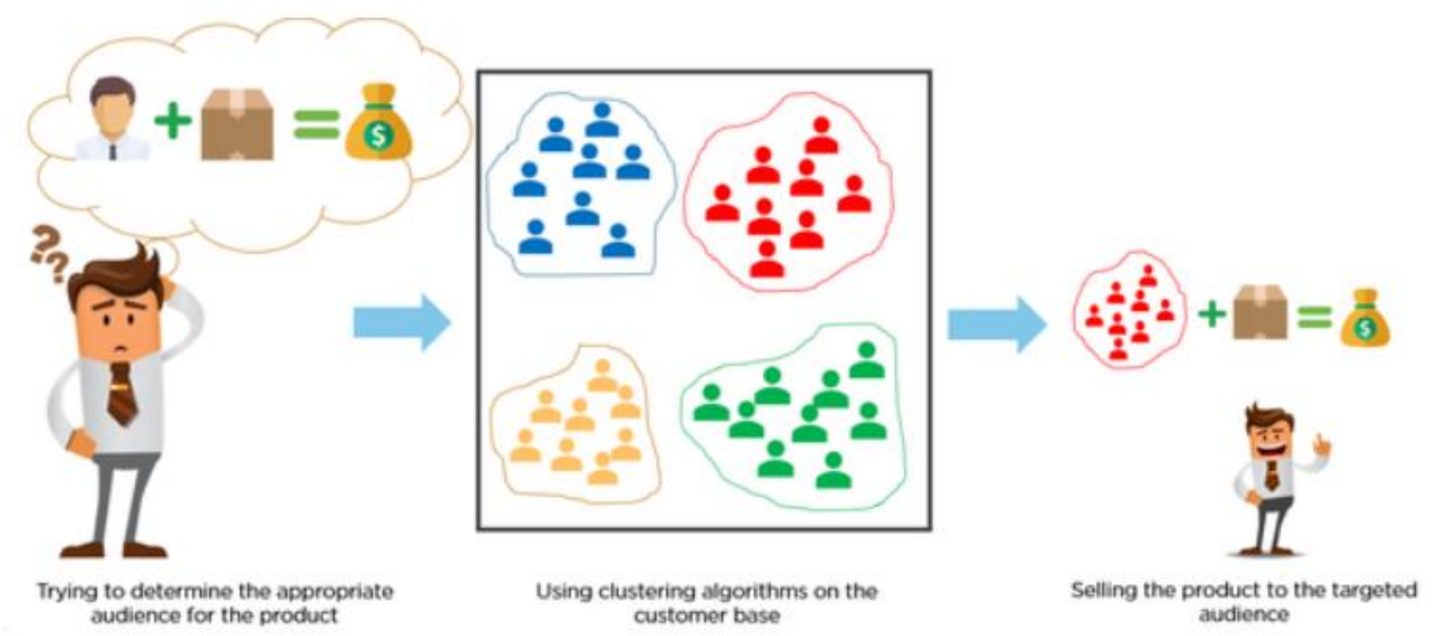
Unsupervised and Unstructured Machine Learning

BA820 – Mohannad Elhamod

Intro to Clustering

Boston University Questrom School of Business

Cluster Analysis



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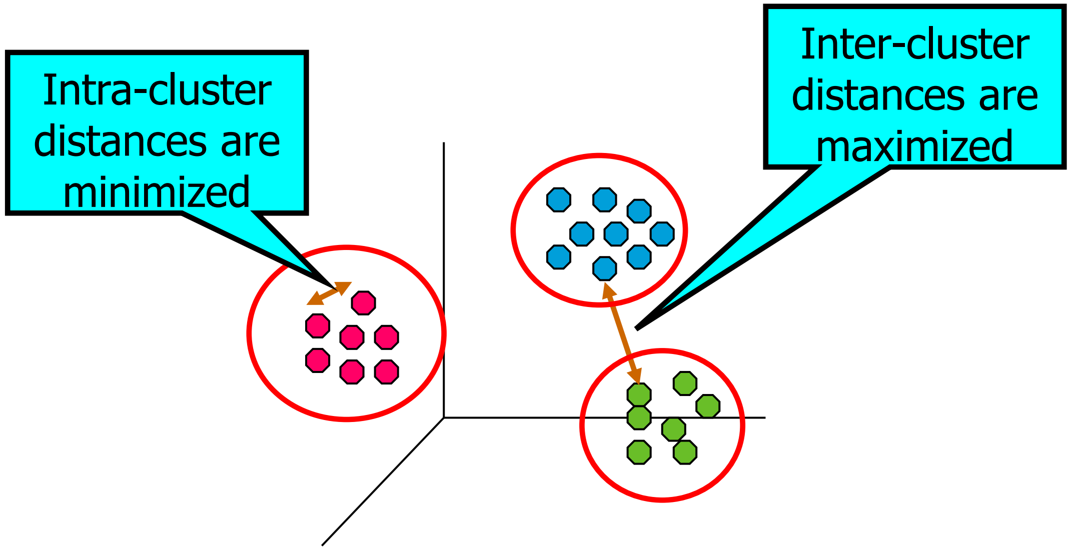
What is Cluster Analysis?

- Placing objects in groups such that:
  - the objects in a group are similar (or related) to one another.
  - They are different from (or unrelated to) the objects in other groups.
- We need a (metric/measure/objective function) to measure the (distance/similarity) of the (objects/clusters).



Clusters are in the eye of the beholder

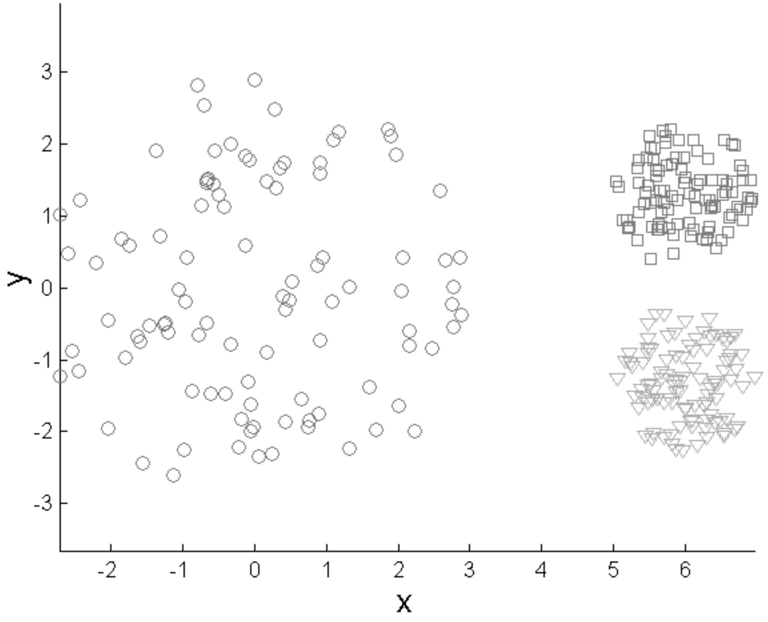
How many clusters?

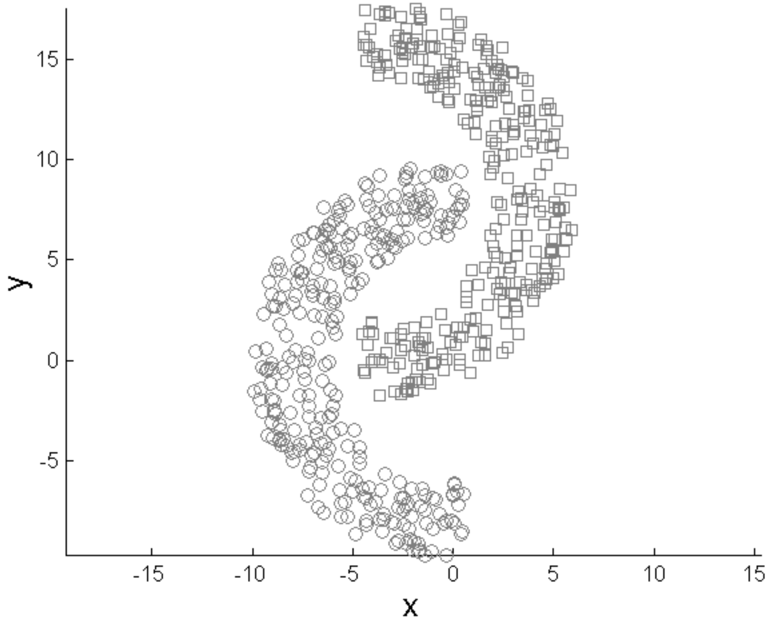
Six Clusters

Two Clusters

Four Clusters

Clusters come in all shapes and sizes





Hierarchical Clustering

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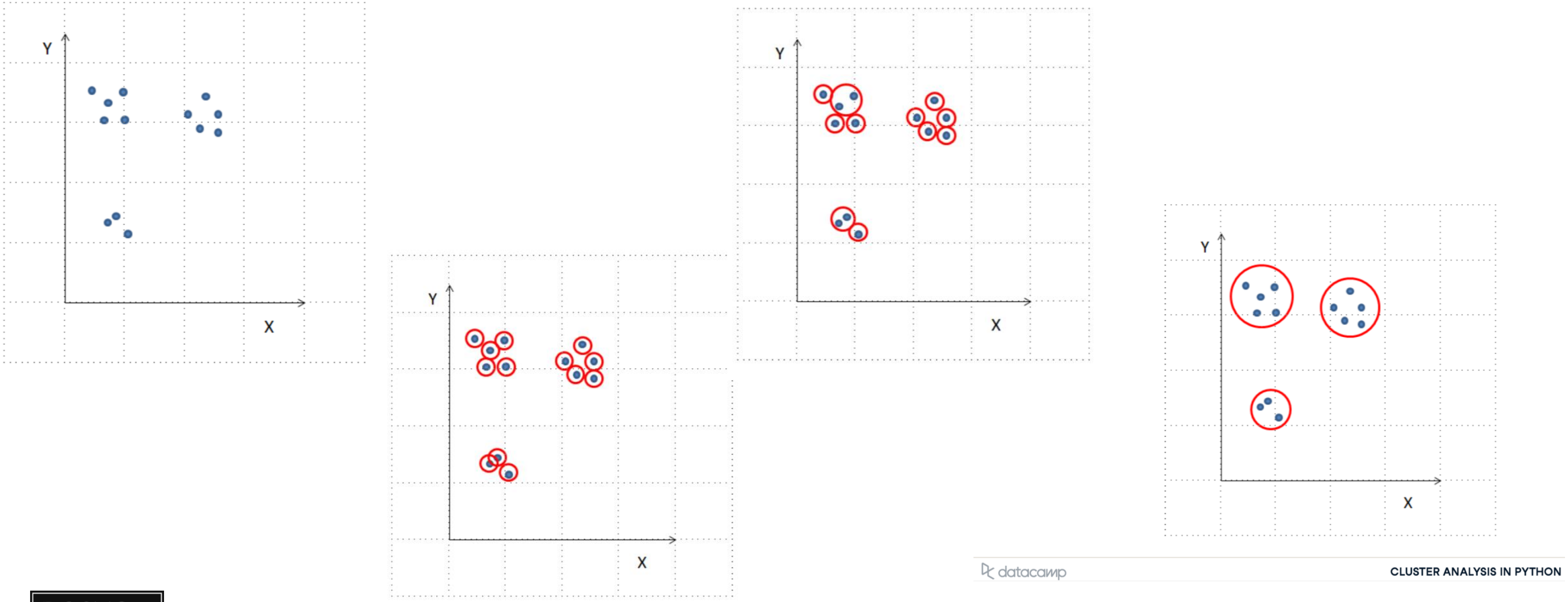
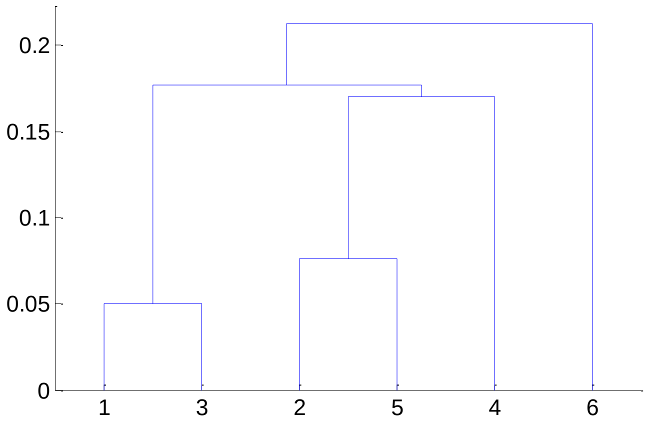
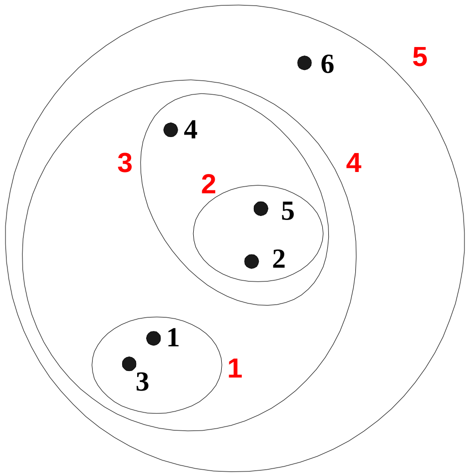
Hierarchical Clustering



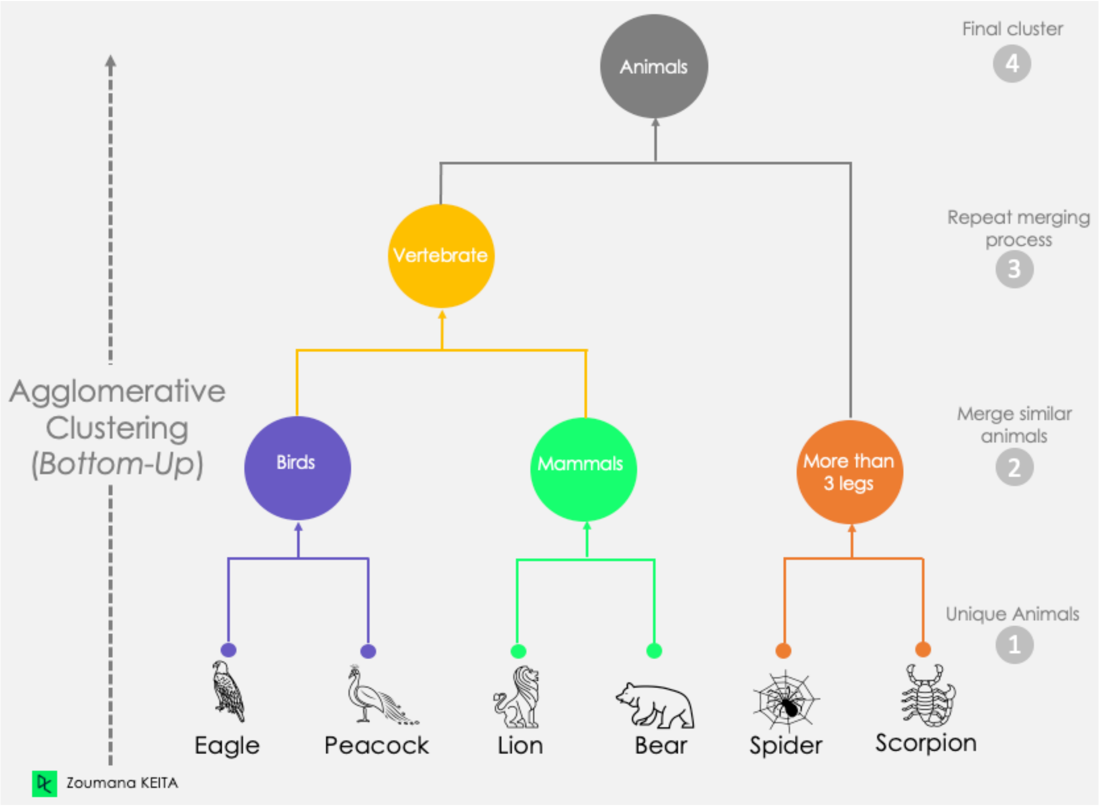
Hierarchical Clustering

- 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.





Hierarchical Clustering

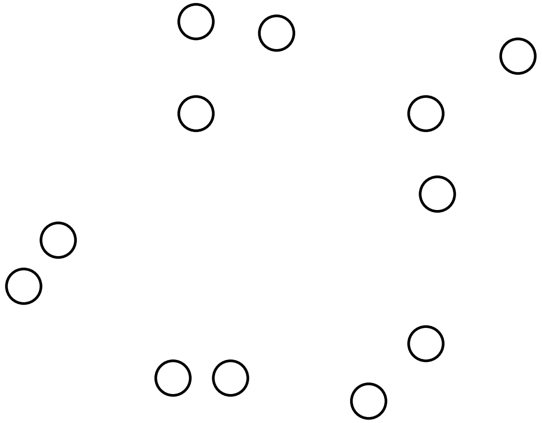


Hierarchical Clustering

- **Key Idea: Successively merge closest clusters**
- 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

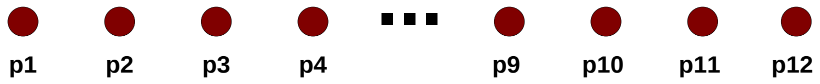
Steps 1 and 2

- Start with clusters of individual points and a proximity matrix



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

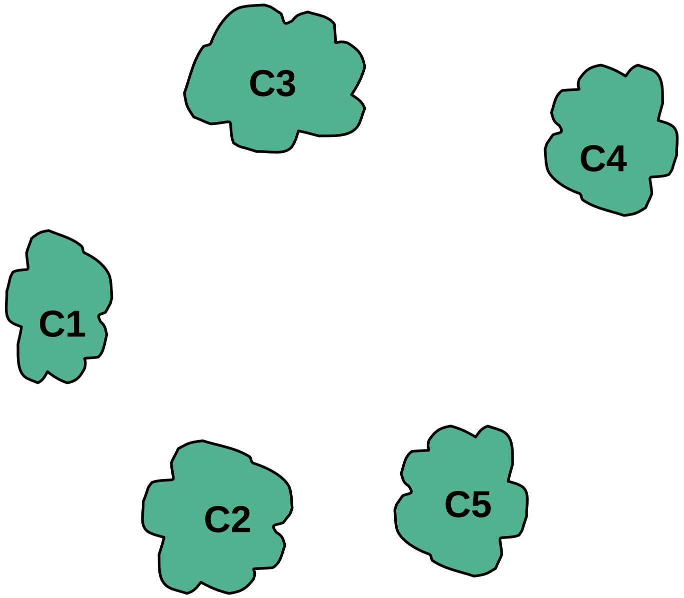
Proximity Matrix

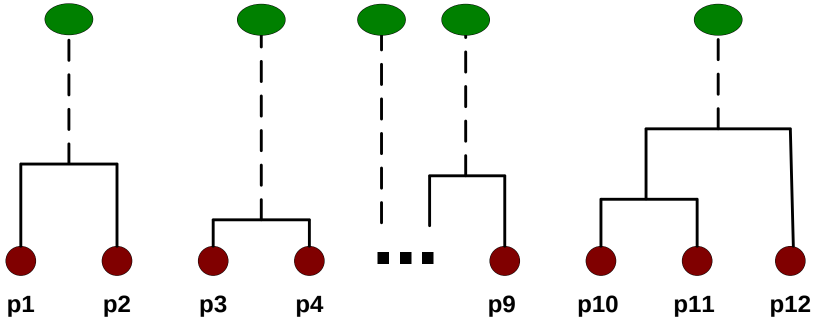


Intermediate Situation

After some merging steps, we have some clusters

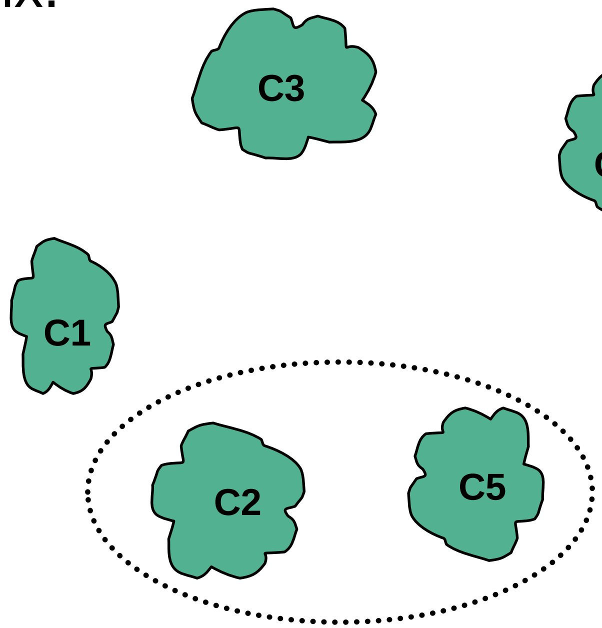
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

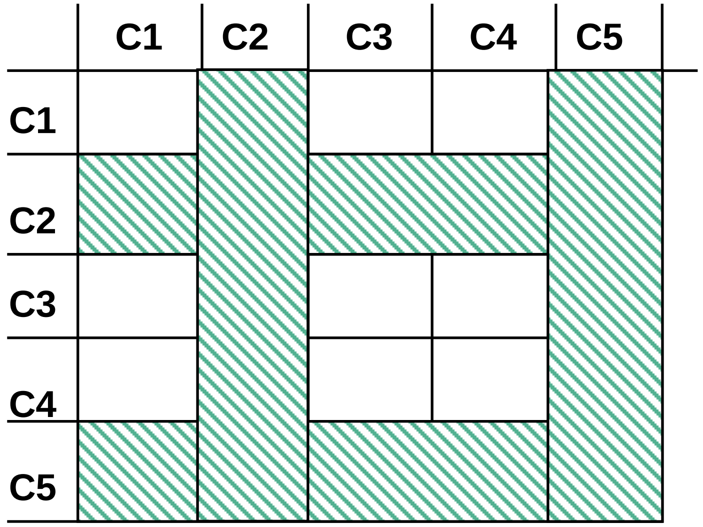




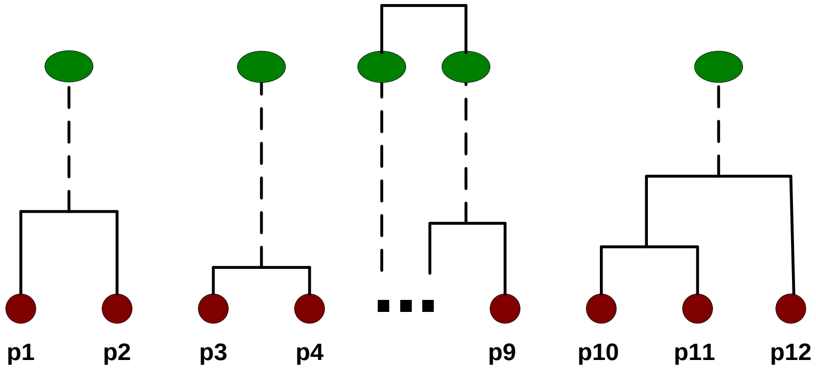
Step 4

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



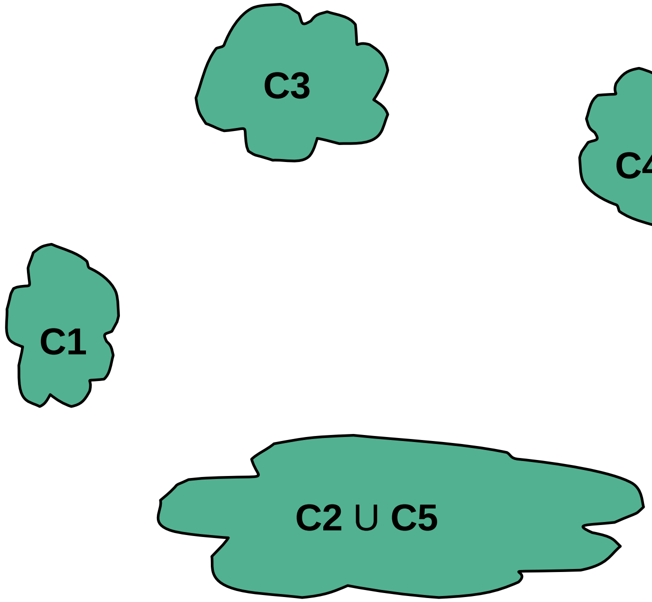


Proximity Matrix



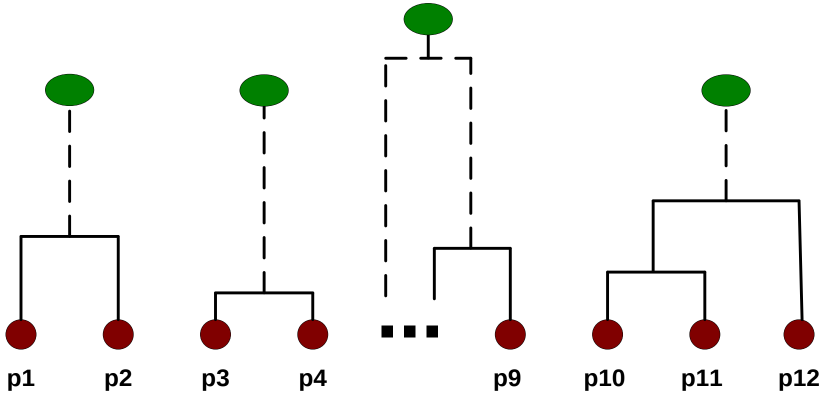
Step 5

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



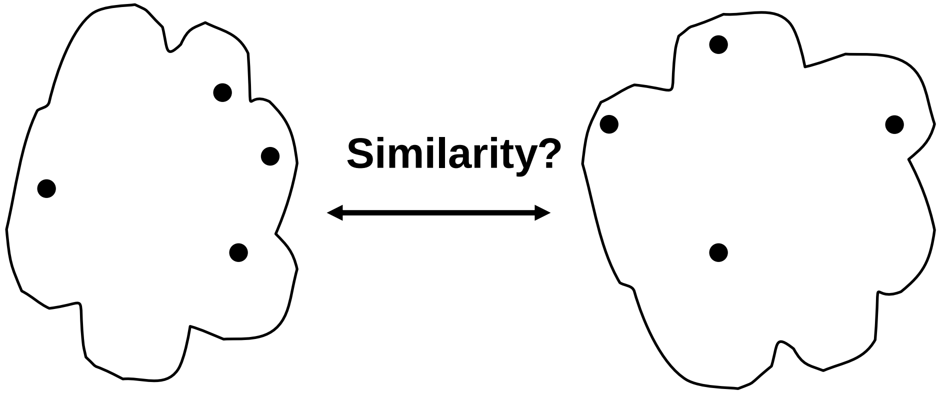
	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		

Proximity Matrix



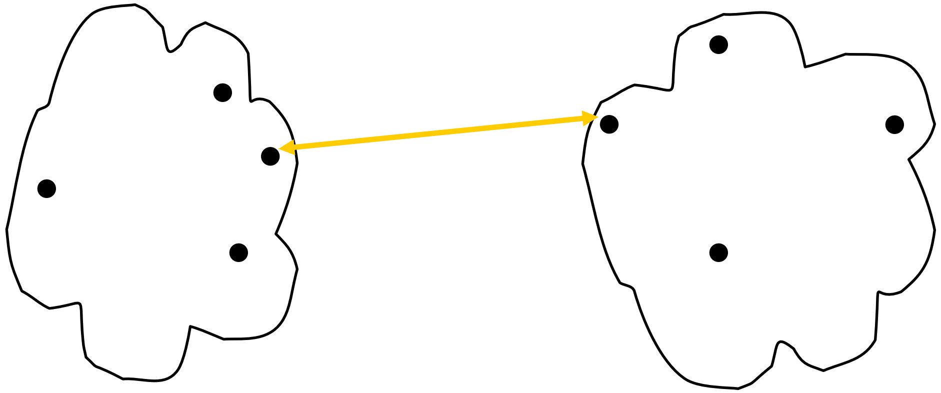
How to Define Inter-Cluster Distance

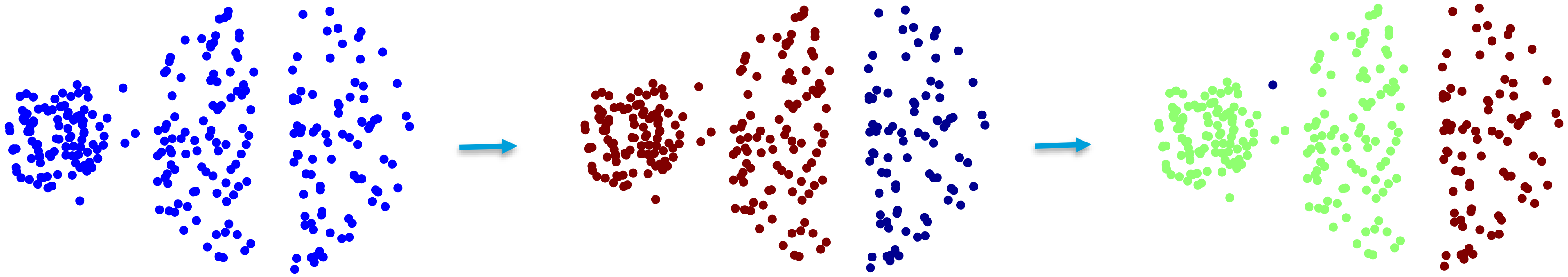
- MIN (Single Link)
- MAX (Complete Linkage)
- Group Average
  - Ward’s Method uses squared error
- Distance Between Centroids



How to Define Inter-Cluster Similarity

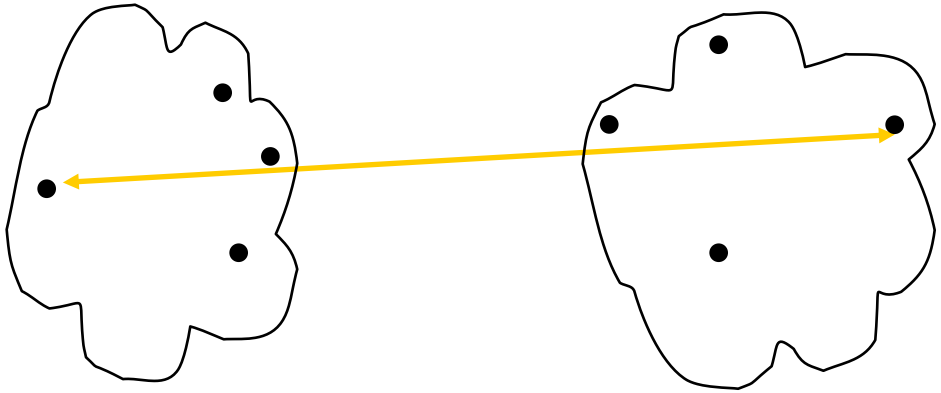
- MIN (Single Link)
  - Sensitive to noise.

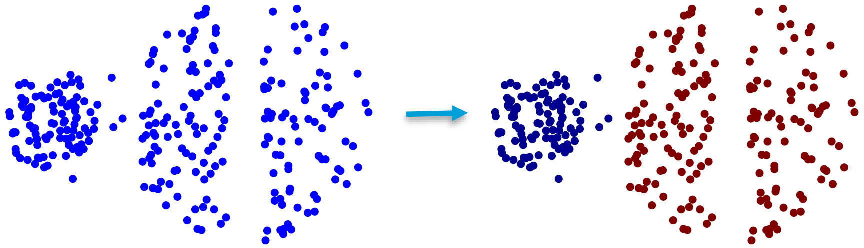


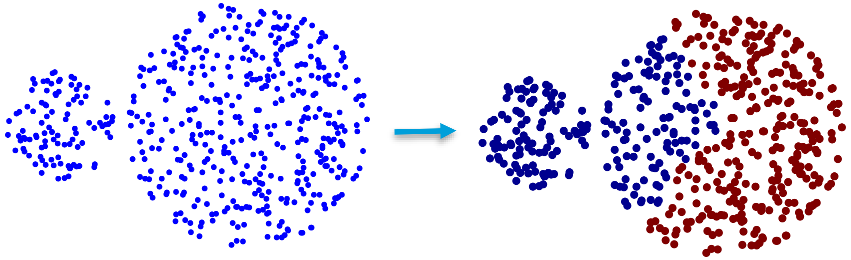


How to Define Inter-Cluster Similarity

- MAX (Complete Linkage)
  - Less susceptible to noise.
  - Breaks larger clusters.

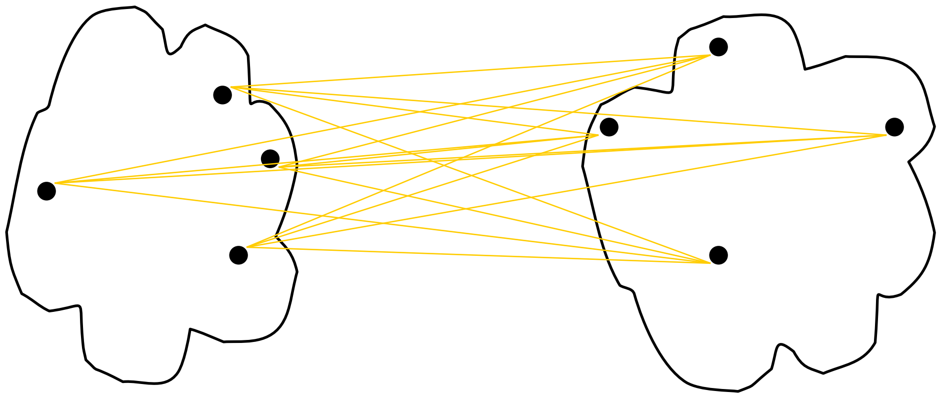






How to Define Inter-Cluster Similarity

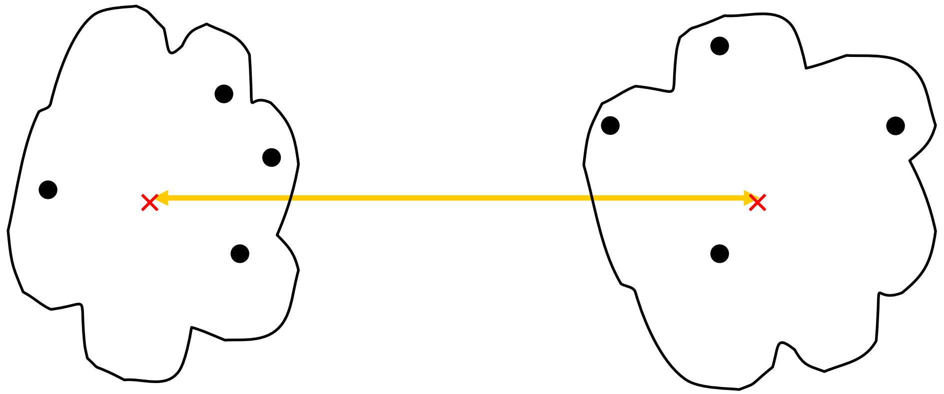
- Group Average
  - Middle ground between MIN and MAX.
  - If square distance is used, it is called Ward method.



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

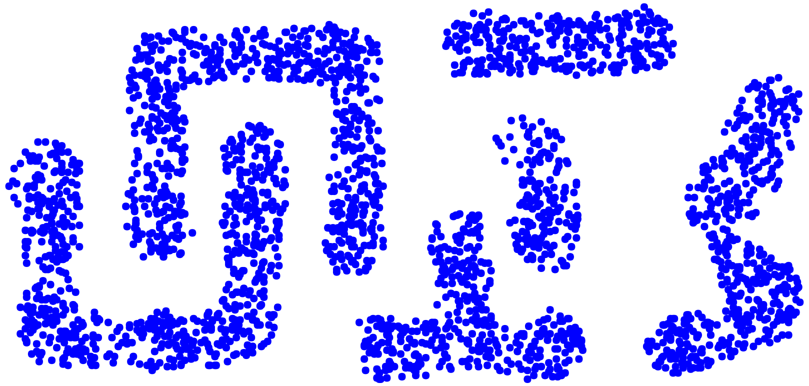
How to Define Inter-Cluster Similarity

- Distance Between Centroids

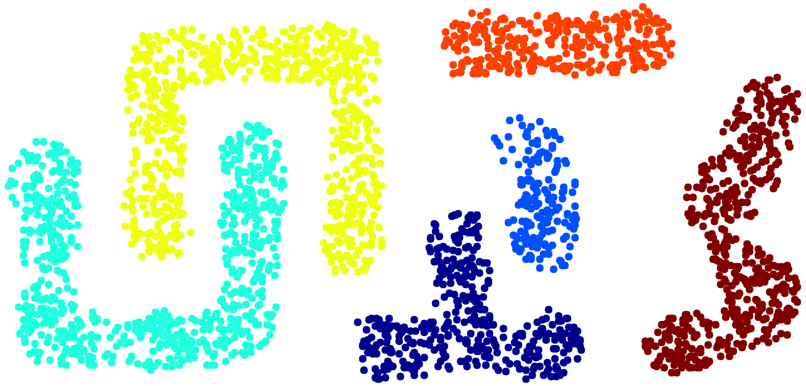


Hierarchical Clustering

Can handle non-elliptical shapes



Original Points



Six Clusters

Hierarchical Clustering

- Visualization + dendograms (easy to find answer when changing number of clusters)
- Hierarchical has a high time complexity (polynomial $O(n^3)$).

Demo time!

Partitional Clustering: K-means

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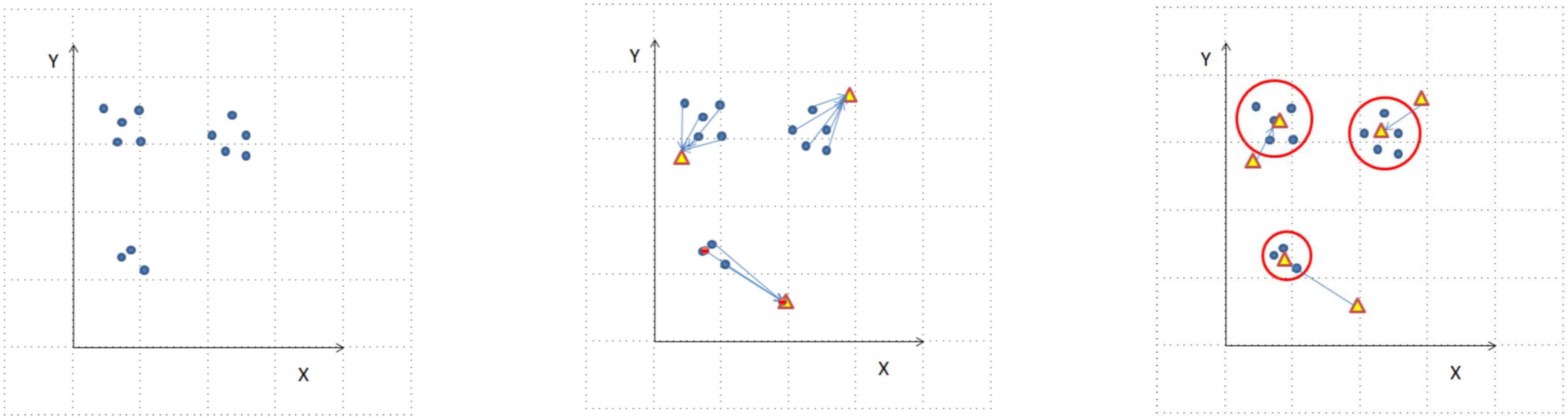
K-means Clustering



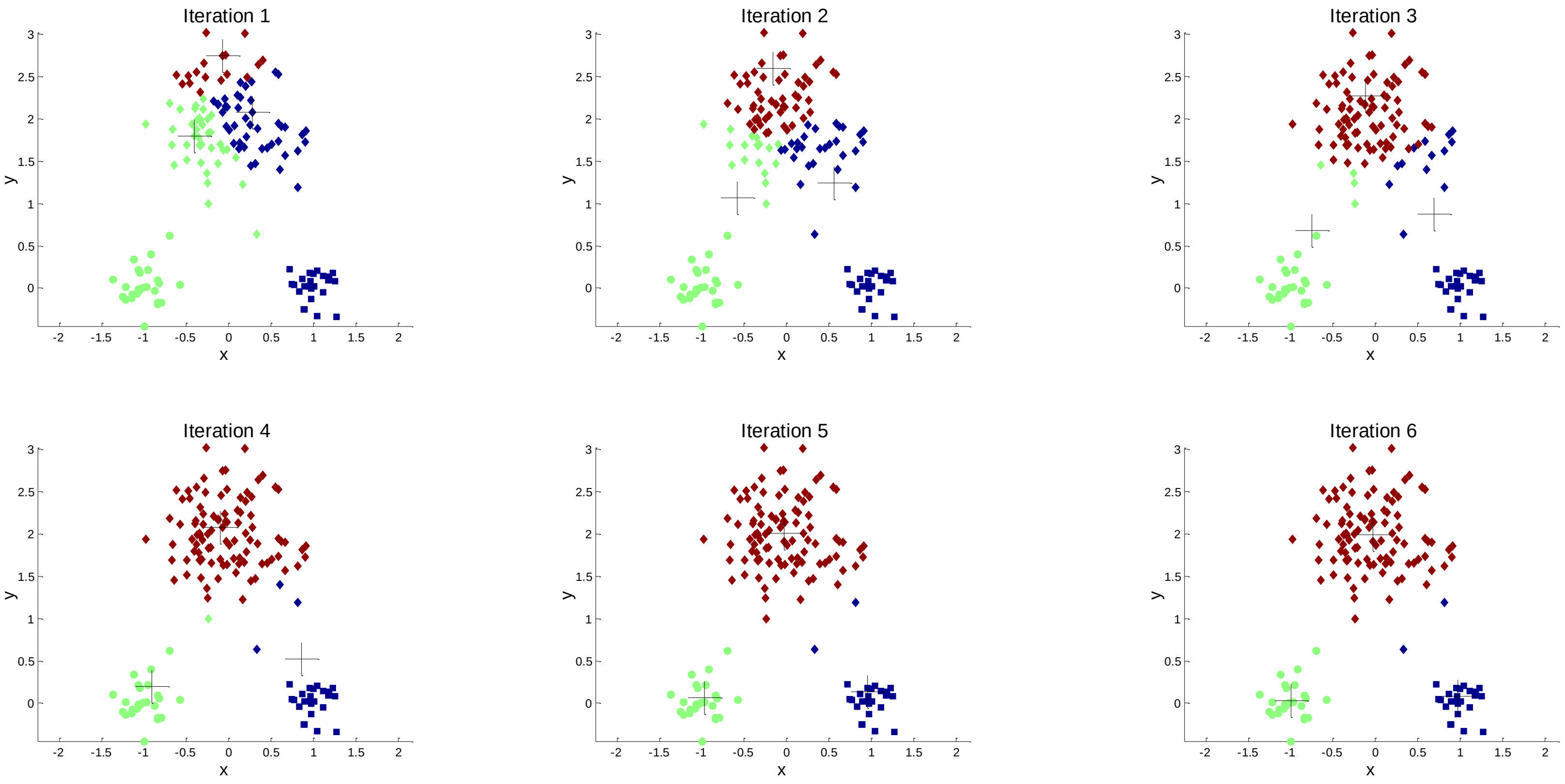
datacamp CLUSTER ANALYSIS IN PYTHON

K-means Clustering

- Number of clusters, K, must be specified in advance.
- 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 Objective Function

- Euclidean 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.

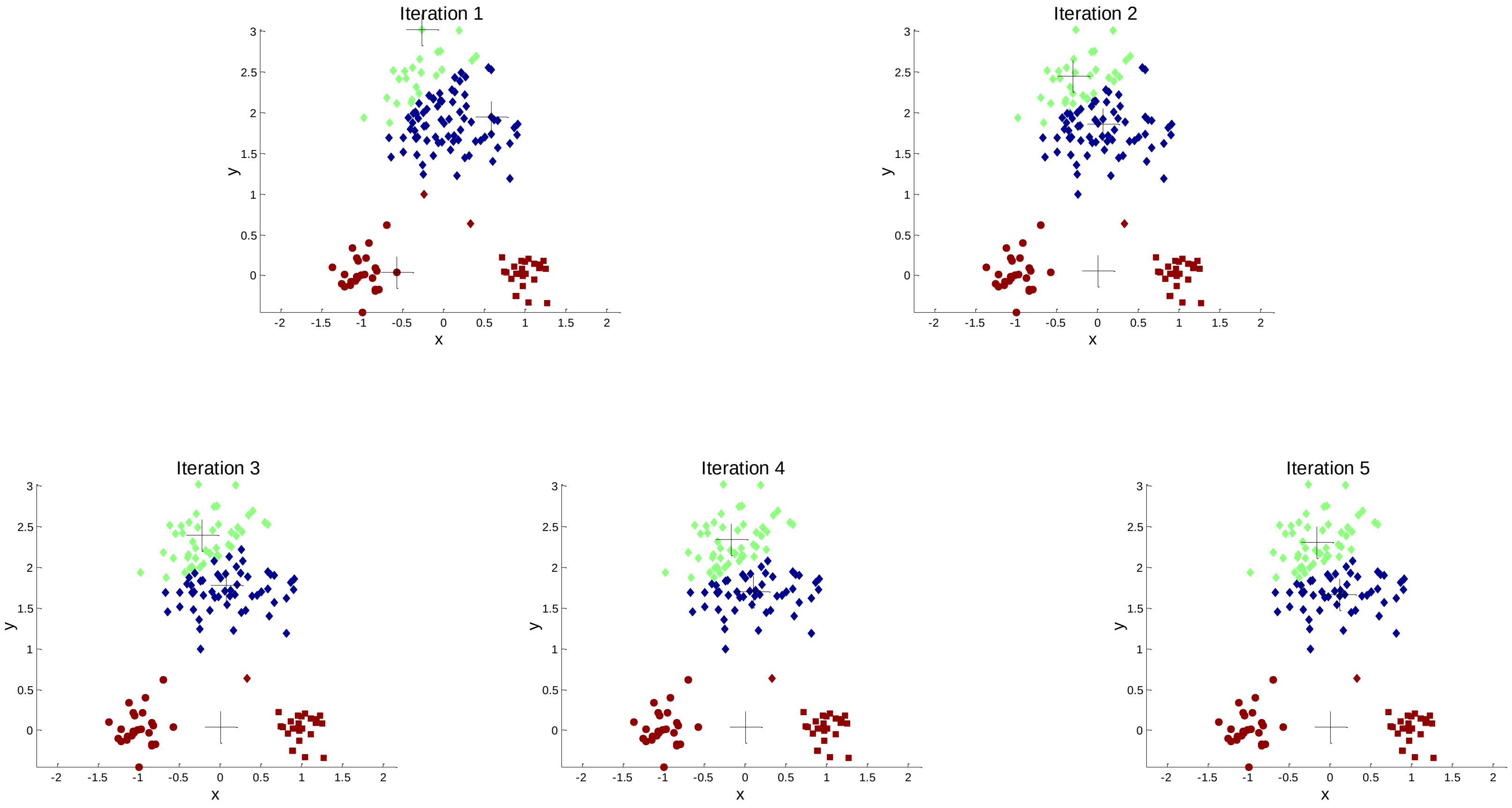
$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(m_i, x)$$

  - This is also called distortion or inertia.
  - 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.

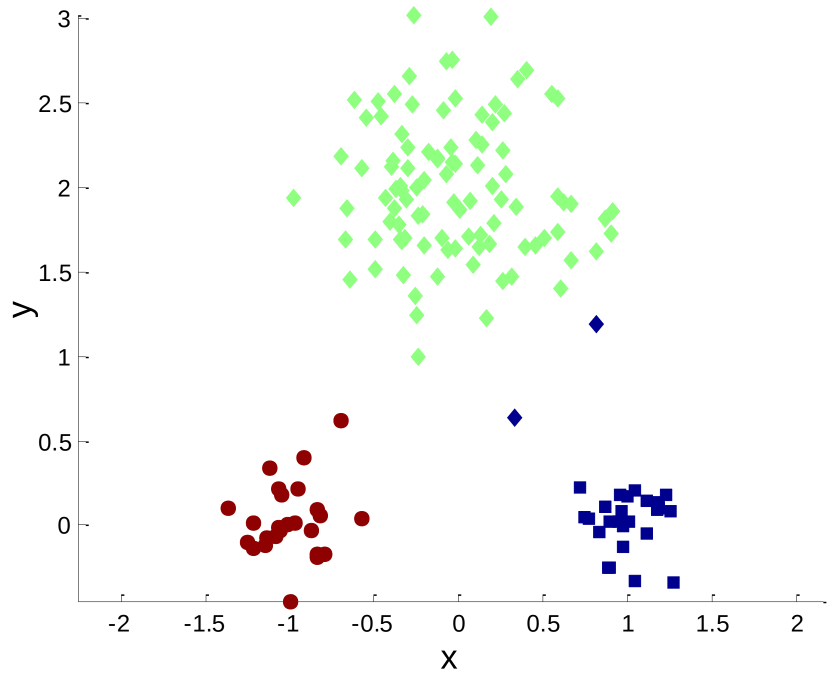
K-means Playground

- This playground helps understand the mechanism of k-means. Use it to better visualize how the distribution of data affects the clustering.

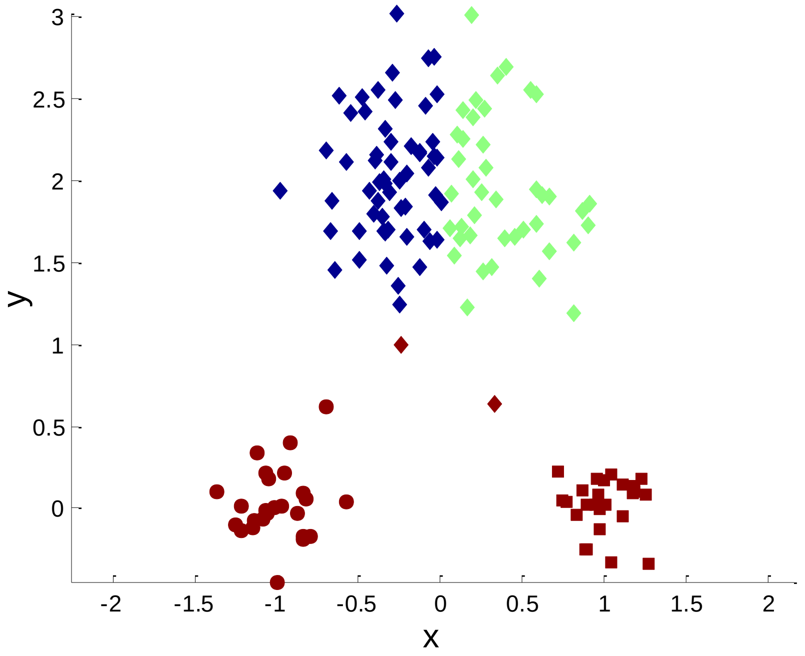
Effect of Random Initialization



Effect of Random Initialization



Optimal Clustering

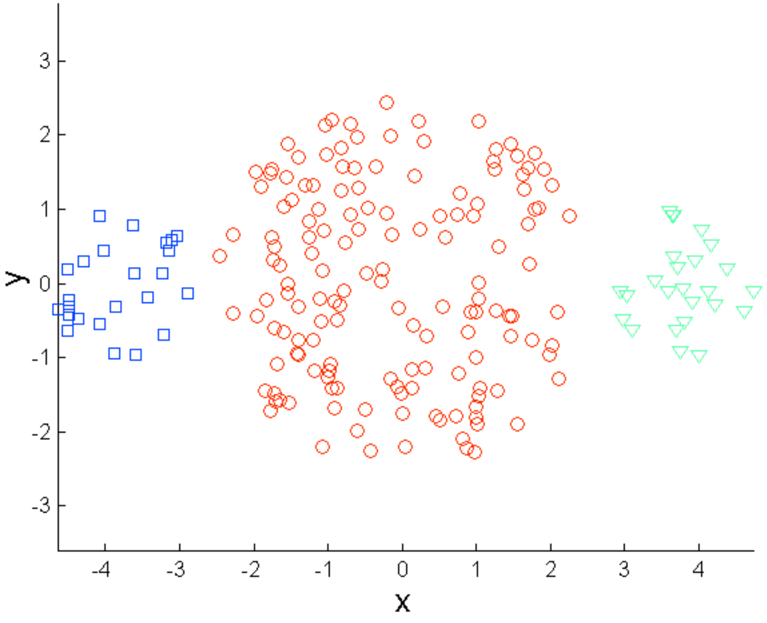


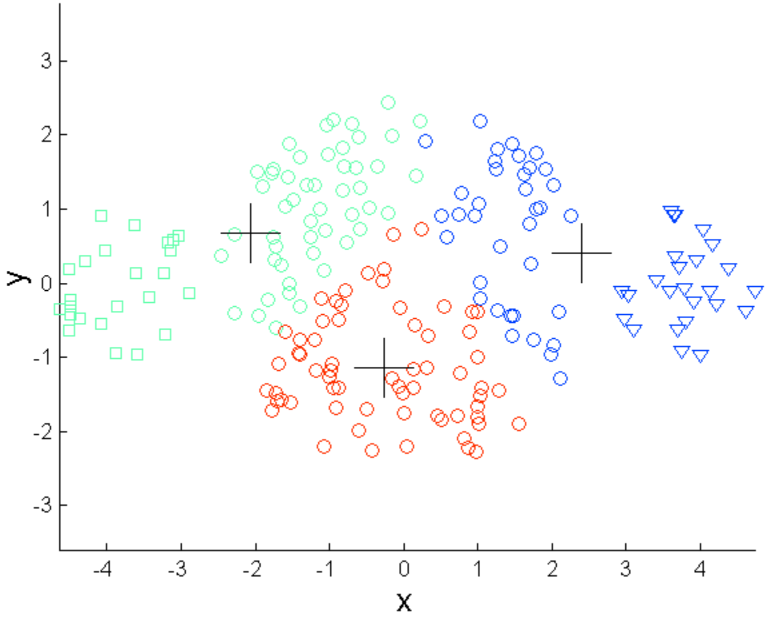
Sub-optimal Clustering

Limitations of K-means

- K-means has problems when clusters are of differing
  - Sizes
  - Densities
  - Non-globular shapes
- K-means is faster than hierarchical clustering.
- K-means is susceptible to suboptimal initialization.
- What do boundaries between clusters look like?
- K-means has problems when the data contains outliers.
  - One possible solution is to remove outliers before clustering

Limitations of K-means: Differing Sizes

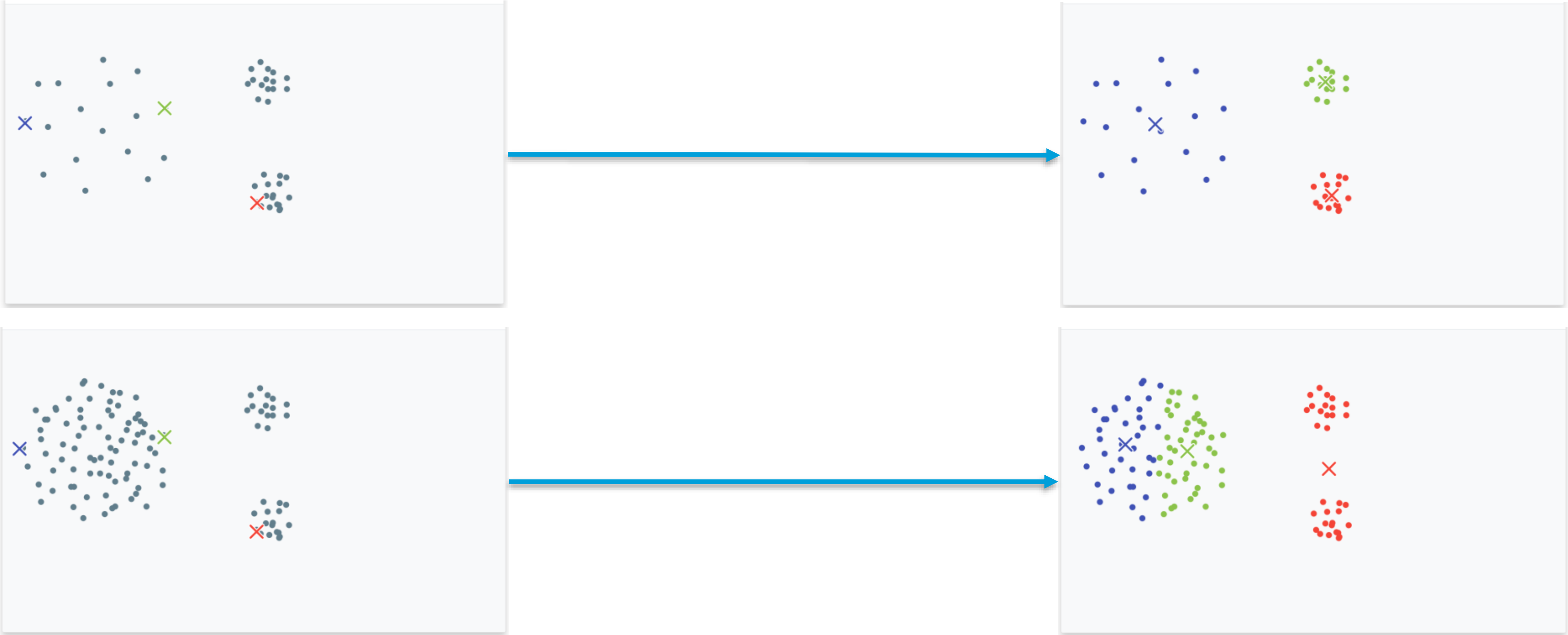




Original Points

K-means (3 Clusters)

Limitations of K-means: Differing Density

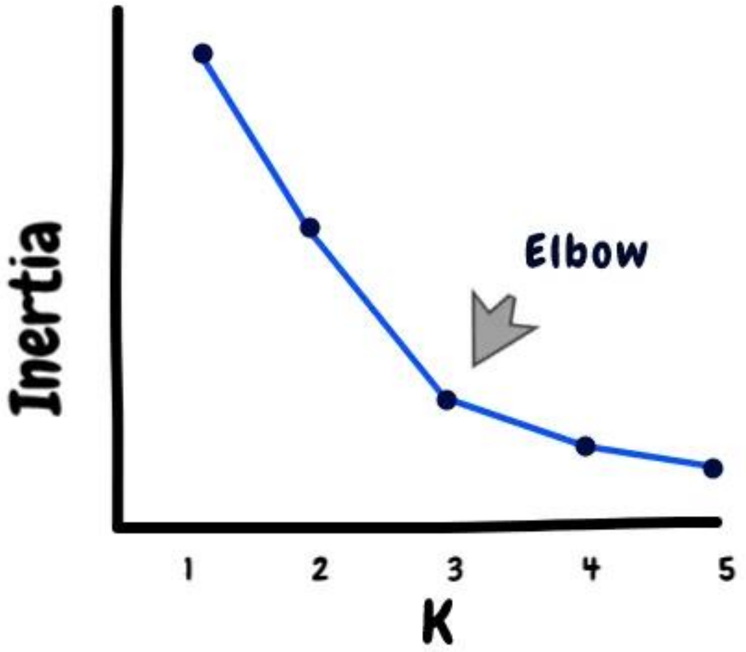


Original Points

K-means (3 Clusters)

Deciding the number of clusters

Inertia: Sum of squared distances of samples to their respective closest cluster centers.



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Measuring Clustering Quality

Method 1: via Labels (Cheating…)

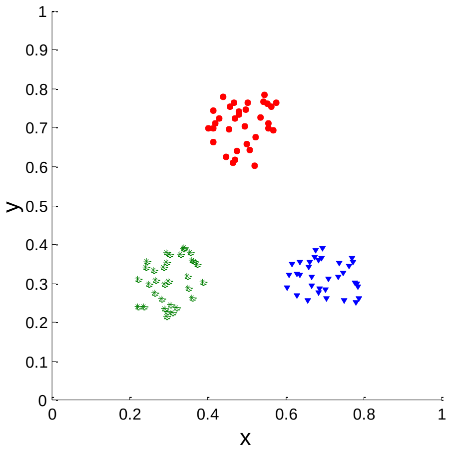
- Testing clustering using supervised learning.
- Calculate the error between ideal labelling and assigned cluster label.

Method 2: via Correlation

- Compute the correlation between the two matrices
- High magnitude of correlation indicates that points that belong to the same cluster are close to each other.
- Not a good measure for hierarchical clustering.
- Similarity can be calculated in many ways.
  - Here, we use $s = \frac{Max - d}{Max}$ or $s = \frac{1}{1+d}$ where *Max* is the maximum possible distance and *d* is the distance measure.

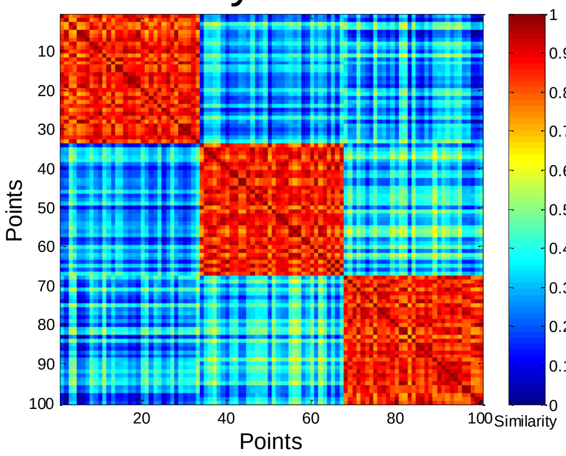
Method 2: via Correlation

- Correlation of ideal similarity and proximity matrices for the K-means clustering



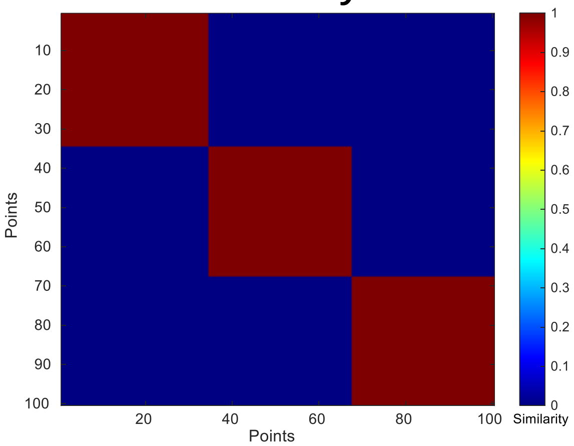
well-clustered data set

Proximity matrix



Corr = 0.9235

Ideal similarity matrix



Method 2: via Correlation

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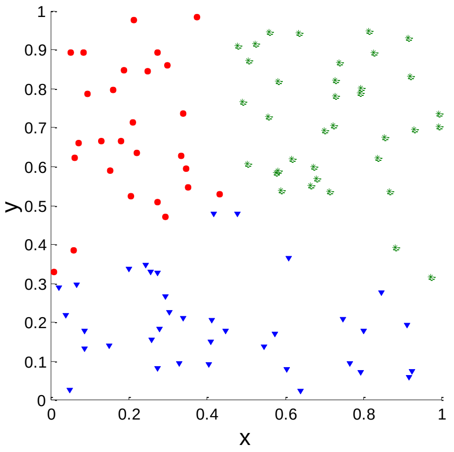
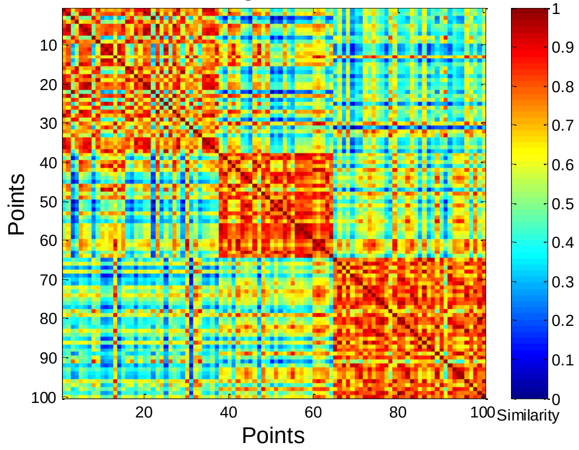
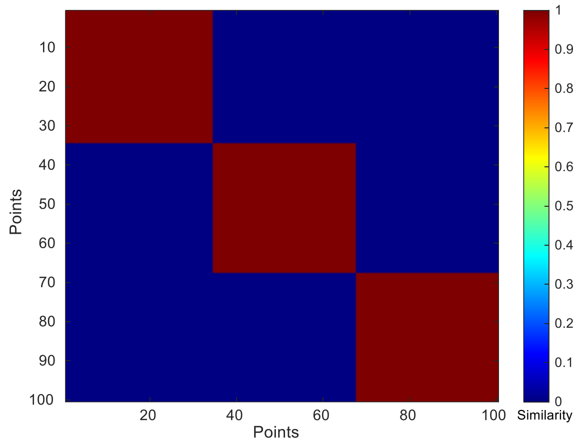


Proximity matrix



Ideal similarity matrix



poorly-clustered data set

Corr = 0.5810