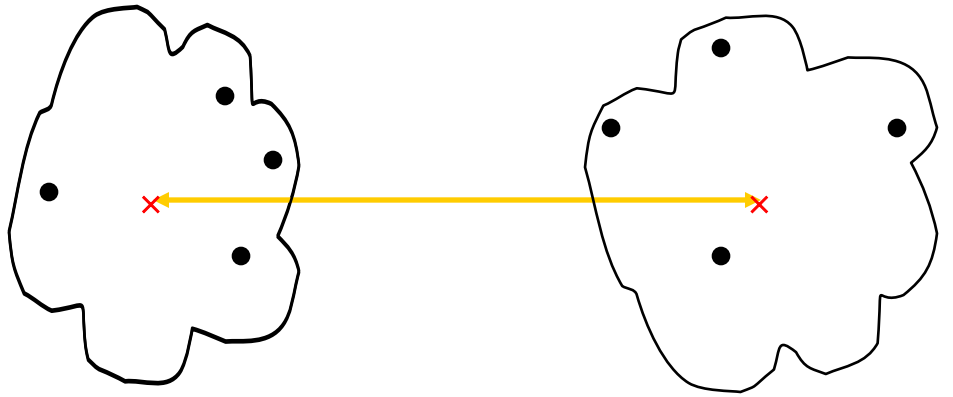
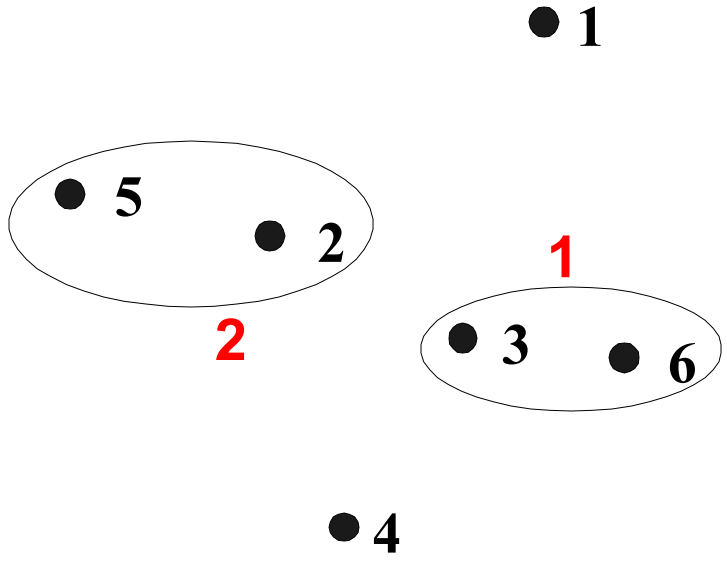


MIN or Single Link

Proximity of two clusters is defined as the minimum of the distance (maximum of the similarity) between any two points in the two different clusters

$$
\begin{aligned}
dist(\{3,6\},\{2,5\}) &= \min(dist(3,2), dist(6,2), dist(3,5), dist(6,5)) \\
&= \min(0.15, 0.25, 0.28, 0.39) \\
&= 0.15.
\end{aligned}
$$



	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

Distance Matrix:

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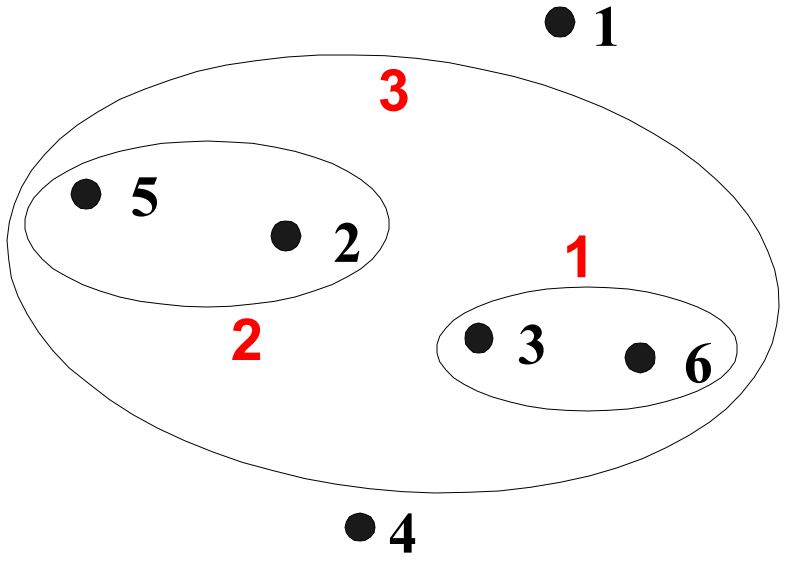
&= 0.15.
\end{aligned}
$$



	p1	p2	p3	p4	p5	p6
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p3	0.22	0.15	0.00	0.15	0.28	0.11
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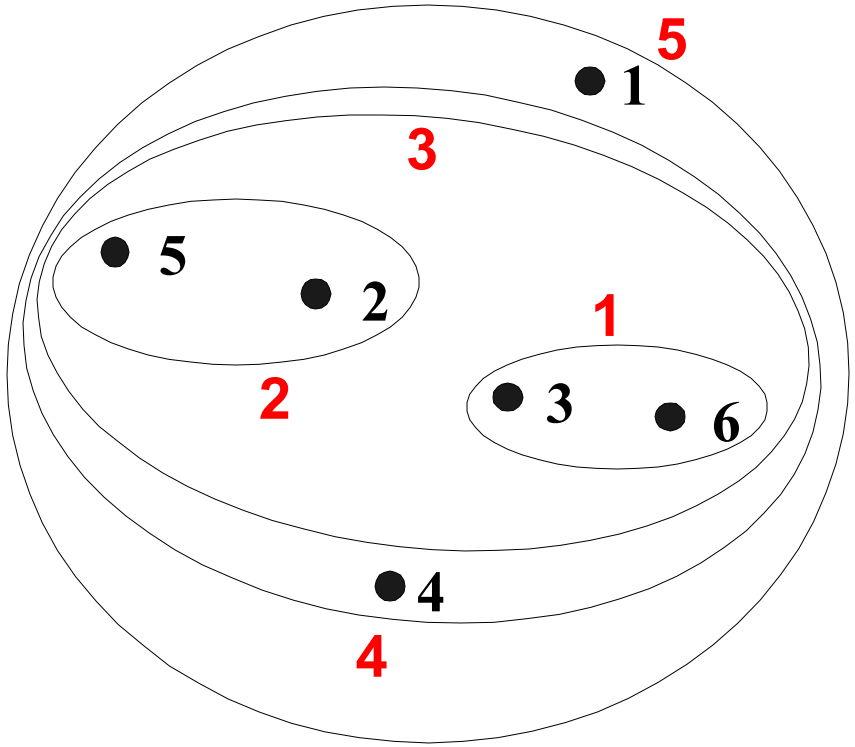
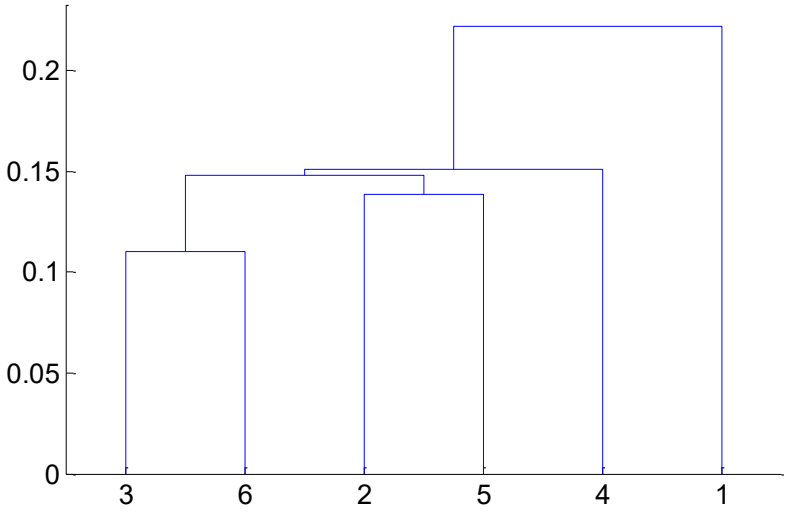
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

Distance Matrix:

MIN or Single Link



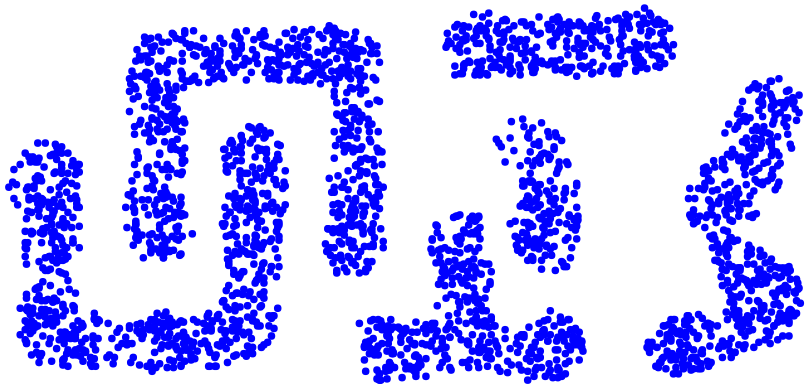
Nested Clusters



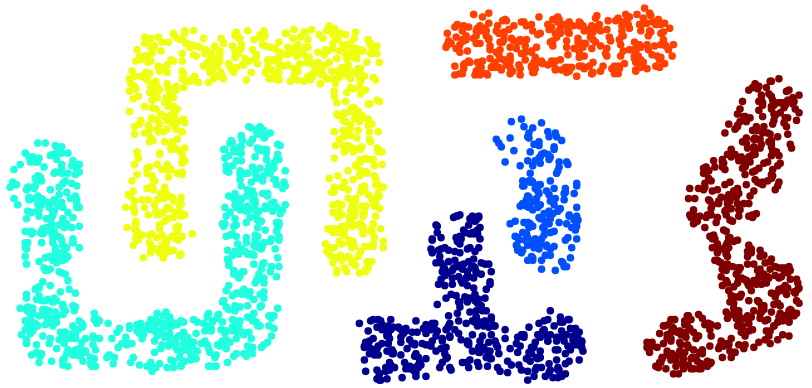
Dendrogram

MIN or Single Link: Strength

- **Can handle non-elliptical shapes**



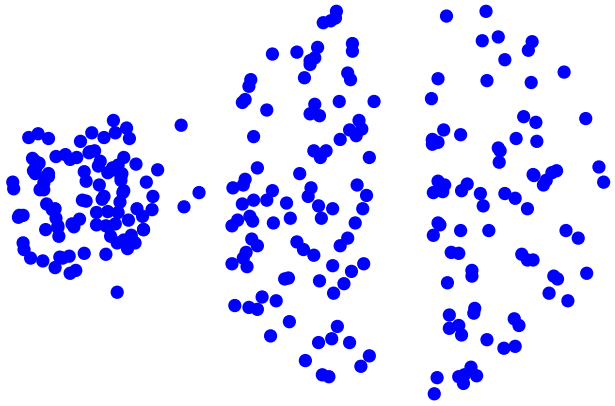
Original Points



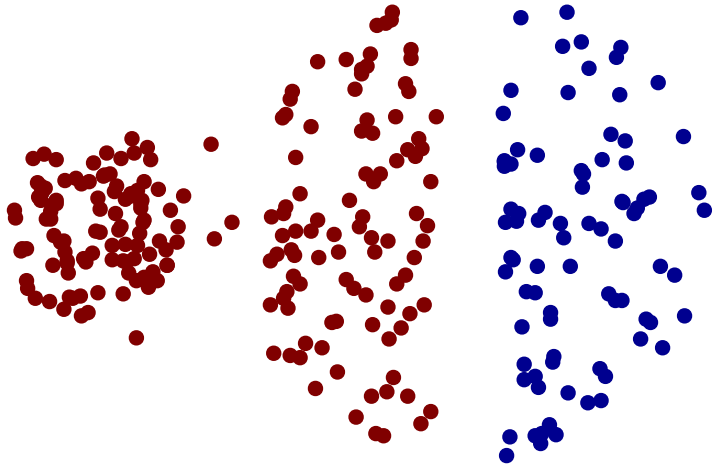
Six Clusters

MIN or Single Link: Limitations

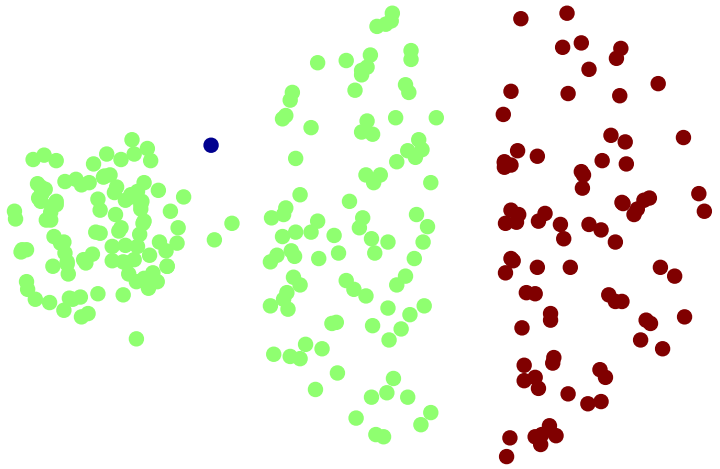
- **Sensitive to noise**



Original Points



Two Clusters



Three Clusters

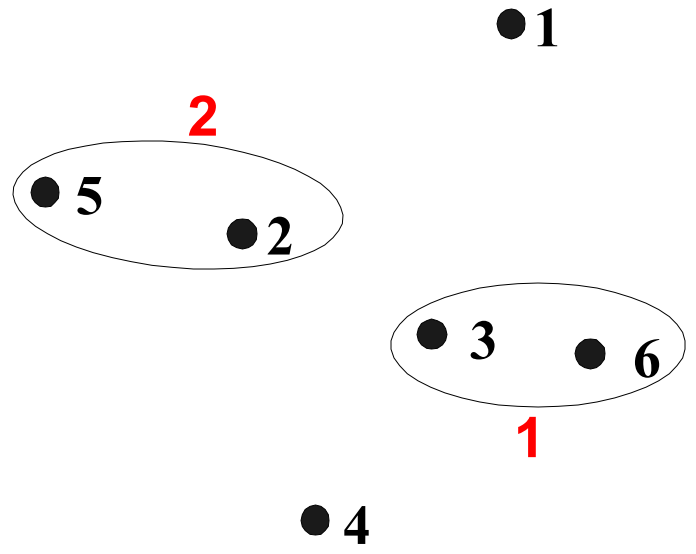
MAX or Complete Linkage

Proximity of two clusters is defined as the maximum of the distance (minimum of the similarity) between any two points in the two different clusters

$$
\begin{aligned}
dist(\{3,6\},\{4\}) &= \max(dist(3,4), dist(6,4)) \\
&= \max(0.15, 0.22) \\
&= 0.22. \\
dist(\{3,6\},\{2,5\}) &= \max(dist(3,2), dist(6,2), dist(3,5), dist(6,5)) \\
&= \max(0.15, 0.25, 0.28, 0.39) \\
&= 0.39. \\
dist(\{3,6\},\{1\}) &= \max(dist(3,1), dist(6,1)) \\
&= \max(0.22, 0.23) \\
&= 0.23.
\end{aligned}
$$

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

Distance Matrix:



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dist(\{3,6\},\{1\}) &= \max(dist(3,1), dist(6,1)) \\
&= \max(0.22, 0.23) \\
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\end{aligned}
$$

	p1	p2	p3	p4	p5	p6
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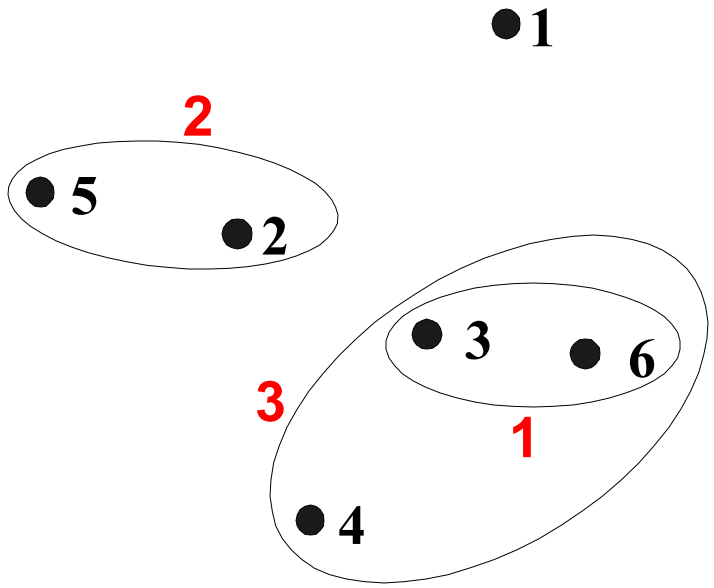
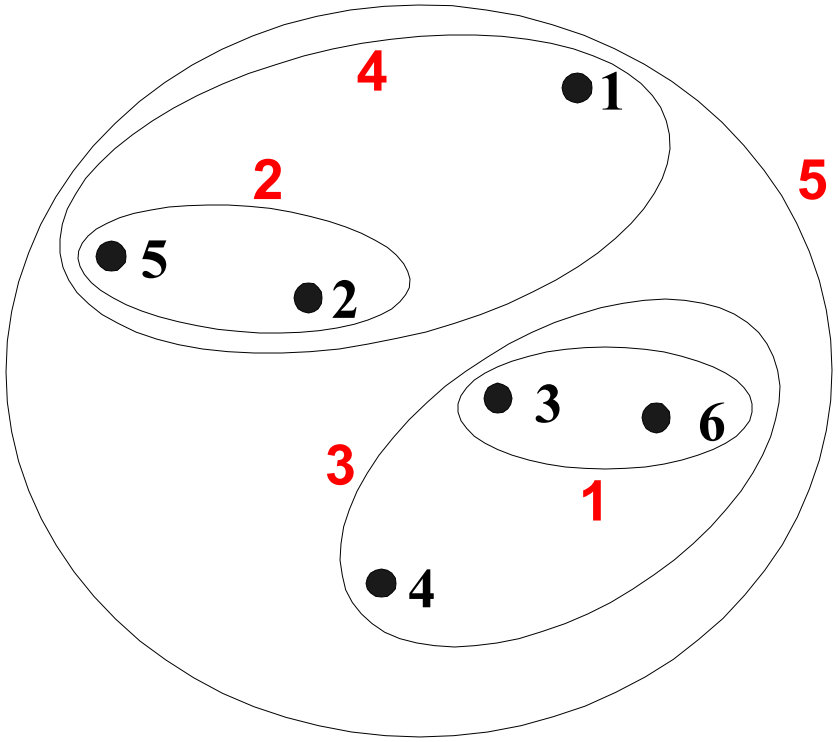
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

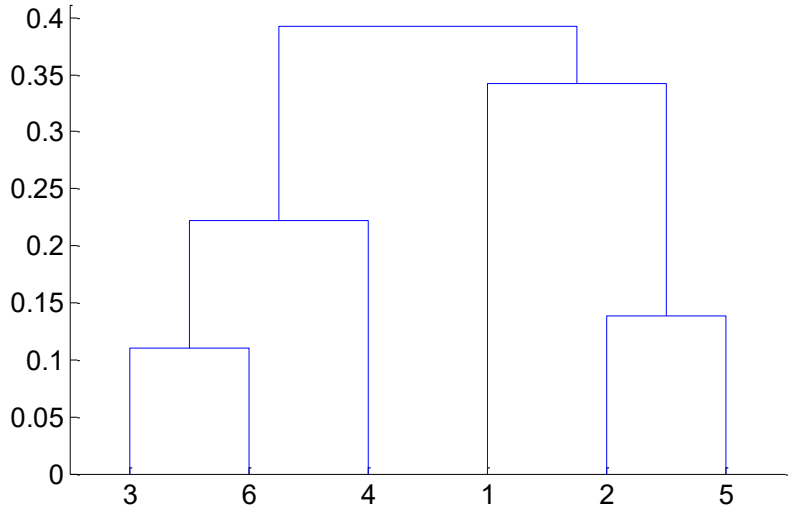
Distance Matrix:



MAX or Complete Linkage



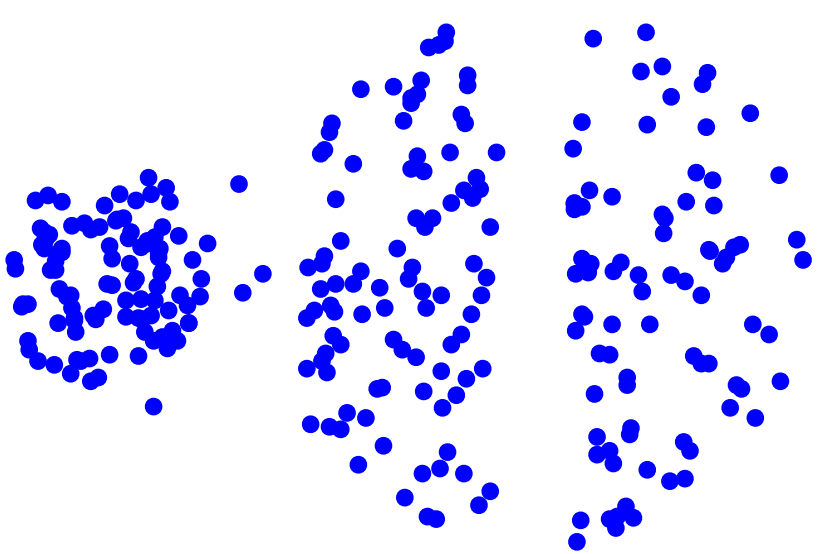
Nested Clusters



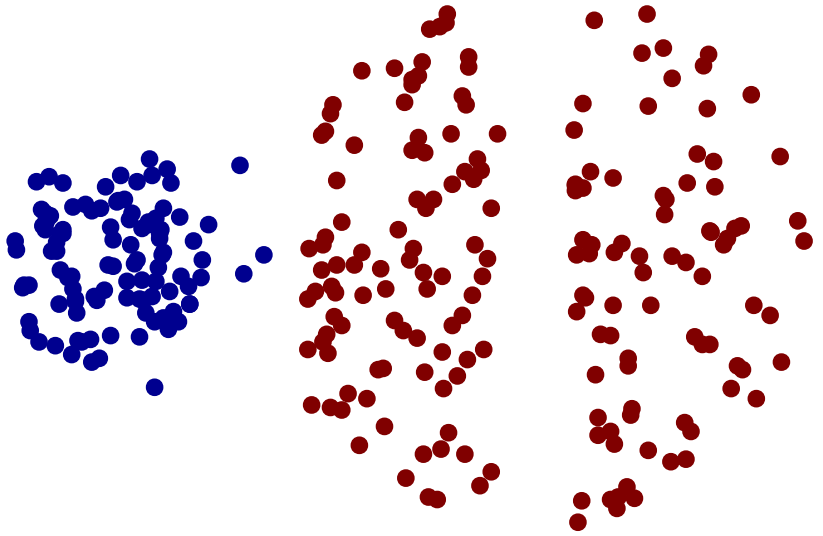
Dendrogram

MAX or Complete Linkage: Strength

- **Less susceptible to noise**



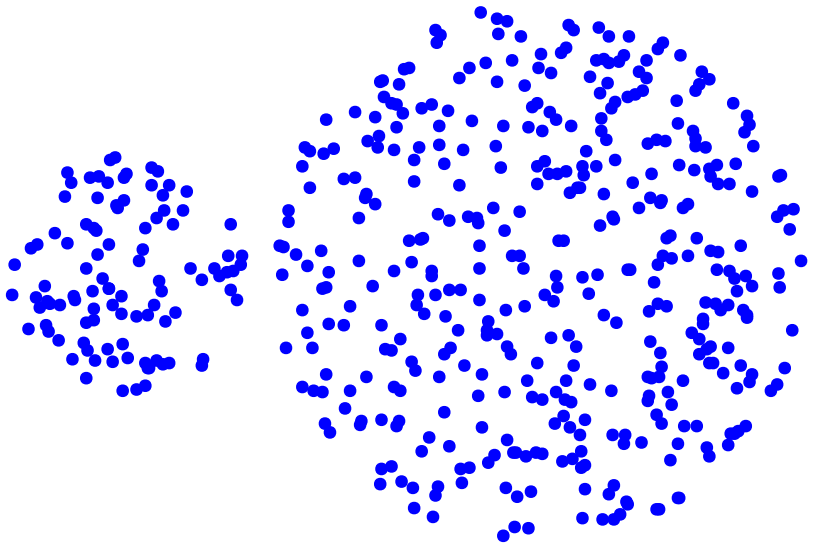
Original Points



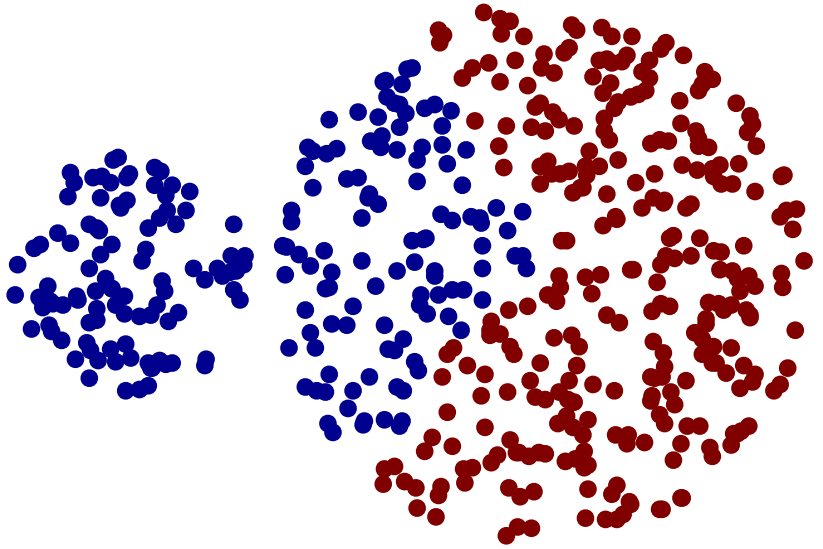
Two Clusters

MAX or Complete Linkage: Limitations

- **Tends to break large clusters**
- **Biased towards globular clusters**



Original Points



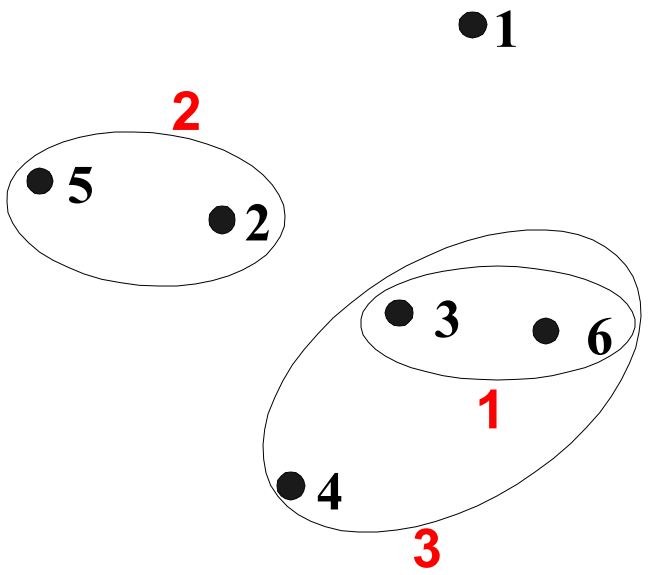
Two Clusters

Group Average

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

$$proximity(C_i, C_j) = \frac{\sum_{\substack{\mathbf{x} \in C_i \\ \mathbf{y} \in C_j}} proximity(\mathbf{x}, \mathbf{y})}{m_i \times m_j}.$$

$$\begin{aligned} dist(\{3,6,4\},\{1\}) &= (0.22 + 0.37 + 0.23)/(3 \times 1) \\ &= 0.28 \\ dist(\{2,5\},\{1\}) &= (0.24 + 0.34)/(2 \times 1) \\ &= 0.29 \\ dist(\{3,6,4\},\{2,5\}) &= (0.15 + 0.28 + 0.25 + 0.39 + 0.20 + 0.29)/(3 \times 2) \\ &= 0.26 \end{aligned}$$



	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

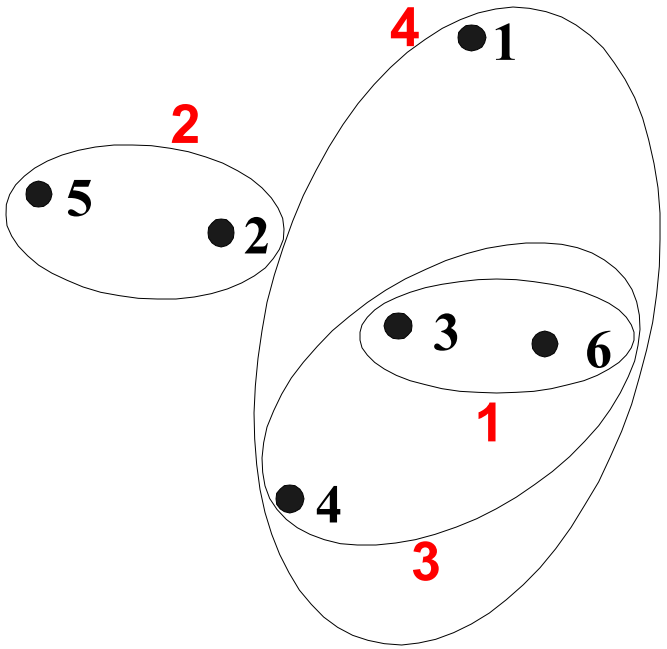
Distance Matrix:

Group Average

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

$$proximity(C_i, C_j) = \frac{\sum_{\substack{\mathbf{x} \in C_i \\ \mathbf{y} \in C_j}} proximity(\mathbf{x}, \mathbf{y})}{m_i \times m_j}.$$

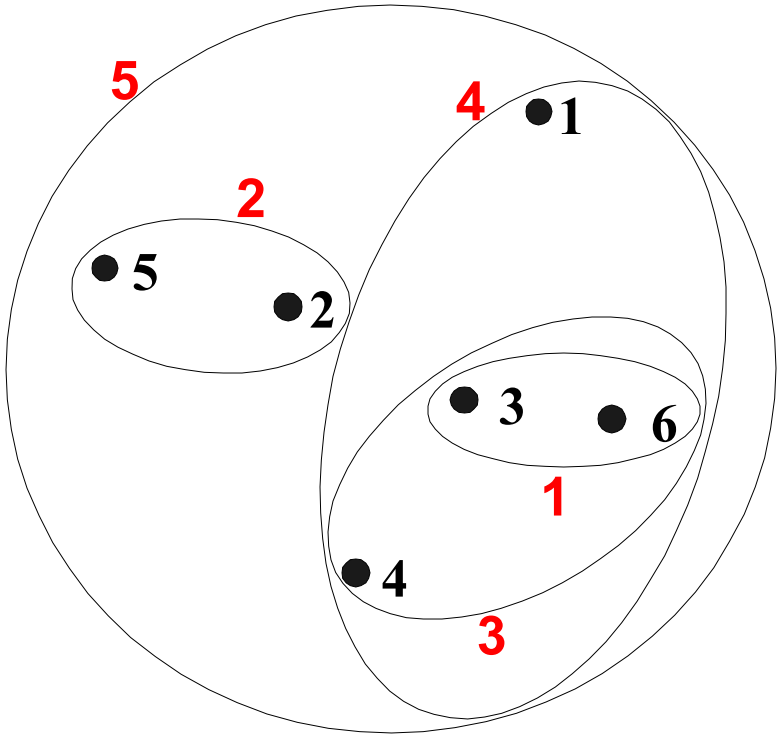
$$\begin{aligned} dist(\{3,6,4\},\{1\}) &= (0.22 + 0.37 + 0.23)/(3 \times 1) \\ &= 0.28 \\ dist(\{2,5\},\{1\}) &= (0.24 + 0.34)/(2 \times 1) \\ &= 0.29 \\ dist(\{3,6,4\},\{2,5\}) &= (0.15 + 0.28 + 0.25 + 0.39 + 0.20 + 0.29)/(3 \times 2) \\ &= 0.26 \end{aligned}$$



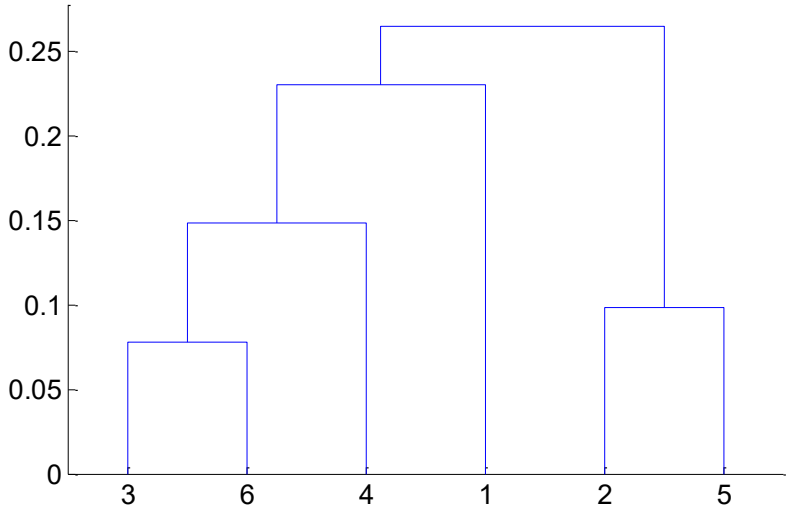
	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

Distance Matrix:

Group Average



Nested Clusters



Dendrogram

Hierarchical Clustering: Group Average

Compromise between Single and Complete Link

Strengths

- Less susceptible to noise

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

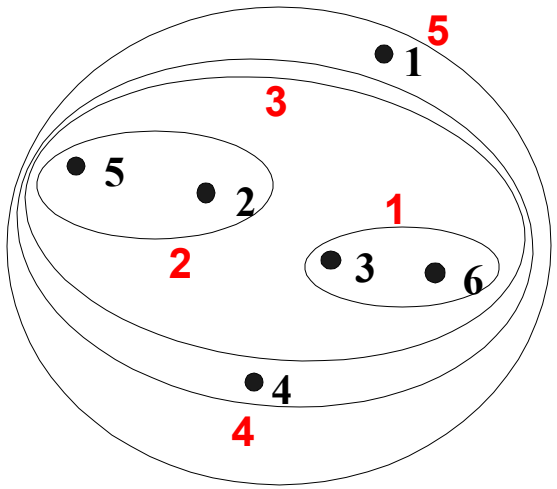
Less susceptible to noise

Biased towards globular clusters

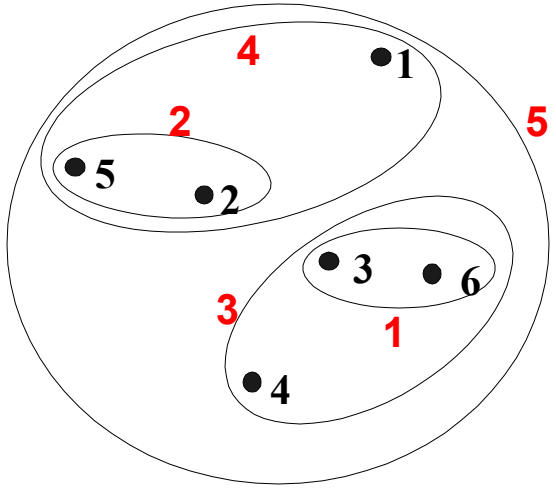
Hierarchical analogue of K-means

- Can be used to initialize K-means

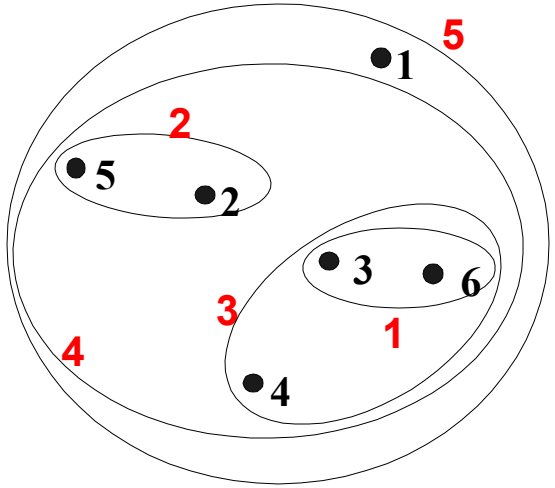
Hierarchical Clustering: Comparison



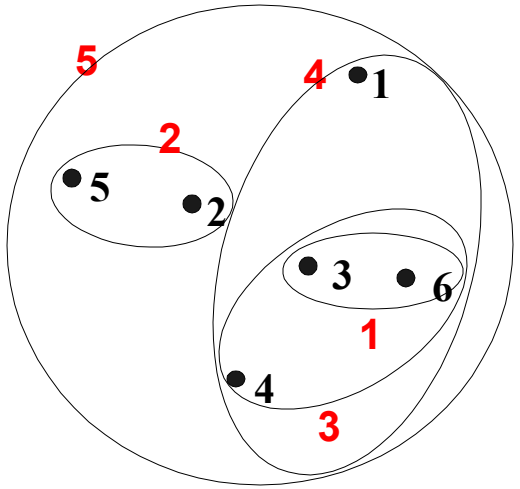
MIN



MAX



Group Average



Ward's Method

Hierarchical Clustering: Problems and Limitations

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

- K-means to create several small clusters -> Hierarchical clustering

No global objective function is directly minimized

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

- Sensitivity to noise -> Outliers increase SSE in Ward's Rule
- Difficulty handling clusters of different sizes and non-globular shapes
- Breaking large clusters

Density Based Clustering

Clusters are regions of high density that are separated from one another by regions on low density.

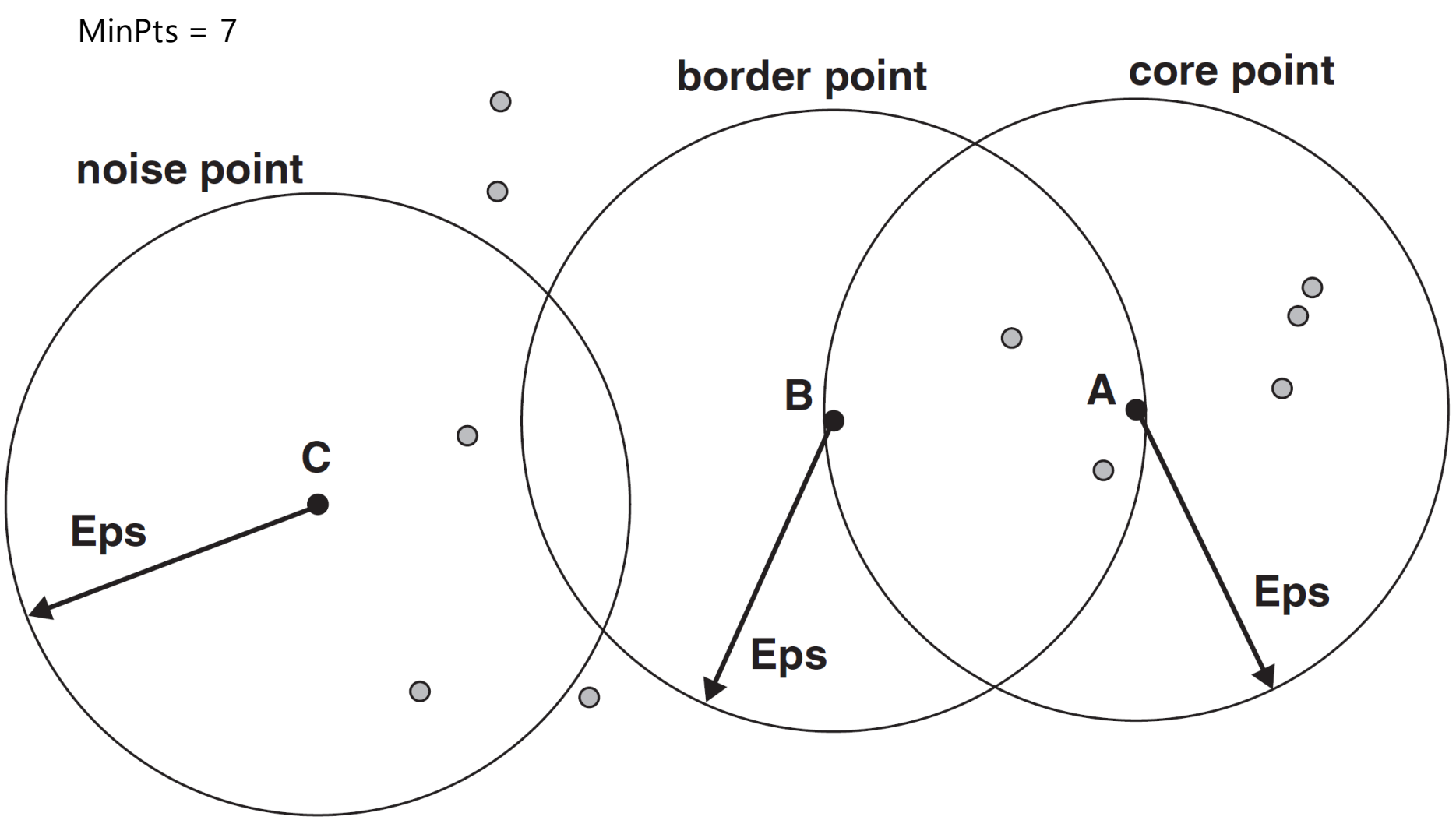
DBSCAN is a simple and effective density-based clustering algorithm

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 at least a specified number of points (MinPts) within Eps
  - These are points that are at the interior of a cluster
  - Counts the point itself
- A border point is not a core point, 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

Form clusters using core points, and assign border points to one of its neighboring clusters

1: Label all points as core, border, or noise points.

2: Eliminate noise points.

3: Put an edge between all core points within a distance *Eps* of each other.

4: Make each group of connected core points into a separate cluster.

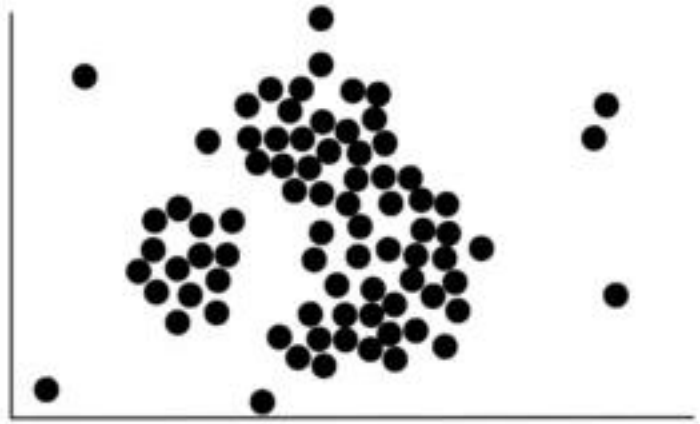
5: Assign each border point to one of the clusters of its associated core points

A simple DBSCAN example

Let's start with a set of points and define eps and minPoints

eps =

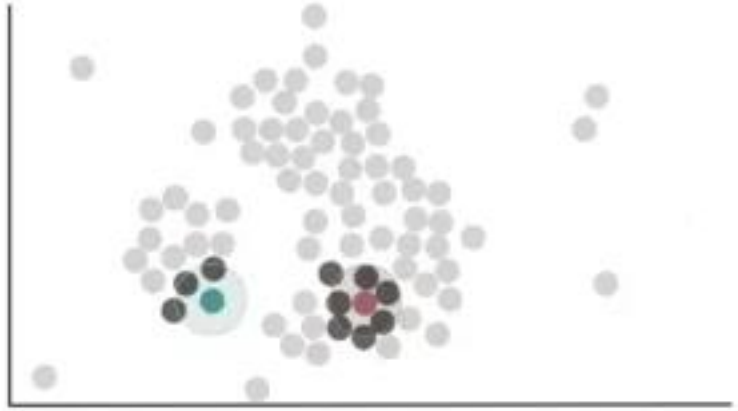
minPoints = 4



The first step is to find all the core points

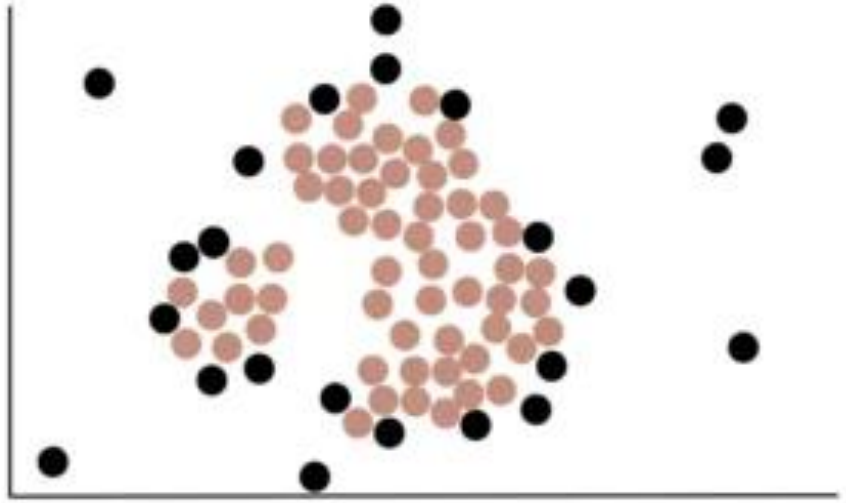
The red point is a core point (close to 7 points)

The green point is not a core point



A simple DBSCAN example

This way we can finally find all the core points

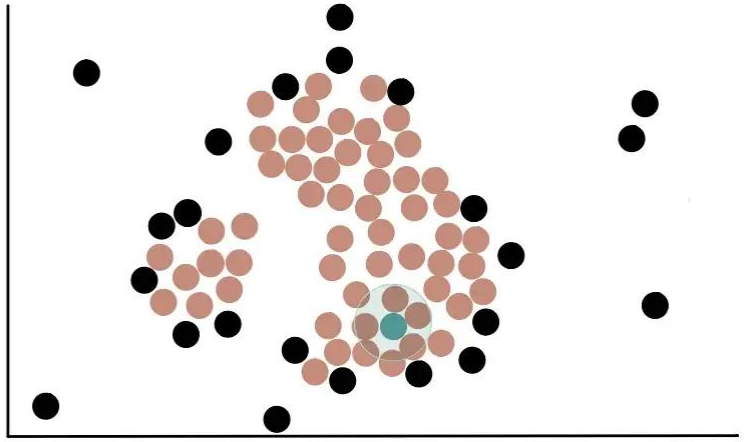


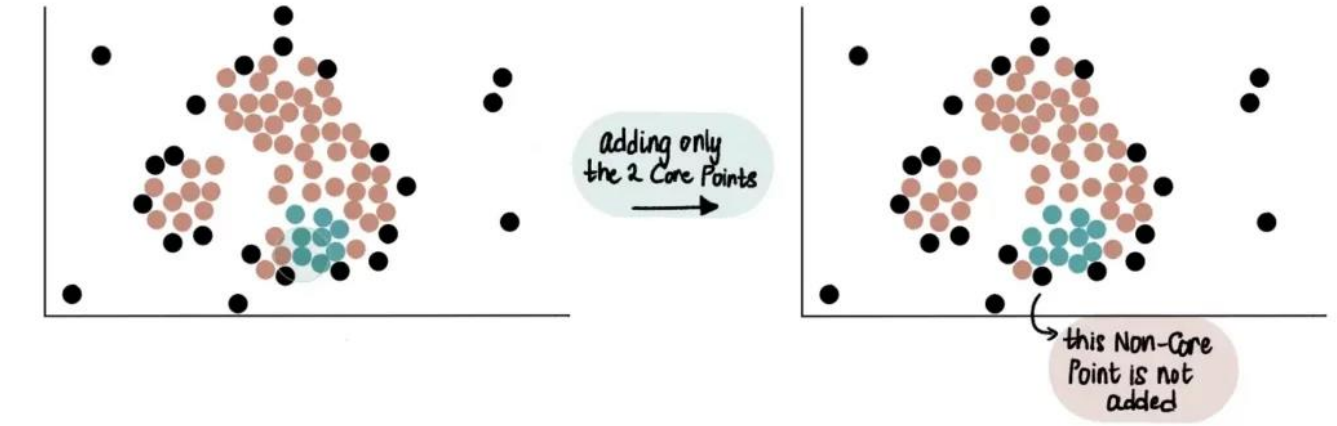
A simple DBSCAN example

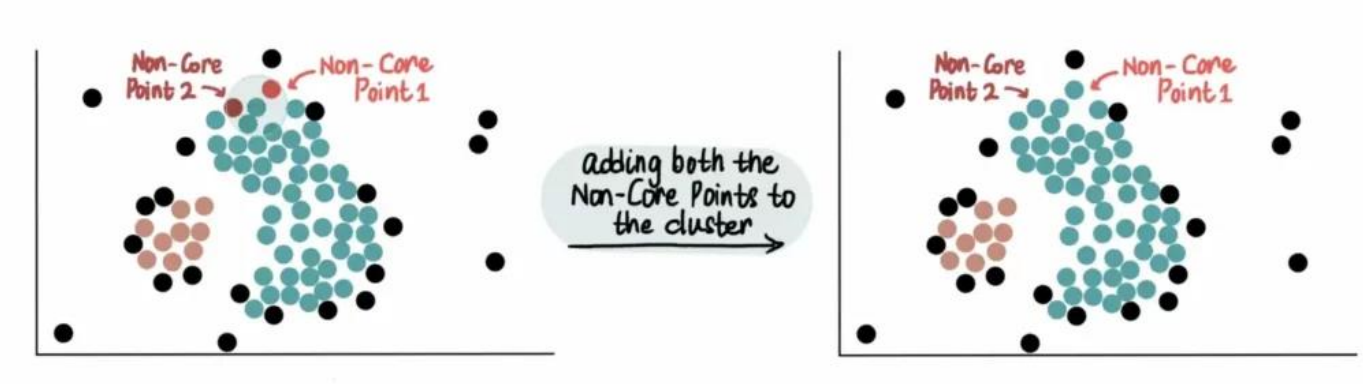
Select a core point to ‘start’ a new cluster

Iteratively add core points within the eps of another core point to the cluster

Finally, add the border points

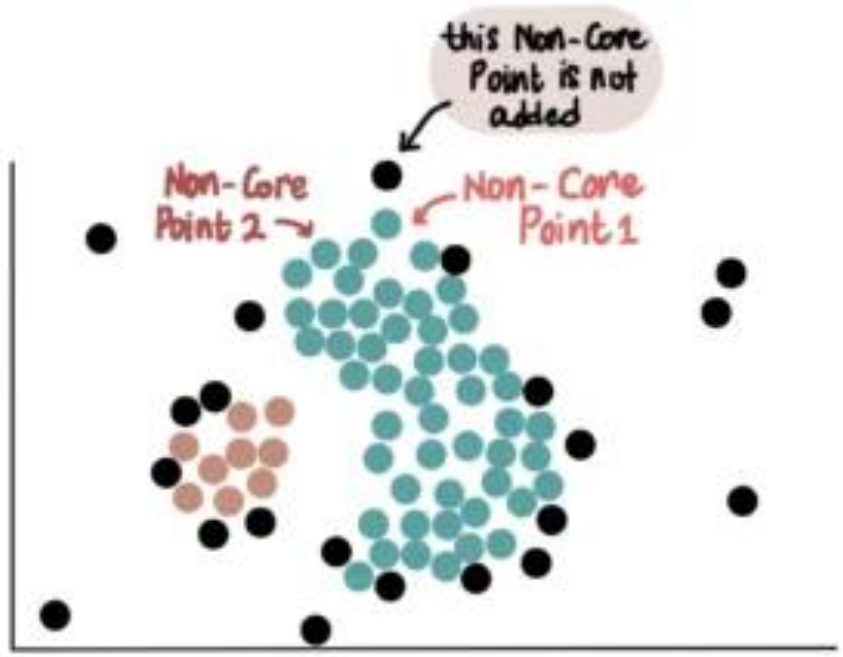






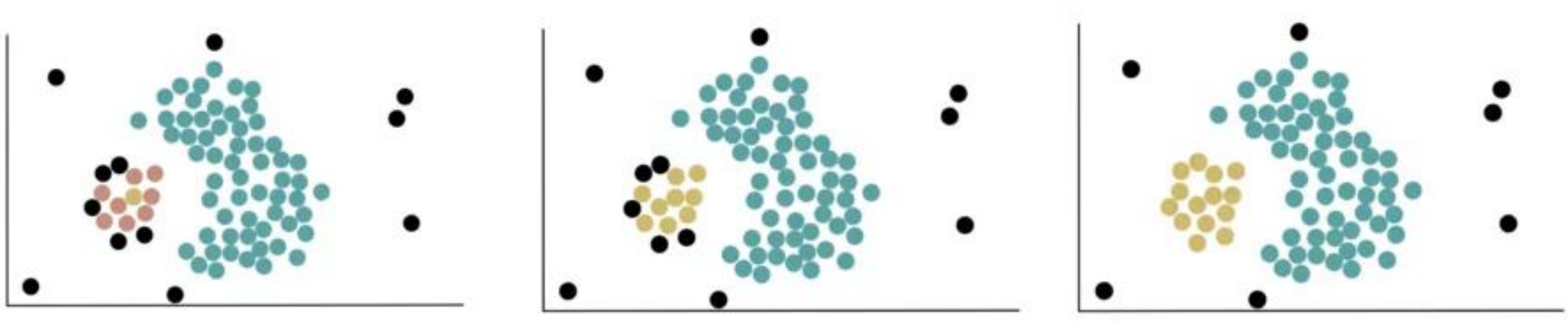
A simple DBSCAN example

Noise points are not added



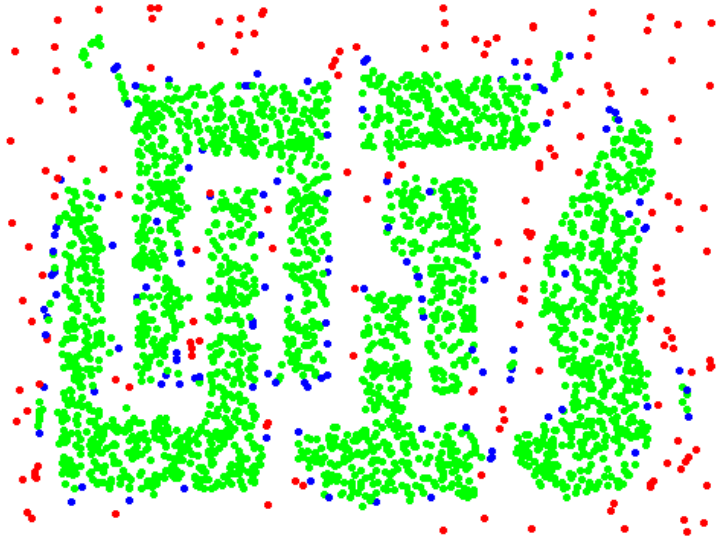
A simple DBSCAN example

Finally, we can repeat the procedure to generate other clusters



When DBSCAN Works Well

Original Points



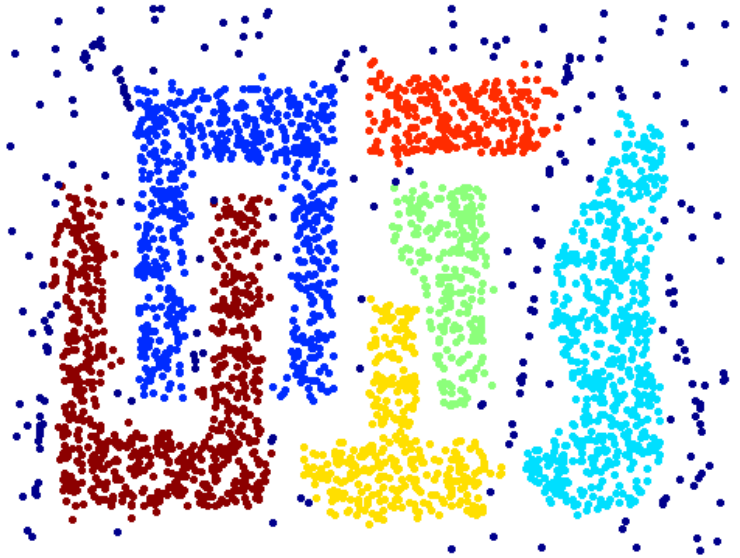
border and noise

Eps = 10, MinPts = 4

When DBSCAN Works Well

- **Can handle clusters of different shapes and sizes**
- **Resistant to noise**

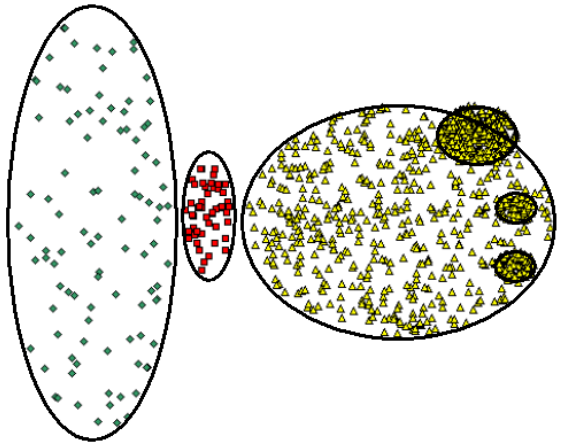
Original Points



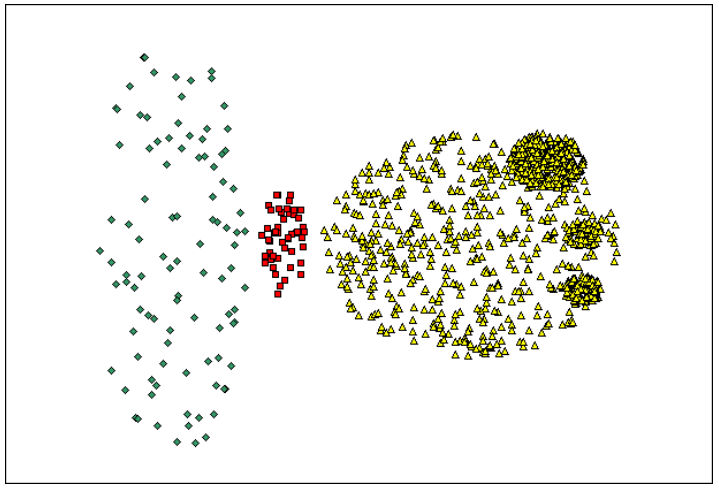
Clusters (dark blue points indicate noise)

When DBSCAN Does NOT Work Well

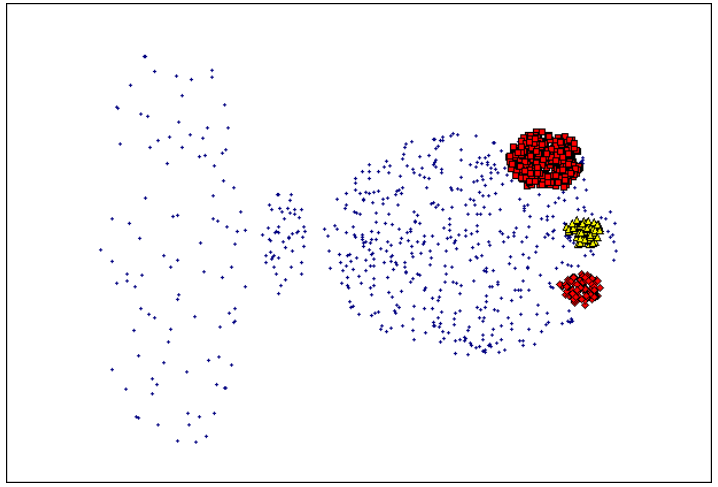
- **Varying densities**
- **High-dimensional data**



Original Points



(MinPts=4, Eps=9.92).



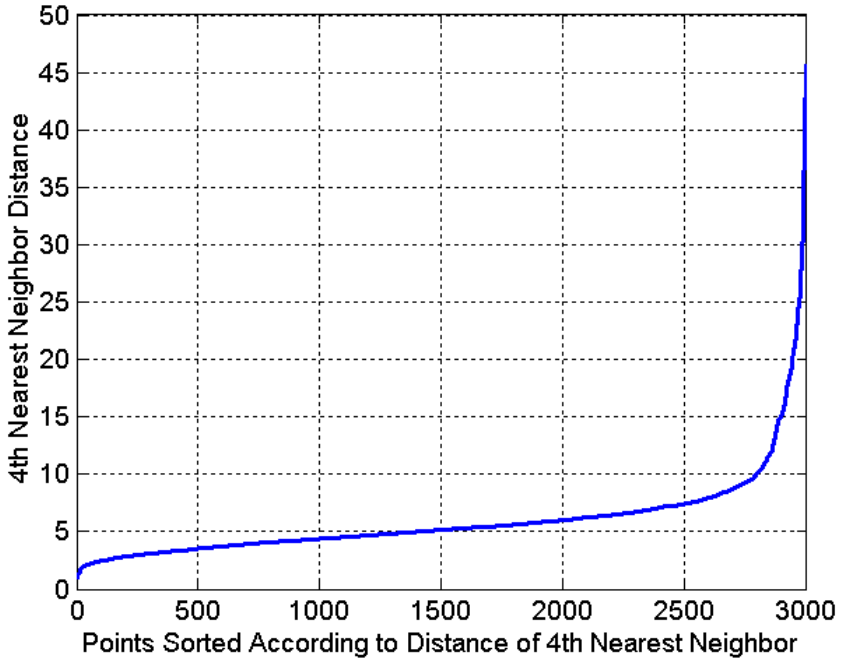
(MinPts=4, Eps=9.75)

DBSCAN: Determining EPS and MinPts

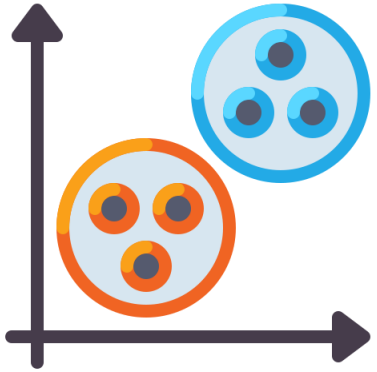
The idea is that for points in a cluster, their k^{th} nearest neighbors are at close distance

Noise points have the k^{th} nearest neighbor at a farther distance

So, plot the sorted distance of every point to its k^{th} nearest neighbor



Cluster Validity



Cluster Validity

For cluster analysis, the question is how to evaluate the "goodness" of the resulting clusters?

But "*clusters are in the eye of the beholder*"!

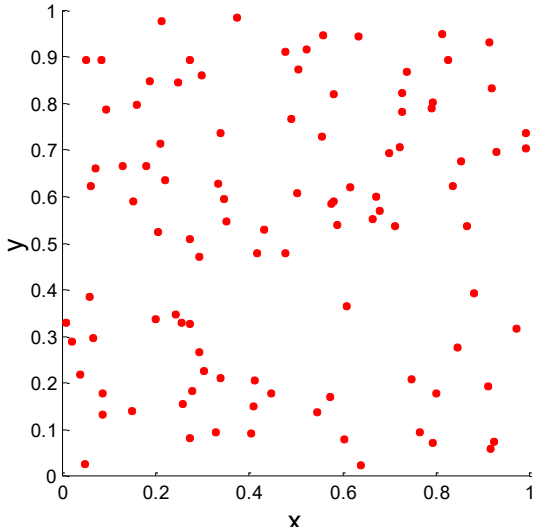
This means that it is mostly impossible to have a correct classification output

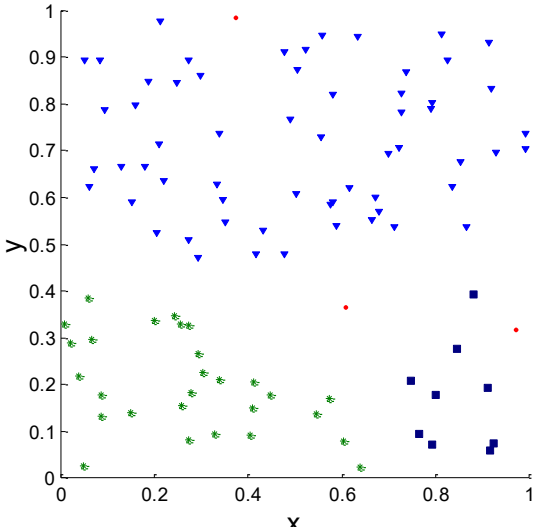
Then why do we want to evaluate them?

- 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

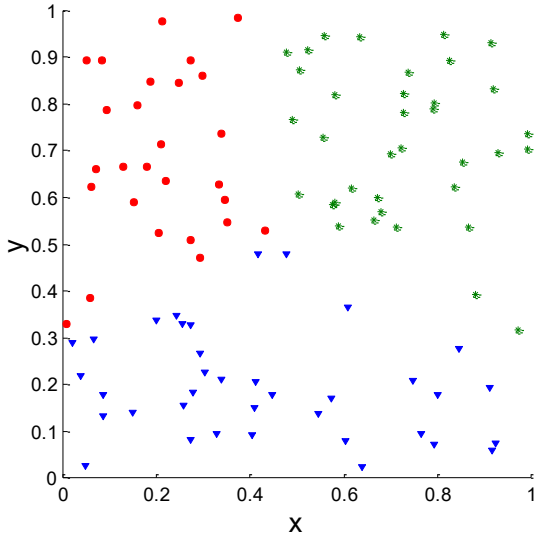
Random Points

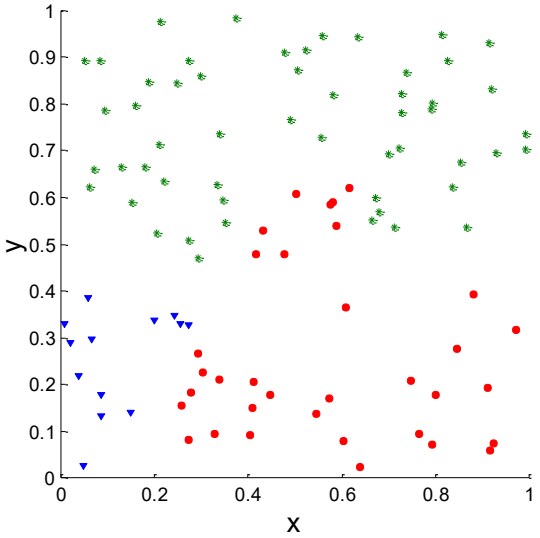




DBSCAN

K-means





Complete Link

Measures of Cluster Validity

Numerical measures that are applied to judge various aspects of cluster validity, are classified into the following two types.

- Supervised: Used to measure the extent to which cluster labels match externally supplied class labels.
  - Entropy
  - Often called ***external indices*** because they use information external to the data
- Unsupervised: Used to measure the goodness of a clustering structure *without* respect to external information.
  - Sum of Squared Error (SSE)
  - Often called ***internal indices*** because they only use information in the data

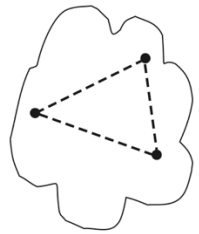
You can use supervised or unsupervised measures to **compare** clusters or clusterings

Unsupervised Measures: Cohesion and Separation

Internal measures of cluster validity for partitional clustering schemes are based on the notions of cohesion or separation

Overall **cluster validity** for a set of K clusters as a *weighted sum* of the validity of individual clusters

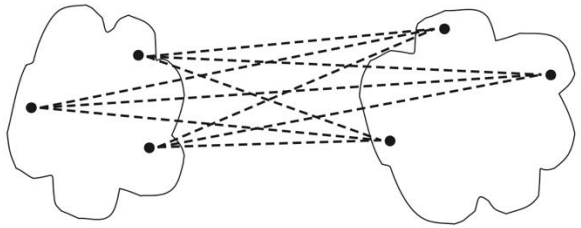
$$overall\ validity = \sum_{i=1}^{K} w_i\ validity(C_i).$$



Cohesion

Validity function can be cohesion, separation, or some combination

- K is the number of clusters
- w_i can be referred to the cluster size or set to 1 to weight equally all the clusters



Separation

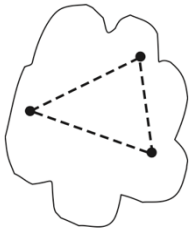
Unsupervised Measures: Cohesion and Separation (graph-based)

A proximity graph-based approach can also be used for cohesion and separation.

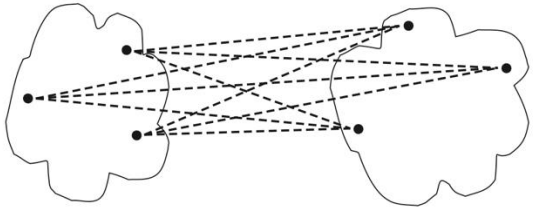
- Cluster cohesion is the sum of the weight of all links within a cluster.
- Cluster separation is the sum of the weights between nodes in the cluster and nodes outside the cluster.

$$cohesion(C_i) = \sum_{\substack{\mathbf{x} \in C_i \\ \mathbf{y} \in C_i}} proximity(\mathbf{x}, \mathbf{y})$$

$$separation(C_i, C_j) = \sum_{\substack{\mathbf{x} \in C_i \\ \mathbf{y} \in C_j}} proximity(\mathbf{x}, \mathbf{y})$$



cohesion



separation

Proximity function can be a similarity or a dissimilarity:

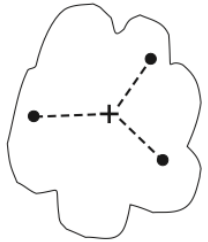
Similarity ➔ Higher values are better for cohesion, Lower values are better for separation.

Dissimilarity ➔ Lower values are better for cohesion, Higher values are better for separation.

Unsupervised Measures: Cohesion and Separation (prototype-based)

In prototype-based clusters:

- Cohesion of a cluster is the sum of the proximities with respect to the prototype (centroid or medoid) of the cluster.
- Separation between two clusters can be measured by the proximity of the two cluster prototypes.

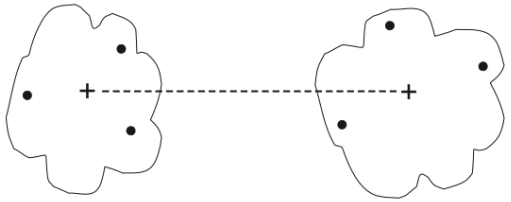


cohesion

$$cohesion(C_i) = \sum_{\mathbf{x} \in C_i} proximity(\mathbf{x}, \mathbf{c}_i)$$

$$separation(C_i, C_j) = proximity(\mathbf{c}_i, \mathbf{c}_j)$$

$$separation(C_i) = proximity(\mathbf{c}_i, \mathbf{c})$$



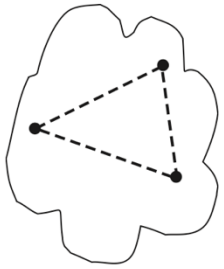
separation

Unsupervised Measures: Cohesion and Separation

- Cluster Cohesion: Measures how closely related are objects in a cluster
- Cluster **Separation**: Measure how distinct or well-separated a cluster is from other clusters

Cohesion is measured by the within cluster sum of squares (SSE)

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

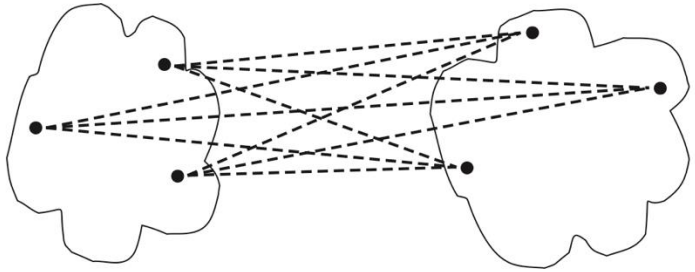


Cohesion

Separation is measured by the between cluster sum of squares

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

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



Separation

Evaluating Individual Clusters and Objects

Cohesion and separation can be used to evaluate individual clusters and objects

- Rank individual clusters according to their specific value of cluster validity (cohesion or separation)
- A cluster that has a *high value* of cohesion may be considered better than a cluster that has a lower value
- If a cluster is not very cohesive, then we may want to split it into several subclusters
- If two clusters are relatively cohesive but not well separated, we may want to merge them into a single cluster

Cluster Object: in terms of their **contribution to the overall cohesion or separation** of the cluster

- **High** contribution to cohesion or separation → **interior** objects
- **Low** contribution to cohesion or separation → **edge** objects

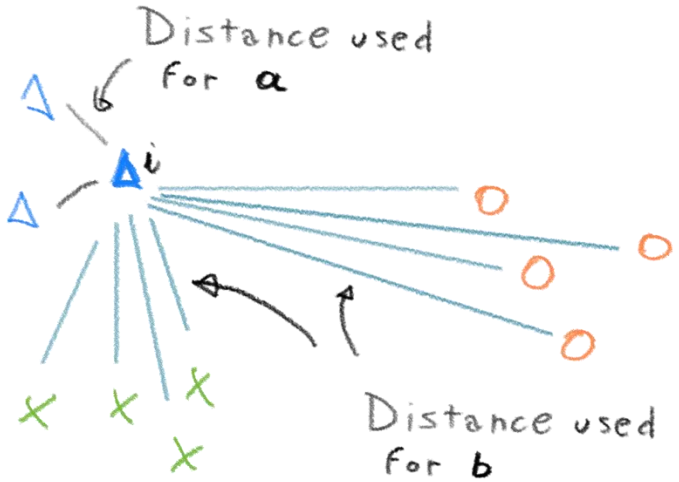
Unsupervised Measures: Silhouette Coefficient

Silhouette coefficient combines ideas of both *cohesion* and *separation*, but for individual points, as well as clusters and clusterings

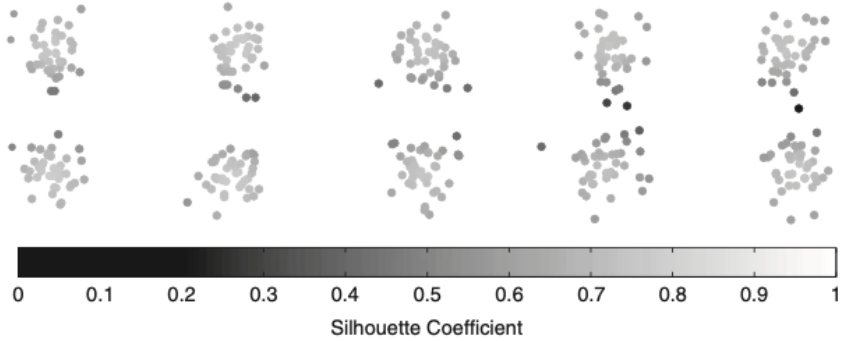
For an individual point $\boldsymbol{i}$

- Calculate $\boldsymbol{a_i}$ = average distance of $\boldsymbol{i}$ to the points in its cluster
- Calculate $\boldsymbol{b_i}$ = min (average distance of $\boldsymbol{i}$ to points in another cluster)
- The silhouette coefficient for a point is then given by

$$\boldsymbol{s_i = \frac{b_i - a_i}{max(b_i, a_i)}}$$



- Value can vary between -1 and 1
- Typically ranges between 0 and 1.
- The closer to 1 the better.



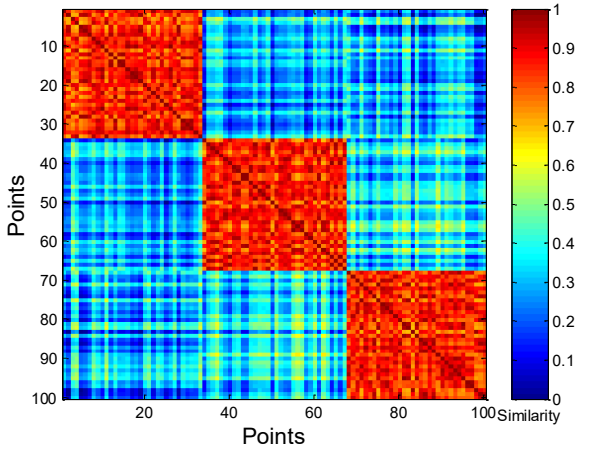
Silhouette coefficient for a **cluster** or a **clustering** is given by the average of of points belonging to the cluster/clustering

Unsupervised Cluster Evaluation Using the Proximity Matrix

Ideal cluster has:

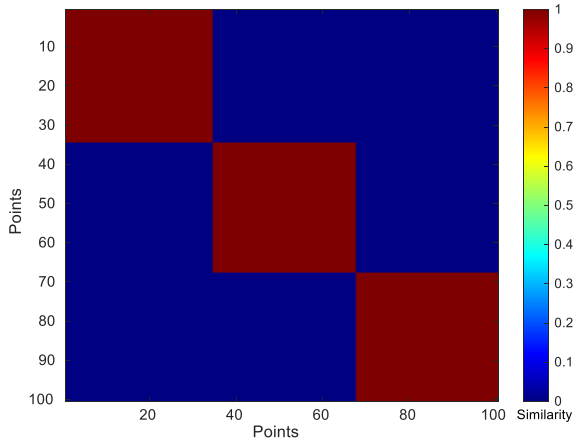
- points with a similarity of 1 to all points in the cluster.
- points with a similarity of 0 to all points in other clusters

Ideal cluster similarity matrix has a block diagonal structure



Two matrices

- **Proximity Matrix**
- **Ideal Similarity 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



Measuring Cluster Validity Via Correlation

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.

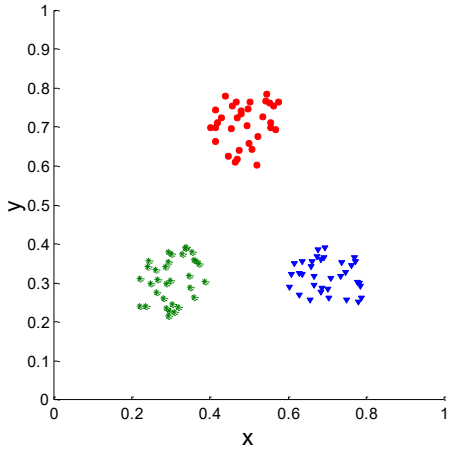
High magnitude of correlation indicates that points that belong to the same cluster are close to each other.

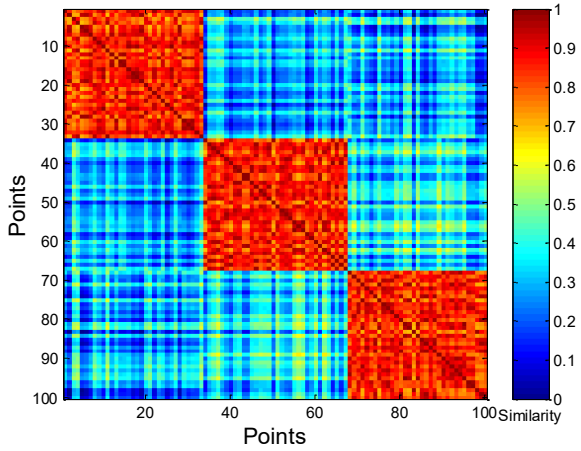
- Correlation may be positive or negative depending on whether the similarity matrix is a similarity or dissimilarity matrix

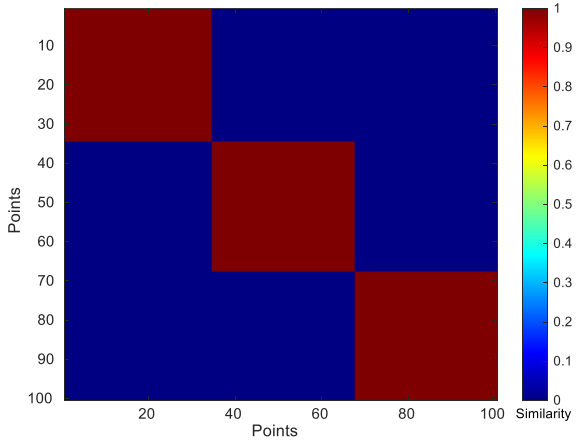
Not a good measure for some density or contiguity-based clusters.

Measuring Cluster Validity Via Correlation

Correlation of ideal similarity and proximity matrices for the K-means clusterings of the following well-clustered data set.



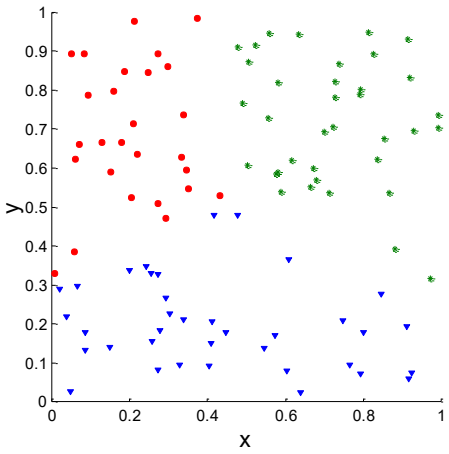




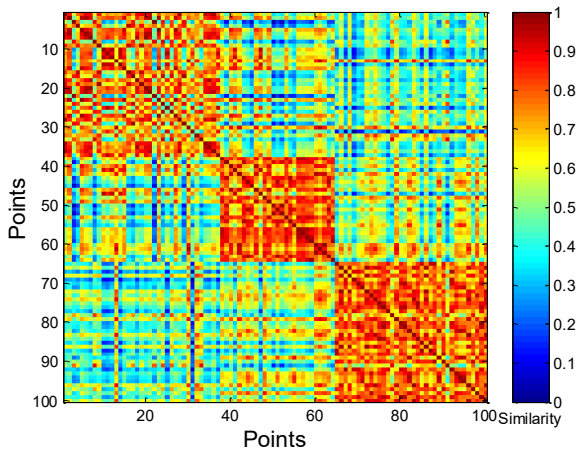
Corr = 0.9235

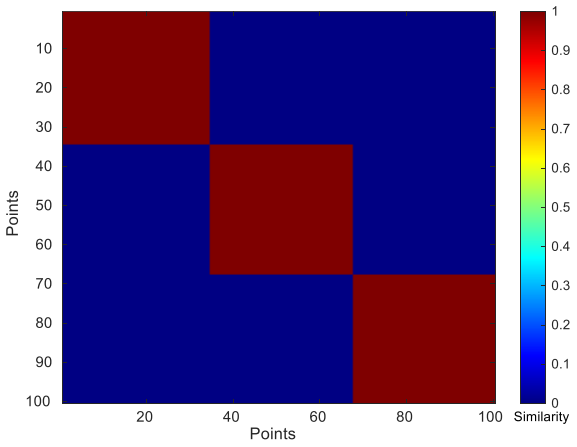
Measuring Cluster Validity Via Correlation

Correlation of ideal similarity and proximity matrices for the K-means clusterings of the following random data set.



K-means



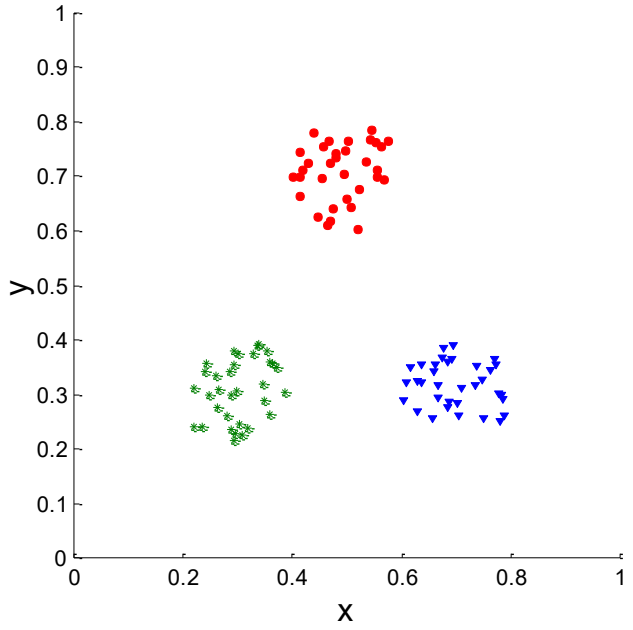


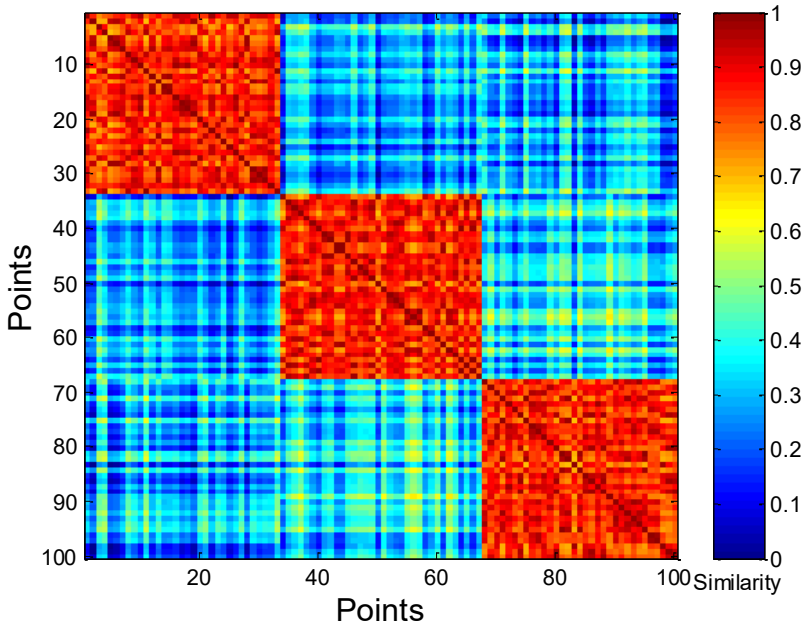
Corr = 0.5810

Judging a Clustering Visually by its Similarity Matrix

Qualitative approach to judging a set of clusters

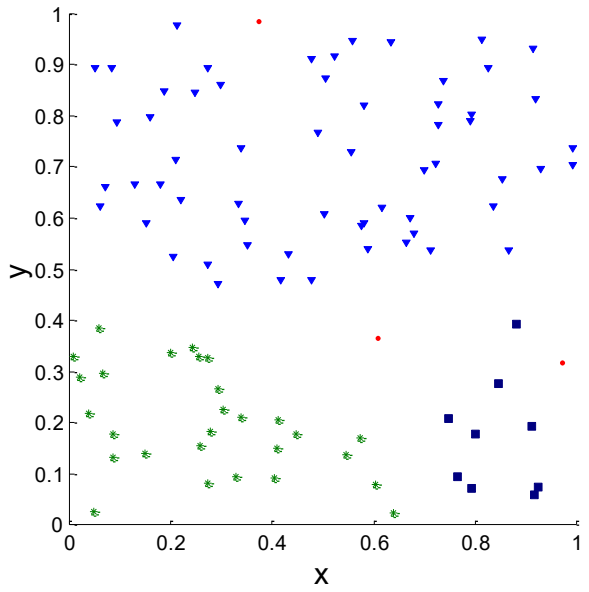
Order the similarity matrix with respect to cluster labels and inspect visually.

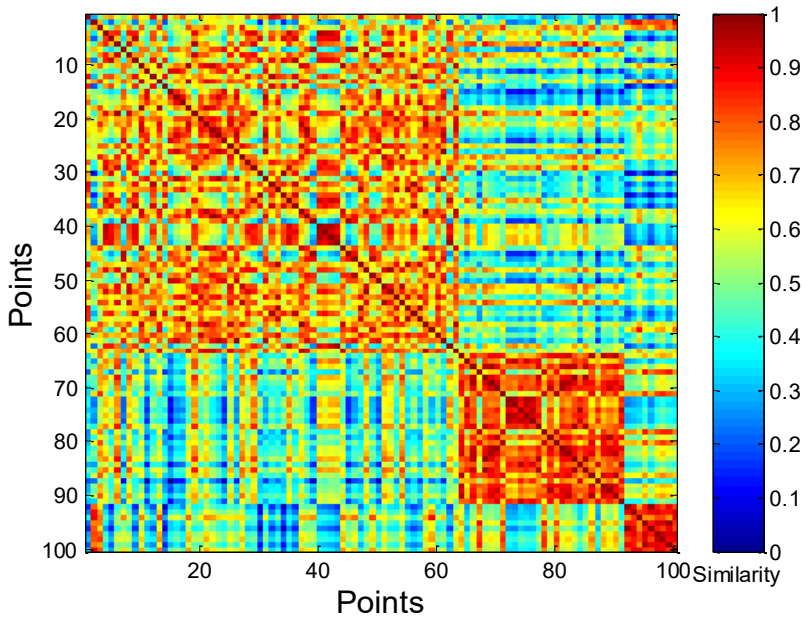




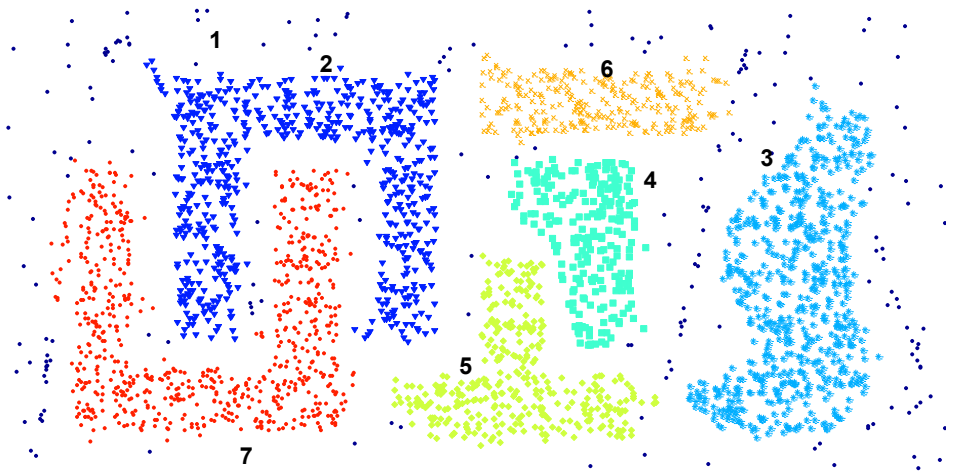
Judging a Clustering Visually by its Similarity Matrix

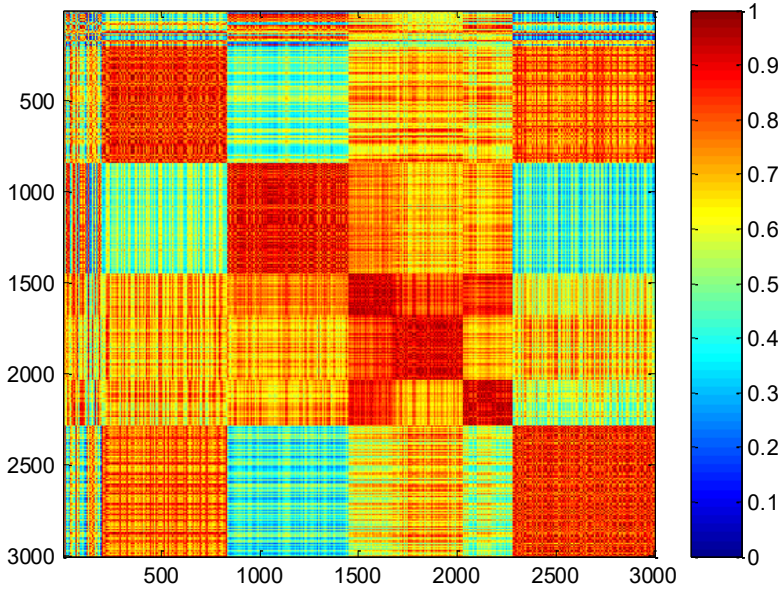
Clusters in random data are not so crisp





Judging a Clustering Visually by its Similarity Matrix



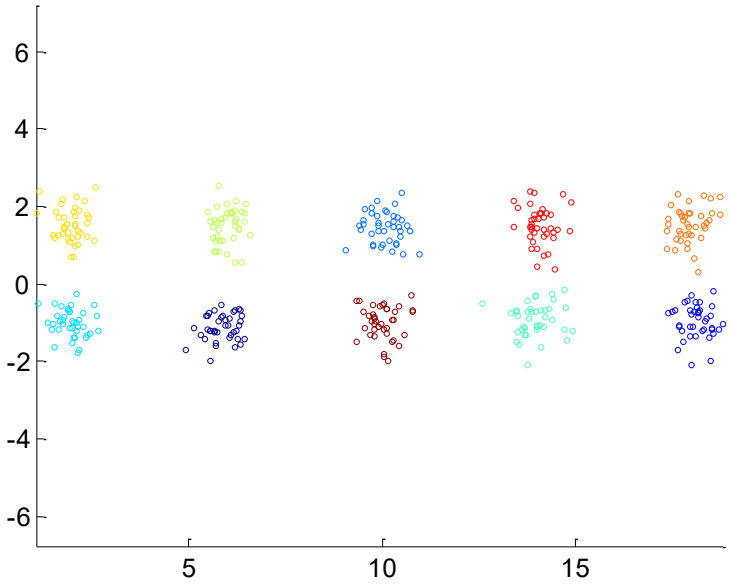


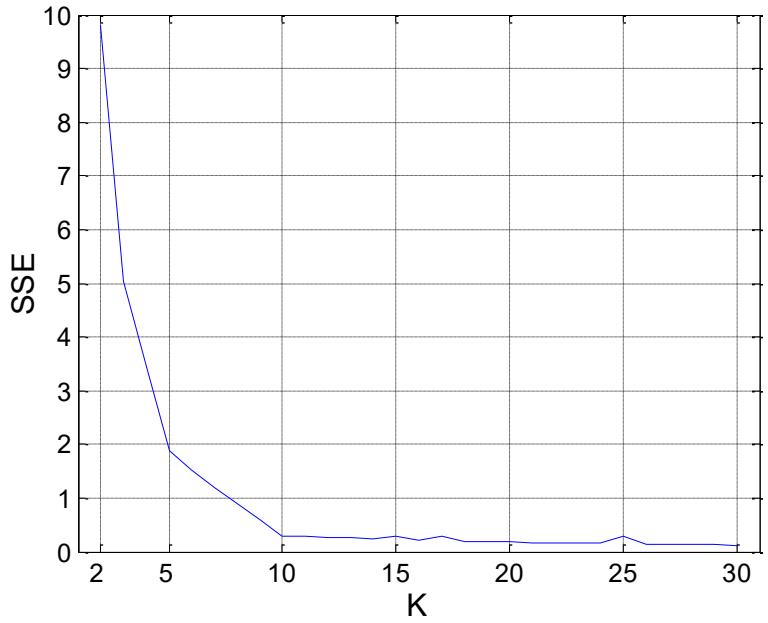
DBSCAN

Determining the Correct Number of Clusters

Unsupervised cluster evaluation measures can be used to approximately determine the correct or natural number of clusters

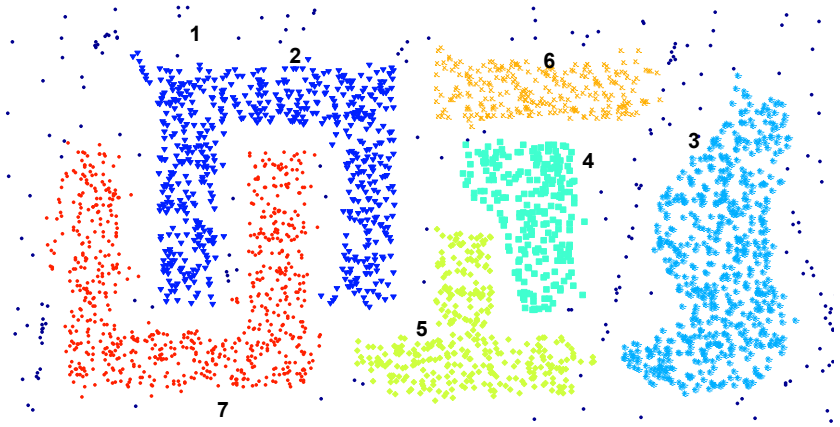
- SSE is good for comparing two clusterings or two clusters
- SSE can also be used to estimate the number of clusters

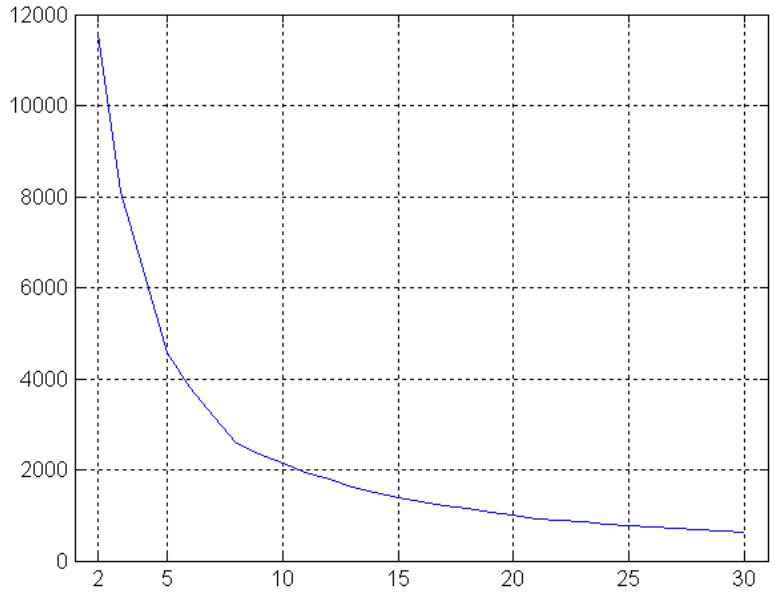




Determining the Correct Number of Clusters

SSE curve for a more complicated data set





SSE of clusters found using K-means

Supervised Measures of Cluster Validity

Supervised measures occur when external information about the data is available

Motivations for such an analysis include:

- Comparison of clustering techniques
- Evaluate whether objects in the same cluster tend to have the same label (semi-supervised learning techniques)

For convenience, we will refer to two types of measures

- **Classification-oriented**: use measures from classification, such as entropy, purity, and the F-measure.
- **Similarity-oriented**: measure the extent to which two objects that are in the same class are in the same cluster and vice versa

Supervised Measures of Cluster Validity: Classification-oriented

In the case of **classification**, we measure the degree to which predicted class labels correspond to actual class labels

In **clustering** we use cluster labels instead of predicted class labels

Entropy: The degree to which each cluster consists of objects of a single class.

- p_{ij} the probability that a member of cluster i belongs to class j
- $p_{ij} = m_{ij}/m\_i$ where m_i is the number of objects in cluster i and m_{ij} is the number of objects of class j in cluster i.
- Entropy(i) → $e_i = -\sum_{j=1}^{L} p_{ij} \log_2 p_{ij}$ where L is the number of classes
- Entropy → $e = \sum_{i=1}^{K} \frac{m_i}{m} e_i$ where K is the number of cluster

Purity: Another measure of the extent to which a cluster contains objects of a single class

- p_{ij} the probability that a member of cluster i belongs to class j
- $p_{ij} = m_{ij}/m\_i$ where m_i is the number of objects in cluster i and m_{ij} is the number of objects of class j in cluster i.
- Purity(i) = $\max_j p_{ij}$
- Purity = $\sum_{i=1}^{K} \frac{m_i}{m} p_i$

Supervised Measures of Cluster Validity: Classification-oriented

Example, we want to cluster 3204 newspaper articles from the Los Angeles Times.

These articles come from six different classes: Entertainment, Financial, Foreign, Metro, National, and Sports

The following table provides a K-means clustering with the cosine similarity measure

Cluster	Enter-tainment	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

Supervised Measures of Cluster Validity: Similarity-oriented

This approach to cluster validity involves the comparison of two matrices:

- The ideal **cluster** similarity matrix:
- A **class** similarity matrix:

We can so compute:

f_{00}= number of pairs of objects having a different class and a different cluster

f_{01} = number of pairs of objects having a different class and the same cluster

f_{10} = number of pairs of objects having the same class and a different cluster

f_{11} = number of pairs of objects having the same class and the same cluster

$$Rand\ Statistic = \frac{f_{00} + f_{11}}{f_{00} + f_{01} + f_{10} + f_{11}}$$

$$Jaccard\ coefficent = \frac{f_{11}}{f_{01} + f_{10} + f_{11}}$$

Point	p1	p2	p3	p4	p5
p1	1	1	1	0	0
p2	1	1	1	0	0
p3	1	1	1	0	0
p4	0	0	0	1	1
p5	0	0	0	1	1

Ideal cluster similarity matrix

Point	p1	p2	p3	p4	p5
p1	1	1	0	0	0
p2	1	1	0	0	0
p3	0	0	1	1	1
p4	0	0	1	1	1
p5	0	0	1	1	1

Class similarity matrix

Assessing the Significance of Cluster Validity Measures

Need a framework to interpret any measure.

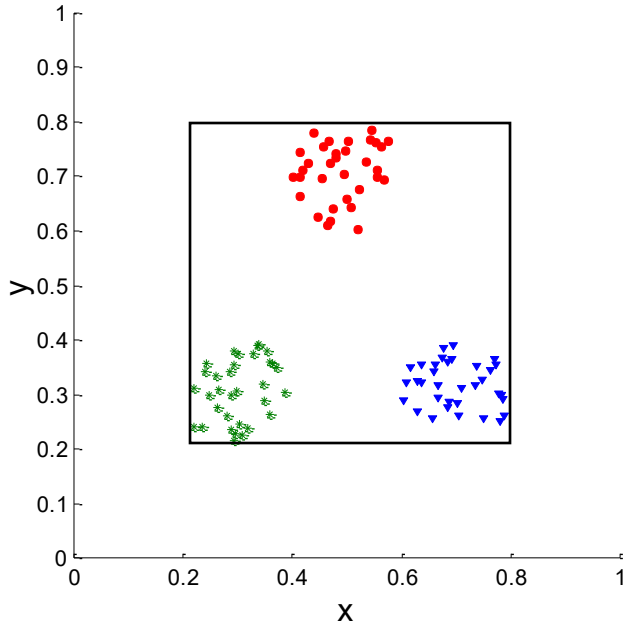
- For example, if our measure of evaluation has the value, 10, is that good, fair, or poor?

Statistics provide a framework for cluster validity

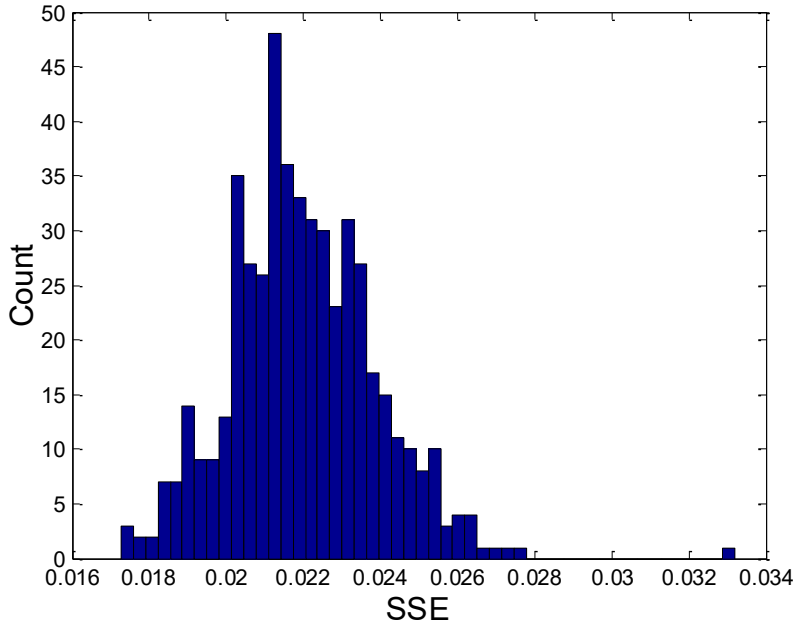
- The more “atypical” a clustering result is, the more likely it represents valid structure in the data
- Compare the value of an index obtained from the given data with those resulting from random data.
    - If the value of the index is unlikely, then the cluster results are valid

Statistical Framework for SSE

Example: Compare SSE of three cohesive clusters against three clusters in random data



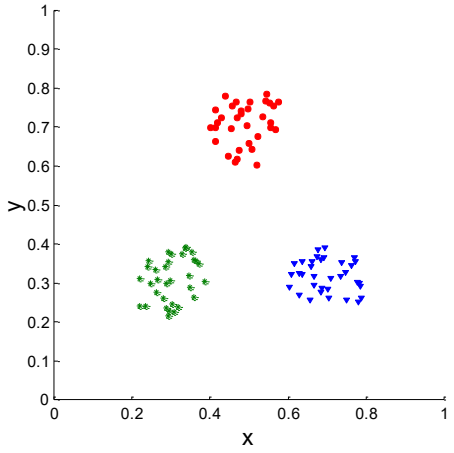
SSE = 0.005



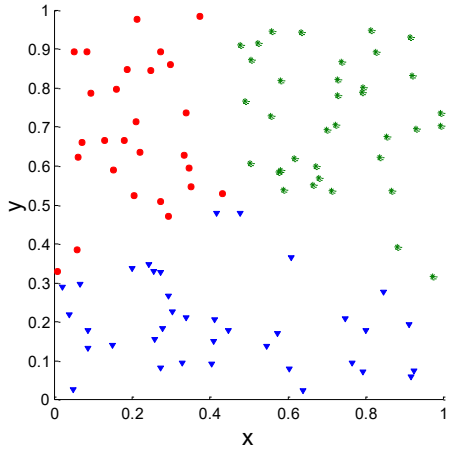
Histogram shows SSE of three clusters in 500 sets of random data points of size 100 distributed over the range 0.2 – 0.8 for x and y values

Statistical Framework for Correlation

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

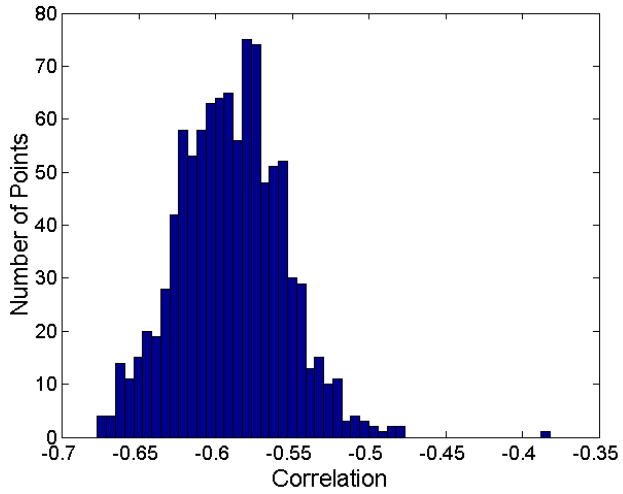


Corr = -0.9235



Corr = -0.5810

Correlation is negative because it is calculated between a distance matrix and the ideal similarity matrix. Higher magnitude is better.



Histogram of correlation for 500 random data sets of size 100 with *x* and *y* values of points between 0.2 and 0.8.

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."