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Machine Learning

Session 5 - T

Unsupervised Learning - Clustering

Degree in Applied Data Science

2024/2025

Unsupervised vs Supervised Learning

- **Unsupervised:** involves working with **unlabeled data**, where the algorithm explores the inherent **structure and patterns** within the input without explicit output guidance.

- **Supervised:** the algorithm is trained on a **labeled dataset**, where the input data is paired with corresponding output labels. The goal is to learn a **mapping from inputs to outputs**, allowing the algorithm to make predictions on new, unseen data.

Unsupervised vs Supervised Learning

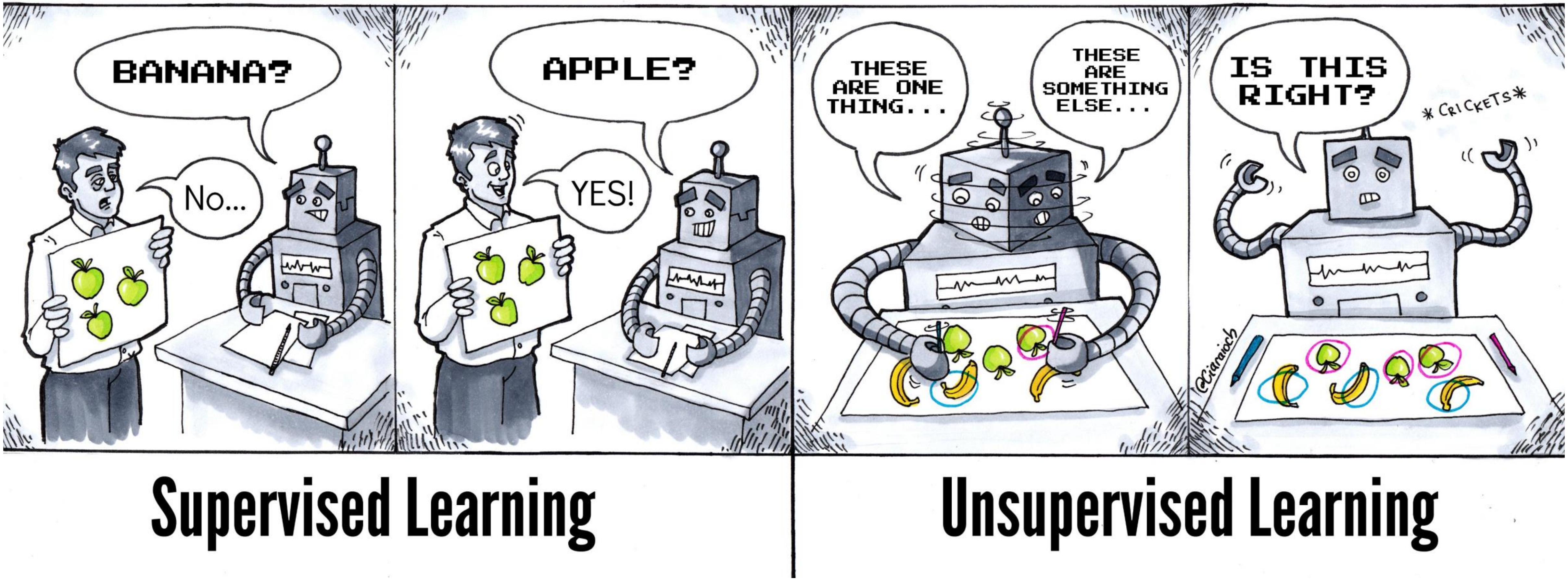
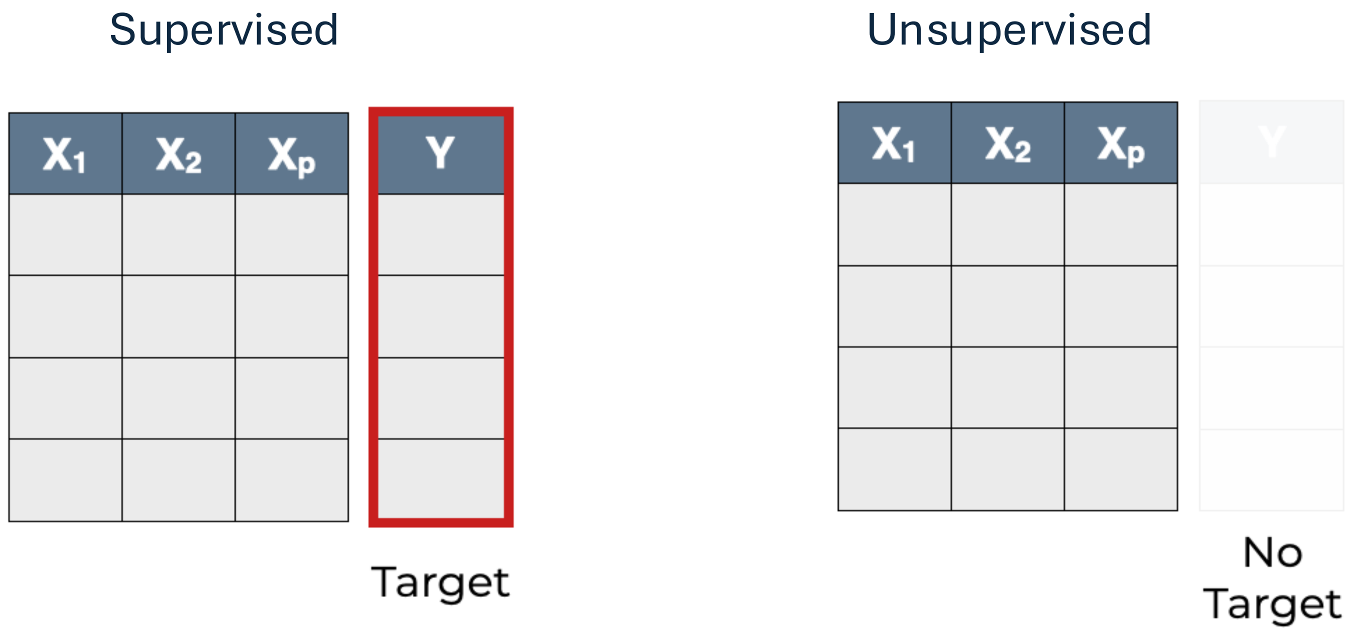


Illustration by @Ciaraioch

Unsupervised Learning

- What can we do in the absence of target labels?
  - Group data based on similarity ⇒ **clustering**
  - Simplify/reduce data ⇒ **dimensionality reduction**
  - Visualize data ⇒ **data visualization**



Clustering

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- Clustering is not a well-defined term with varying definitions in the literature:
  - Finding **groups in data**;
  - Dividing data into homogeneous groups;
  - Dividing data into groups where **points within each group are close or similar**;
  - Dividing data into groups where points within each group are close or similar, and **points of different groups are far or dissimilar**;
  - Dividing the feature space into regions with relatively **high density of points**, separated by regions with relatively **low density of points**.

Our First Clustering Task

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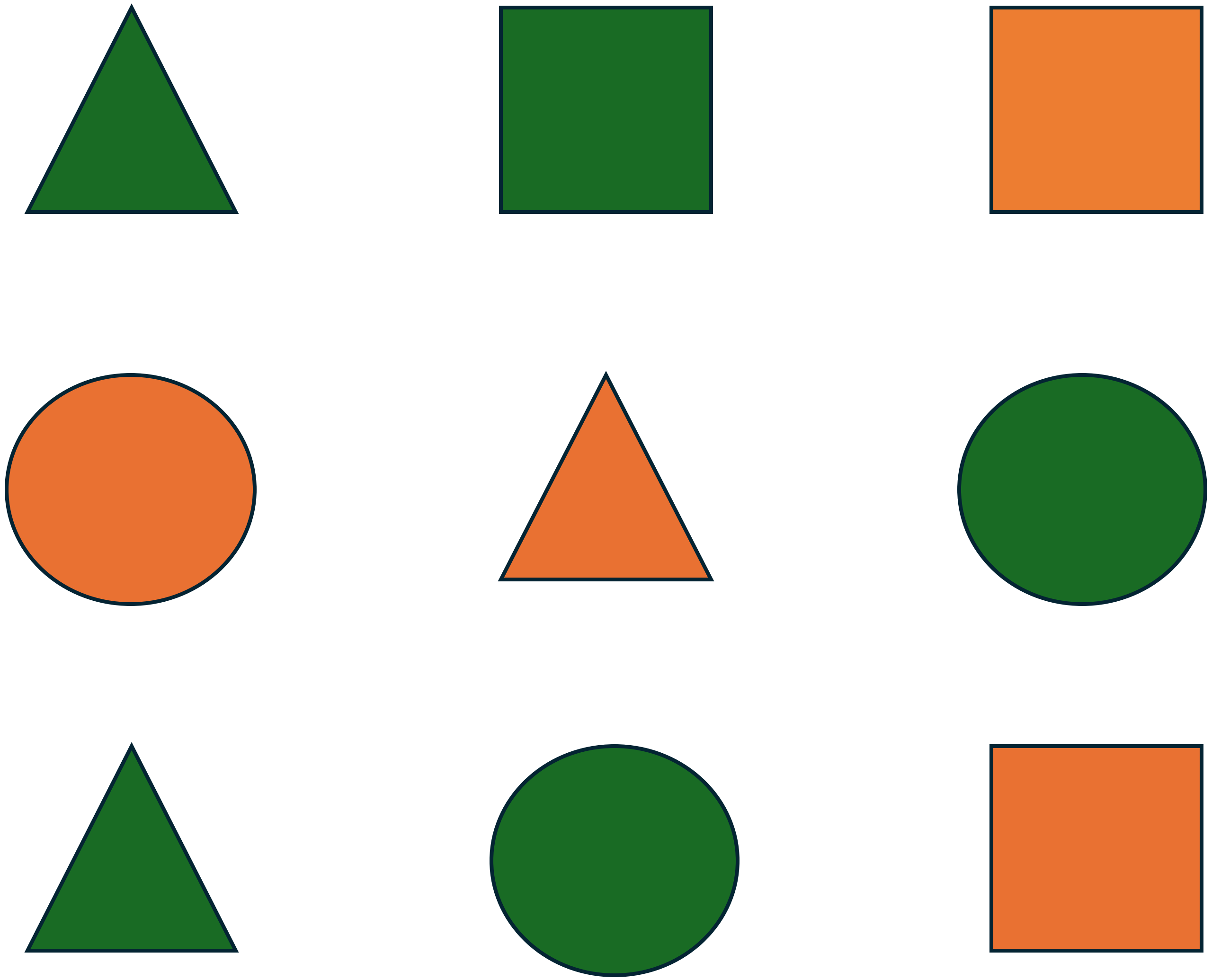
How many clusters?

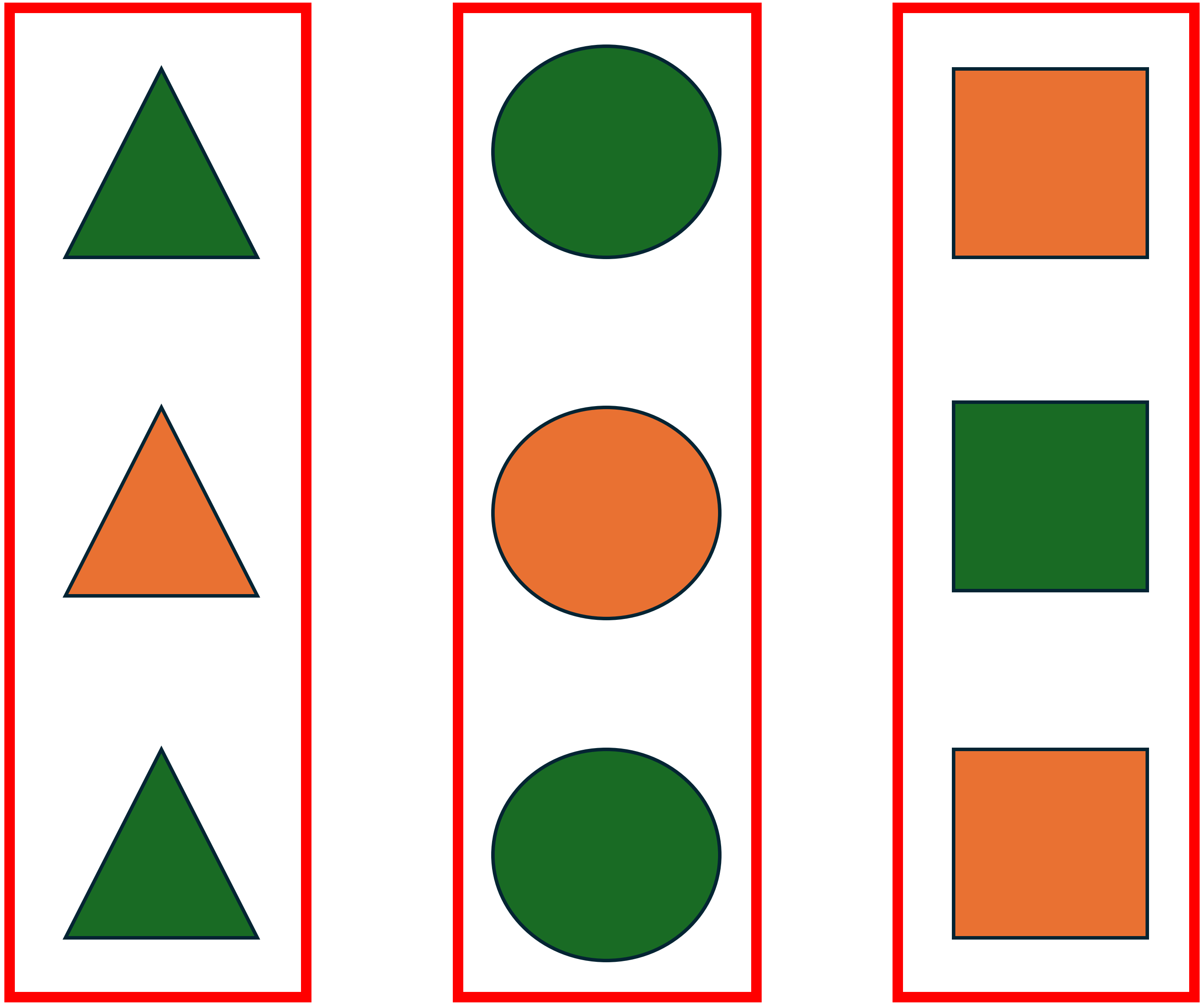
Which forms belong to each cluster?



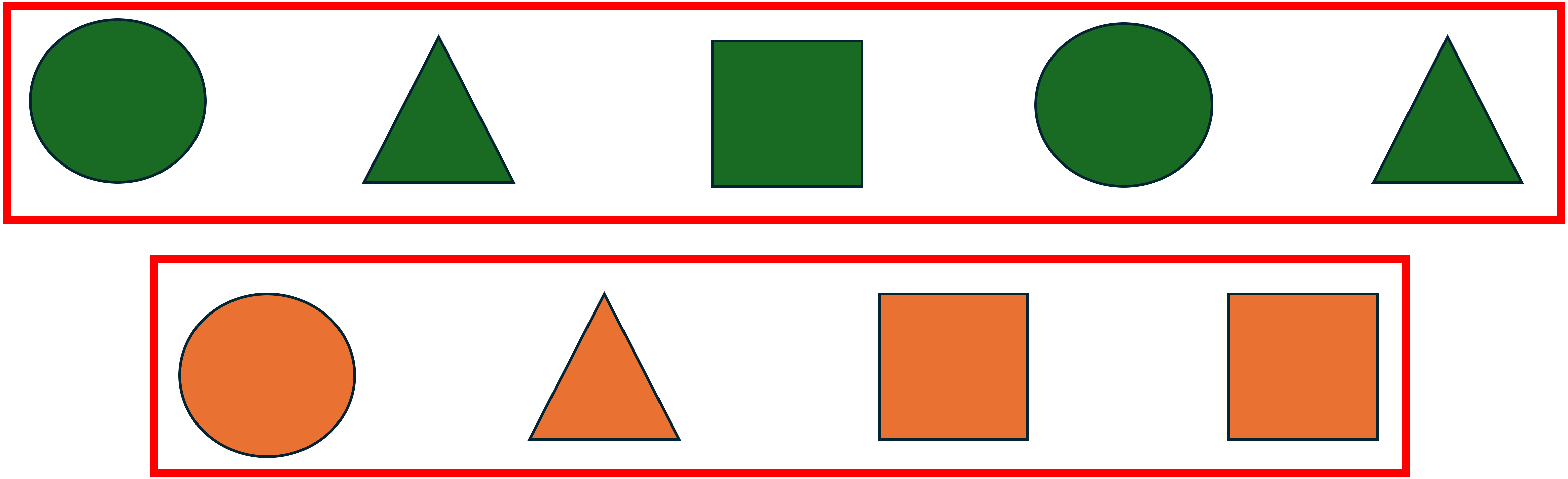
Our first clustering task

3 clusters

by shape



Our first clustering task



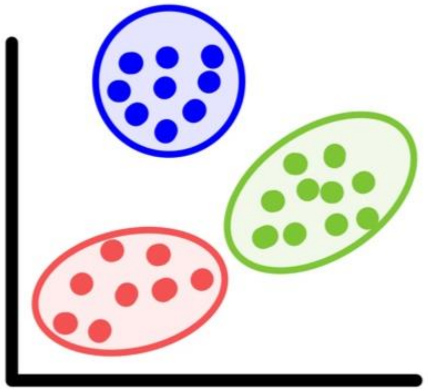
2 clusters **by color**

Clustering

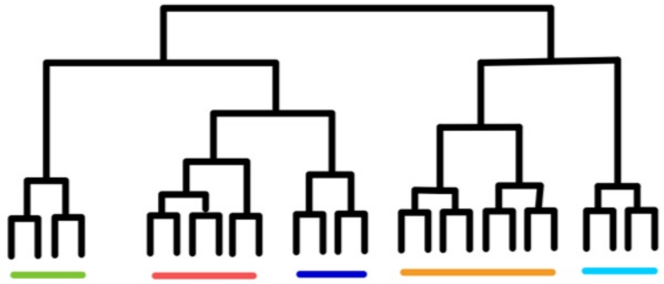
- Mathematically, clustering can be defined as a set of **optimization problems** with several variants.
- The clustering thecnique to use depens on:
  - **Data type** (e.g. numeric, nominal);
  - Desired **output format** (e.g. exclusive clusters, probabilities, hierarchies);
  - **Objective function** (e.g. homogeneity vs separation);
  - **Similarity/distance measure** (e.g. euclidean, manhattan distance).

Defining Clusters

- **Partitional clustering:**
  - Data is divided into groups at the same level.

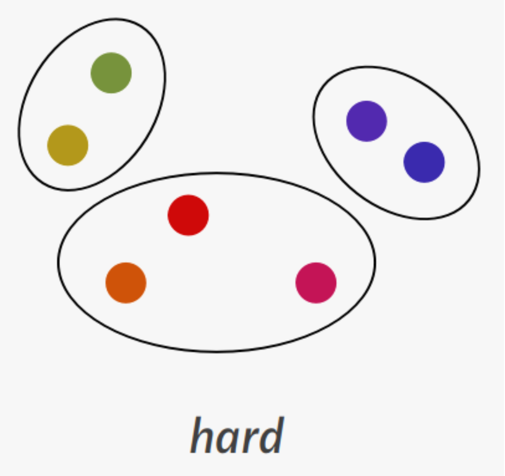


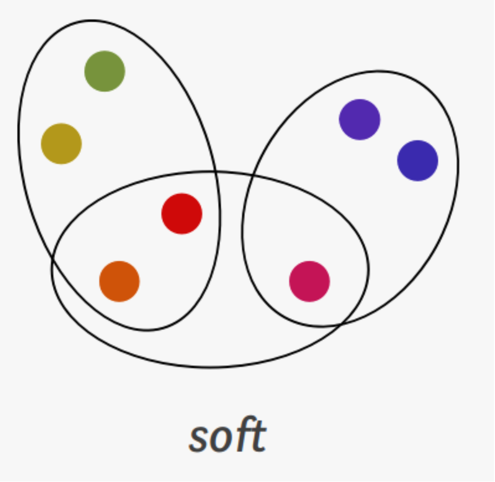
- **Hierarchical clustering:**
  - Clusters are nested within larger clusters, in a tree.



Clustering Membership

- **Hard clustering:**
  - Each example belongs only to one cluster.
- **Soft clustering:**
  - Examples may belong to more than one cluster.
- **Fuzzy clustering:**
  - Each example belongs to clusters with probabilities.





Clustering Coverage

- **Complete clustering:**
  - All examples are assigned to cluster (or clusters);

- **Partial clustering:**
  - Some examples unassigned (e.g. noise, irrelevant data)

Types of Clustering

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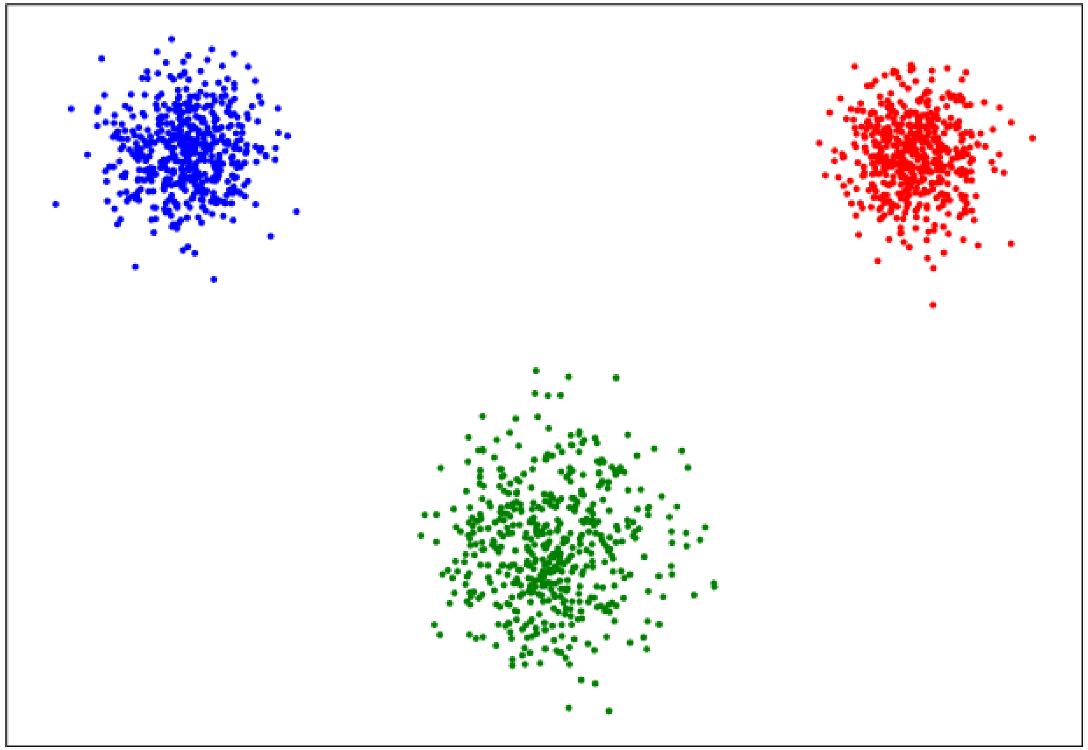
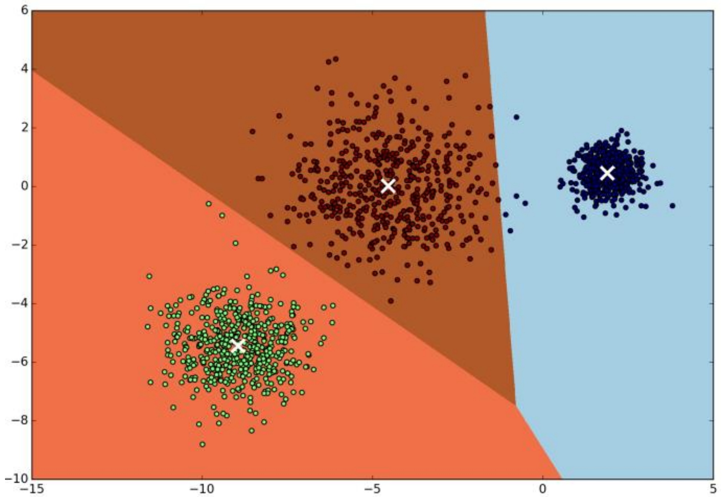
- **Well separated clusters:**
  - Distance between any two points in different clusters is larger than the distance between any two points in the same group.



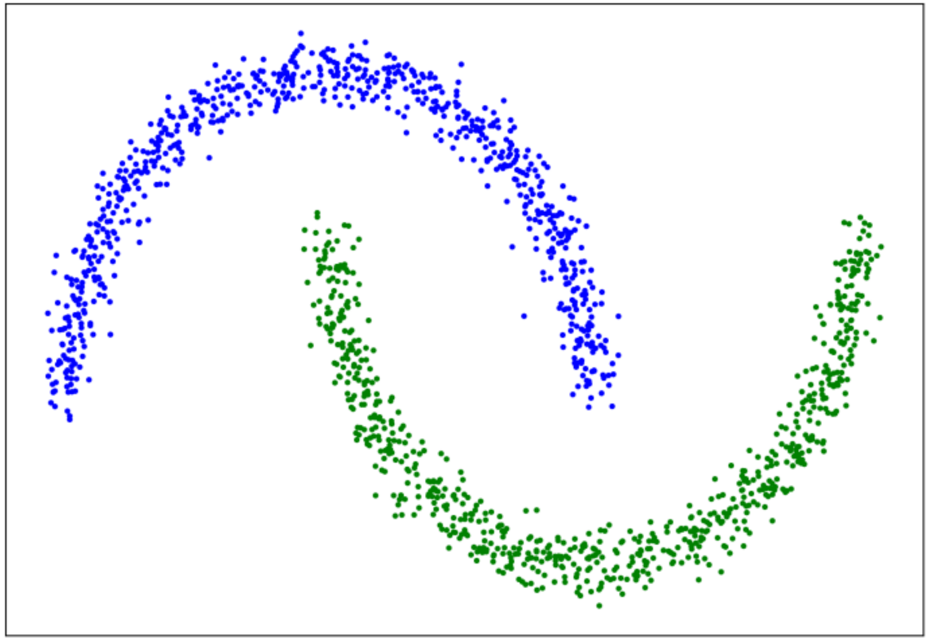
Types of Clustering

- **Prototype-based clustering:**
  - Examples in a cluster are closer to the prototype of the cluster than to the prototype of any other cluster.
  - If the data is **numerical**, the prototype of the cluster is often a **centroid** i.e., the average of all the points in the cluster.
  - If the data has **categorical** attributes, the prototype of the cluster is often a **mode** i.e., the most representative point of the cluster.



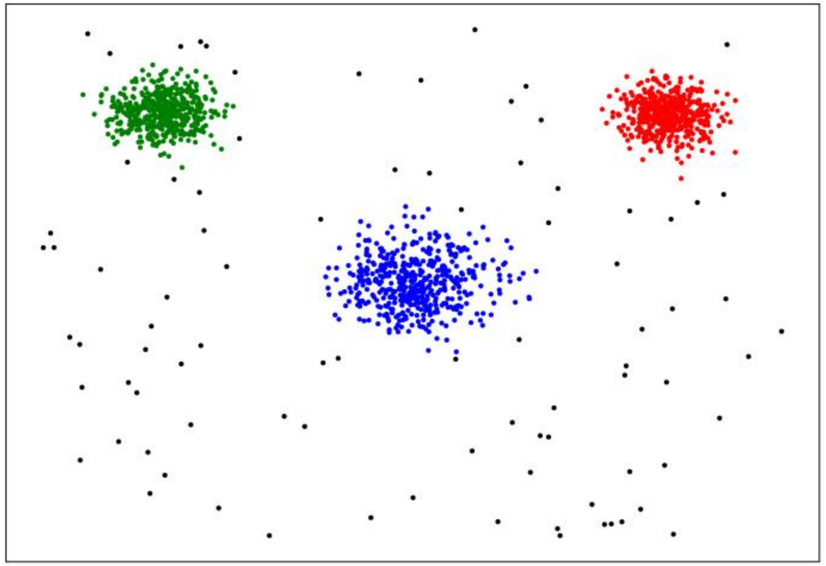
Types of Clustering

- **Contiguity-based clustering:**
  - Each example in a cluster is closer to at least one example in the same cluster than to any example in a different cluster.
  - Useful when clusters are irregular and intertwined.
  - Does not work well when there is noise in the data.



Types of Clustering

- **Density-based clustering:**
  - Cluster is a dense region of examples that is surrounded by a region of low density.
  - Used when the clusters are irregular, intertwined and when noise and outliers are present.
  - Examples in low density region are classified as noise and omitted.



Similarity

- Sometimes is difficult to determine what is similar or not!

- Distance measures:

  - **Euclidean distance:**

$$d(i,j)=\sqrt{(|x_{i_1}-x_{j_1}|^2+|x_{i_2}-x_{j_2}|^2+\ldots+|x_{i_p}-x_{j_p}|^2)}$$

  - **Manhattan distance:**

$$d(i,j)=|x_{i_1}-x_{j_1}|+|x_{i_2}-x_{j_2}|+\ldots+|x_{i_p}-x_{j_p}|$$

Similarity

- Sometimes is difficult to determine what is similar or not!

- Similarity measures:
  - **Jaccard similarity:**

$$J(A,B) = \frac{|A \cap B|}{|A \cup B|} = \frac{|A \cap B|}{|A| + |B| - |A \cap B|}.$$

  - **Pearson correlation:**

$$r = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum (x_i - \bar{x})^2 (y_i - \bar{y})^2}}$$

Homogeneity and Separation

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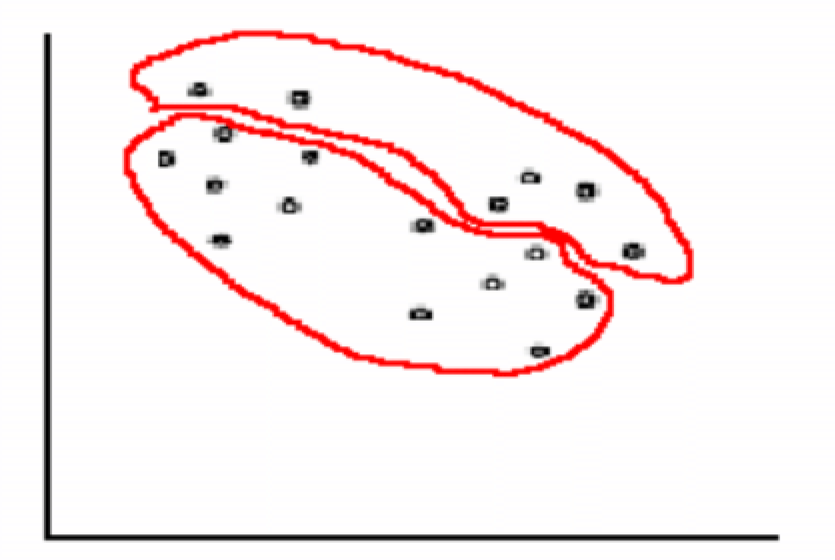
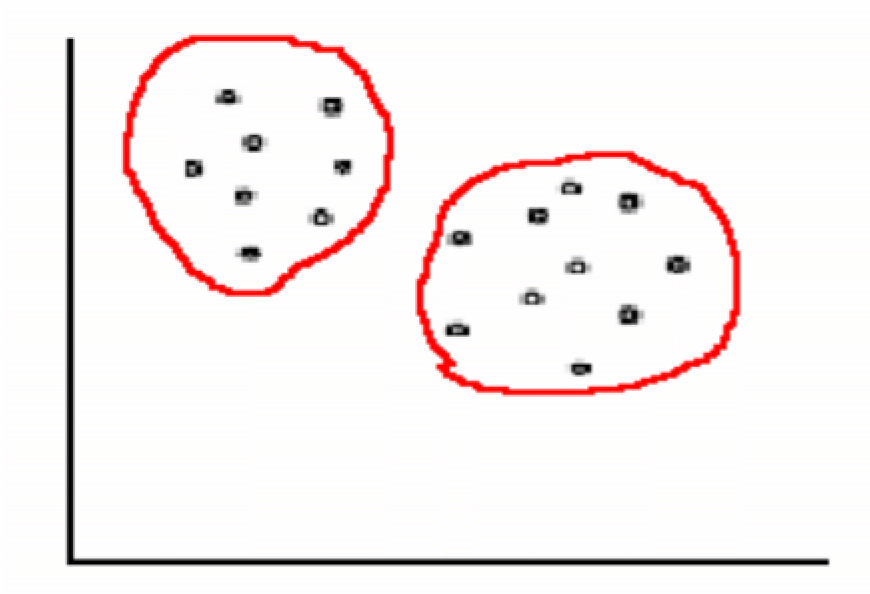
- **Homogeneity:** elements within a cluster must be close to each other (low distances) – intra-cluster

- **Separation:** elements in different clusters should be quite separate from each other (high distances) - inter-cluster

Which clustering would you choose (and why)?

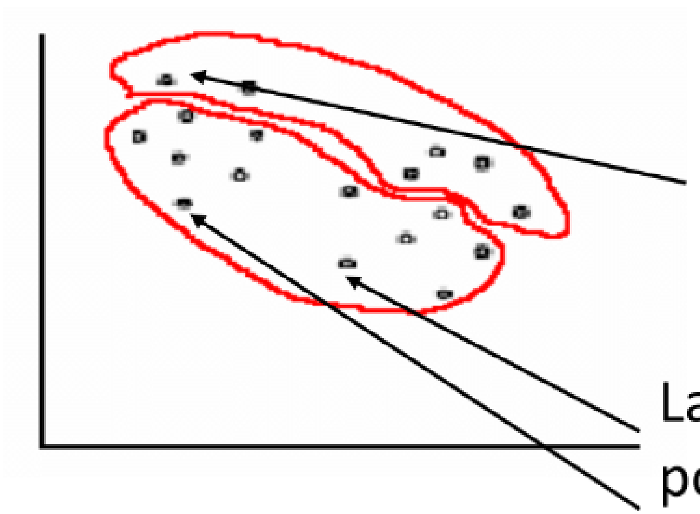


vs



Clustering: "bad" solution

Violates homogeneity and separation

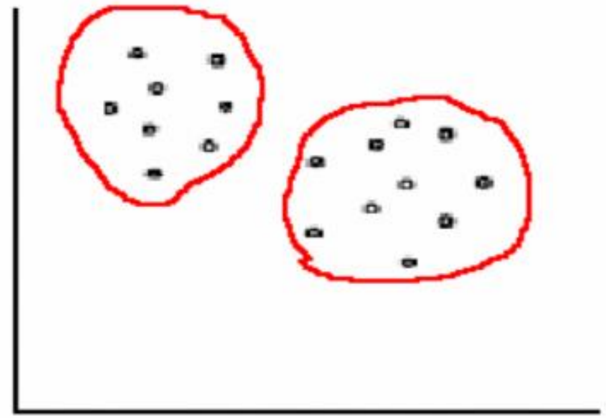


Short distances for points in different clusters

Large distances for points in the same cluster

Clustering: "good" solution

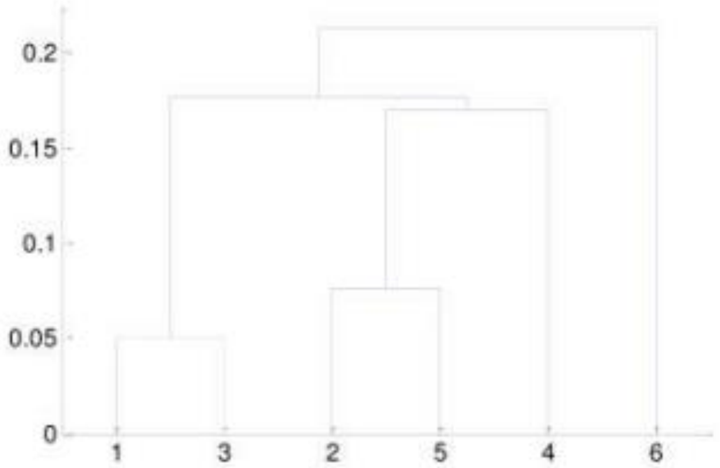
Solution with good homogeneity and separation

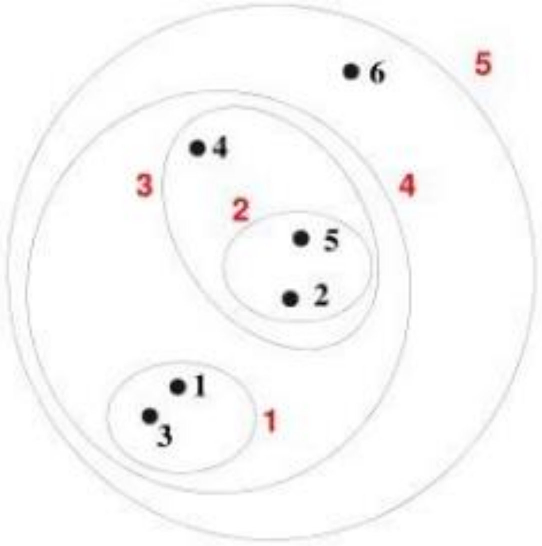


Still, some pairs of points would be better grouped together in the previous solution

Hierarchical Clustering

- Generates a set of **nested clusters** organized as a **hierarchical tree**;
- Visual representation often depicted as a **dendrogram**:
  - A tree like diagram representing a hierarchy of nested clusters
  - Clustering obtained by cutting at desired level





Hierarchical Clustering - Advantages

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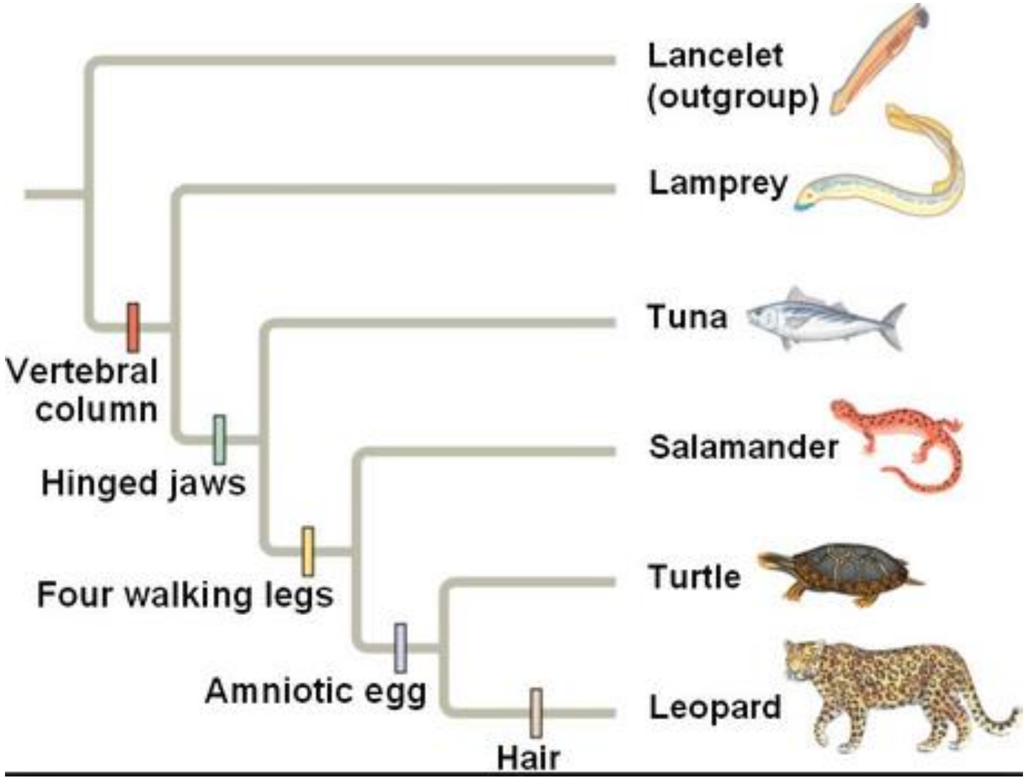
- Do not have to assume any particular number of clusters;

- May correspond to meaningful taxonomies.



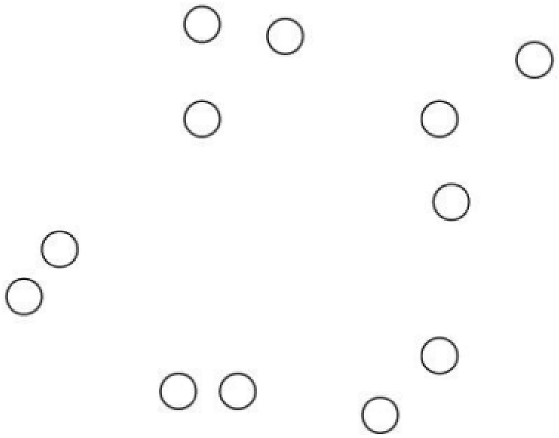
Hierarchical Clustering Types

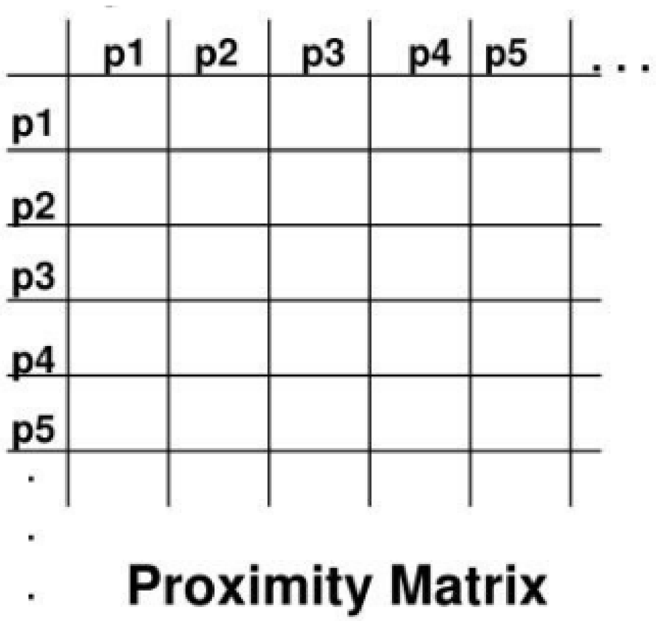
- **Agglomerative:**
  - Start with the examples as individual clusters;
  - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left.

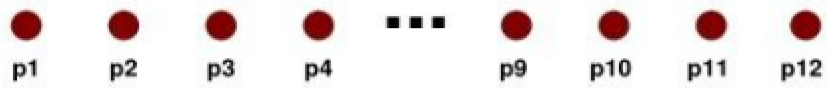
- **Divisive:**
  - Start with one cluster with all examples;
  - At each step, split a cluster until each cluster contains a example (or there are k clusters).

Agglomerative Hierarchical Clustering

1. **Compute the proximity matrix;**
2. **Let each example be a cluster;**
3. Merge the two closest clusters;
4. Update the proximity matrix;
5. Repeat 3 and 4 until a single cluster remains (or k clusters).





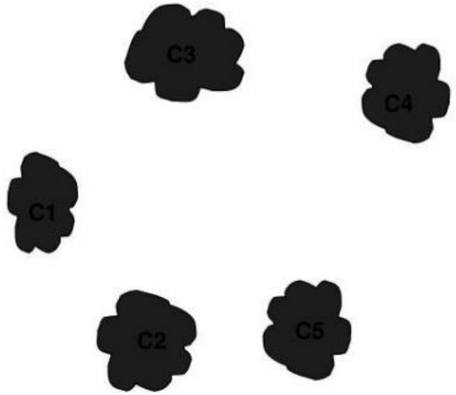


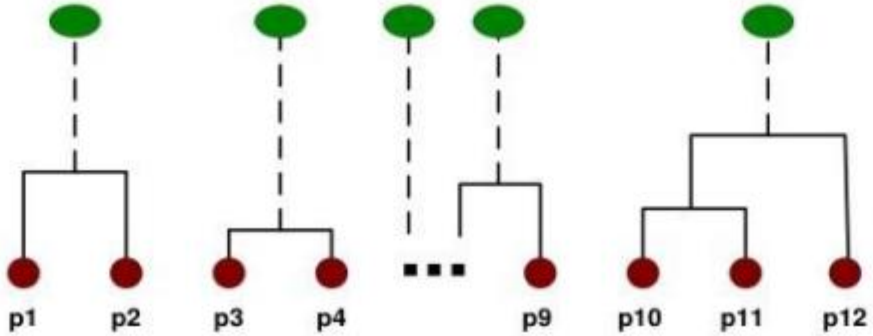
Agglomerative Hierarchical Clustering

1. Compute the proximity matrix;
2. Let each example be a cluster;
3. **Merge the two closest clusters;**
4. **Update the proximity matrix;**
5. **Repeat 3 and 4 until a single cluster remains (or k clusters).**

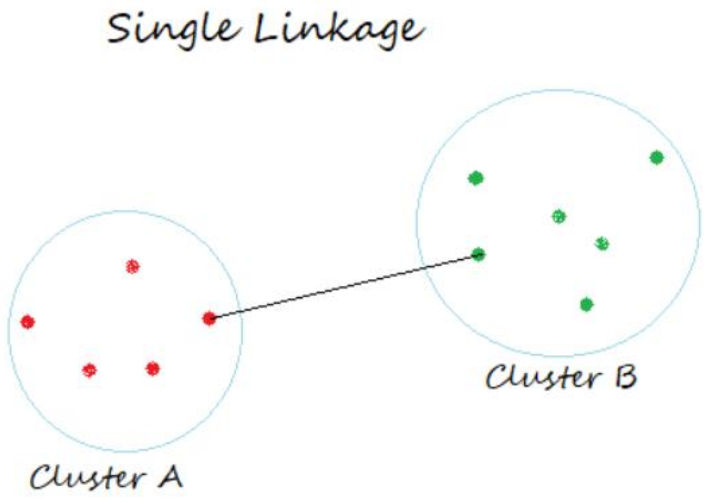
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

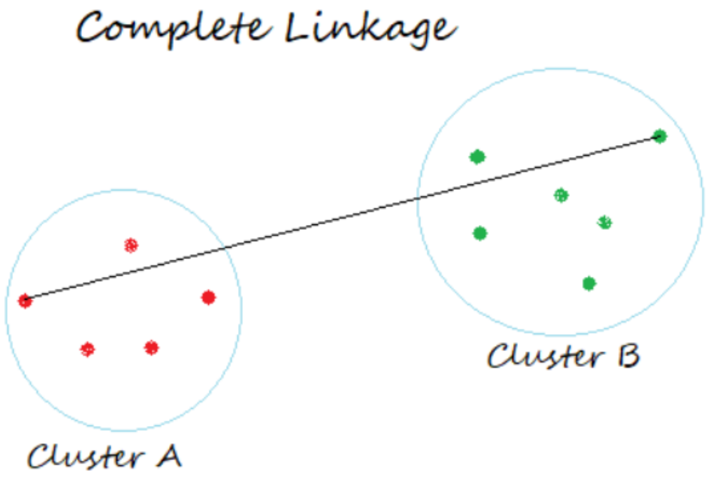
Proximity Matrix

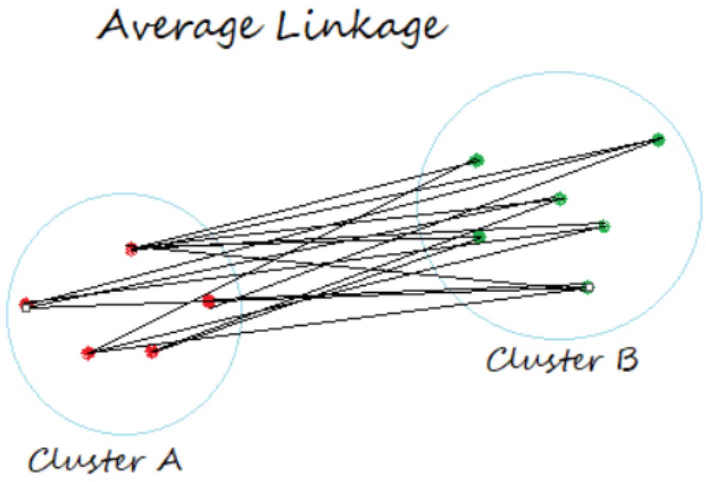


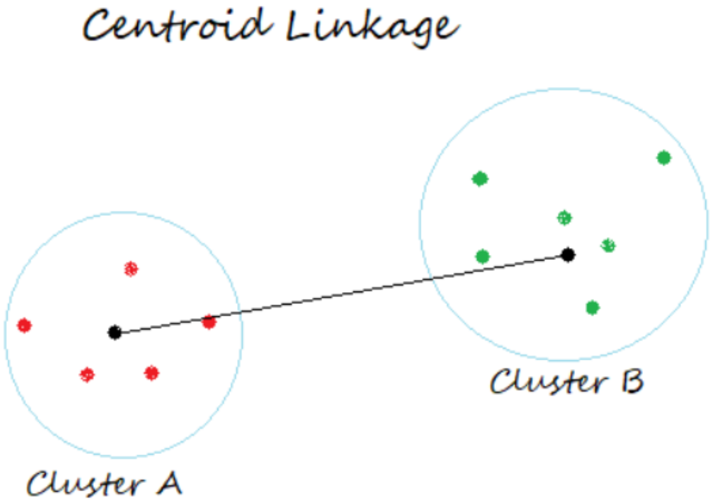


Hierarchical Clustering – Cluster Similarity

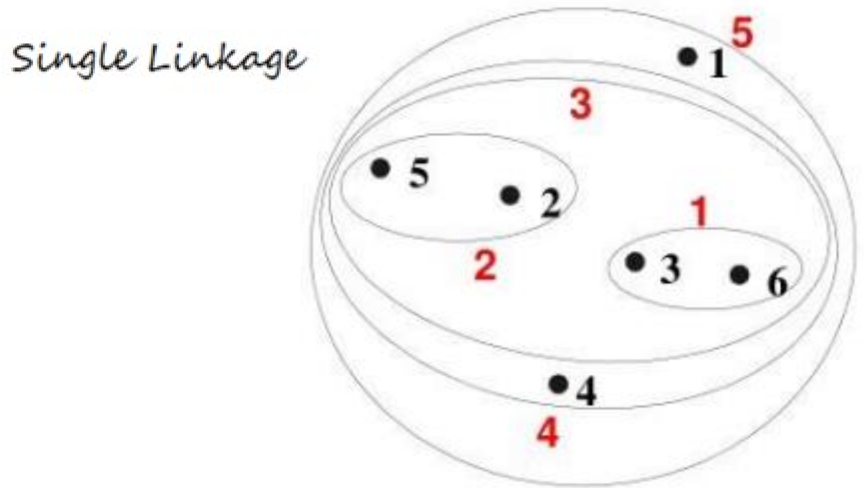


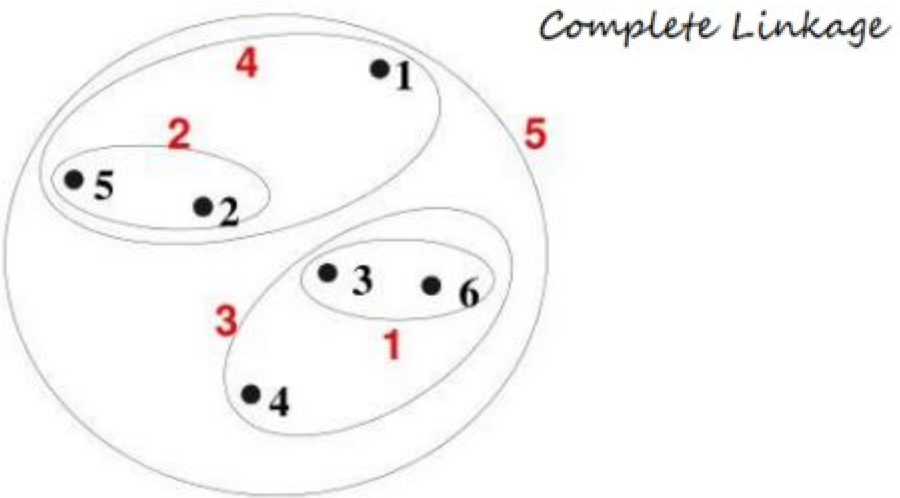


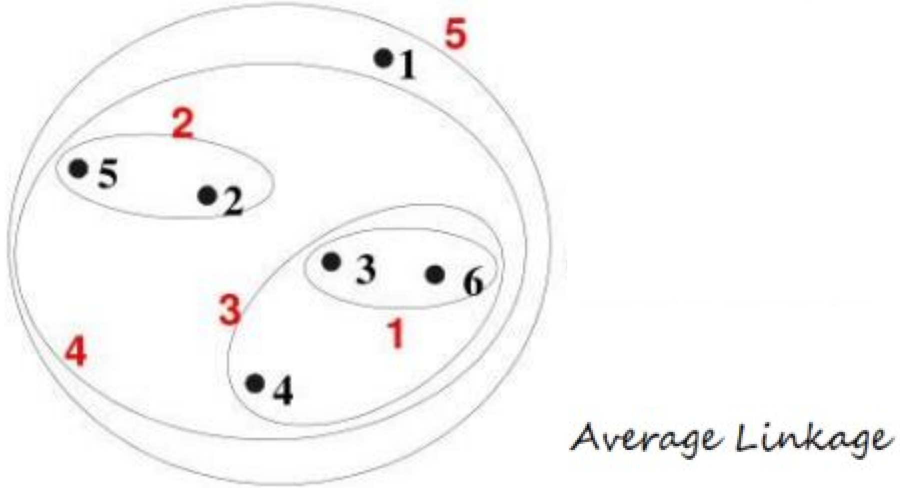




Hierarchical Clustering – Single vs Complete vs Average







Hierarchical Clustering – Single vs Complete vs Average

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- **Single Linkage**:
  - Can handle non-eliptical shapes;
  - Sensitive to noise and outliers.

- **Complete Linkage:**
  - Less susceptible to noise and outliers;
  - Tends to break large clusters;
  - Biased towards globular clusters.

- **Average Linkage:**
  - Compromise between single and complete linkage;
  - Less susceptible to noise and outliers;
  - Biased towards globular clusters.

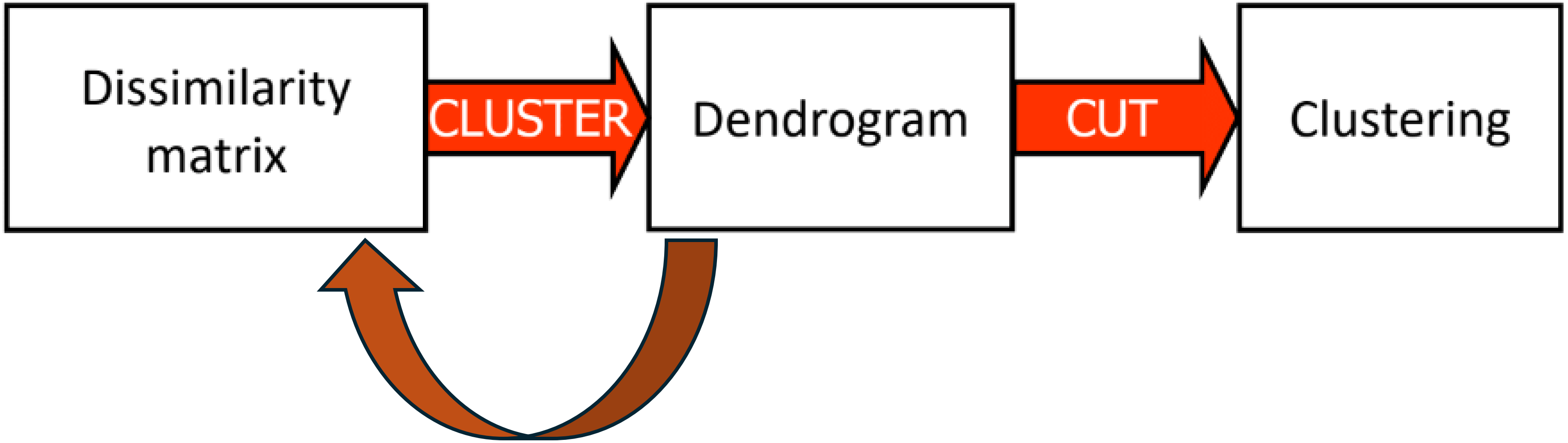
Hierarchical Clustering – Limitations

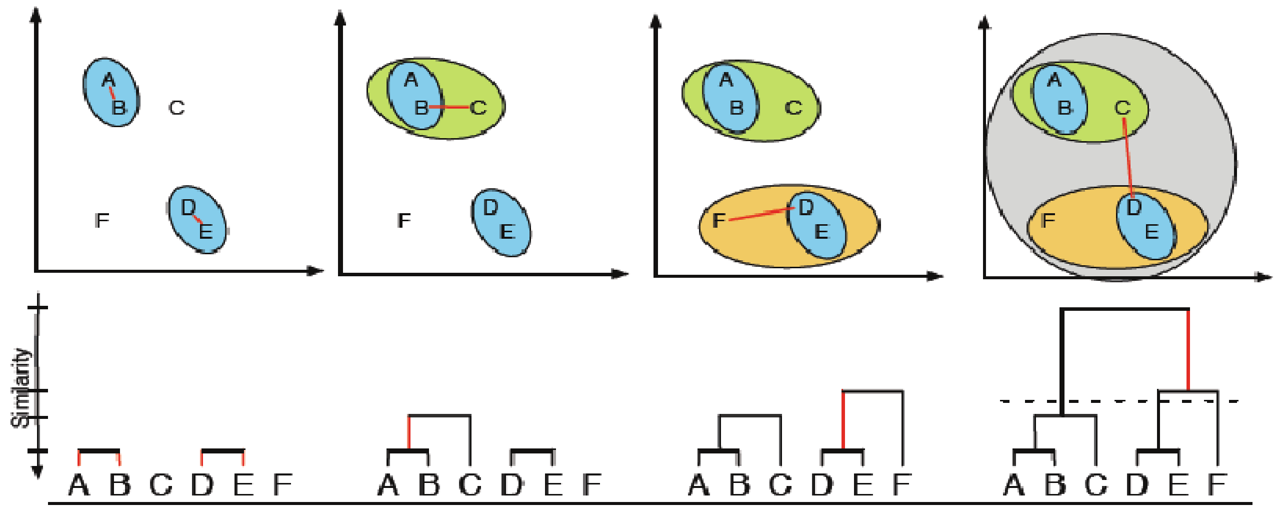
- **Do not scale well:**
  - Space complexity: $O(N^2)$
  - Time complexity: $O(N^3)$
    - $O(N^2 \log(N))$ for some approaches.

- **Cannot undo what was previosly done**;

- **Quality varies** a lot in terms of distance measure used.

Hierarchical Clustering - Summary





Hierarchical Clustering – Applications

- **Biology:** Used in genomics for grouping genes with similar expression patterns, clustering protein sequences, and phylogenetic analysis.
- **Marketing:** Segmentation of customers based on purchasing behavior or demographic characteristics to tailor marketing strategies.
- **Image Analysis:** Grouping similar images together for tasks such as image retrieval, object recognition, and image compression.
- **Document Clustering:** Organizing documents by topic for information retrieval, text mining, and document summarization.
- **Anomaly Detection:** Identifying outliers or unusual patterns in data, such as detecting fraudulent transactions or network intrusions.
- **Finance:** Segmenting financial data for portfolio optimization, risk assessment, and fraud detection.

K-Means Clustering

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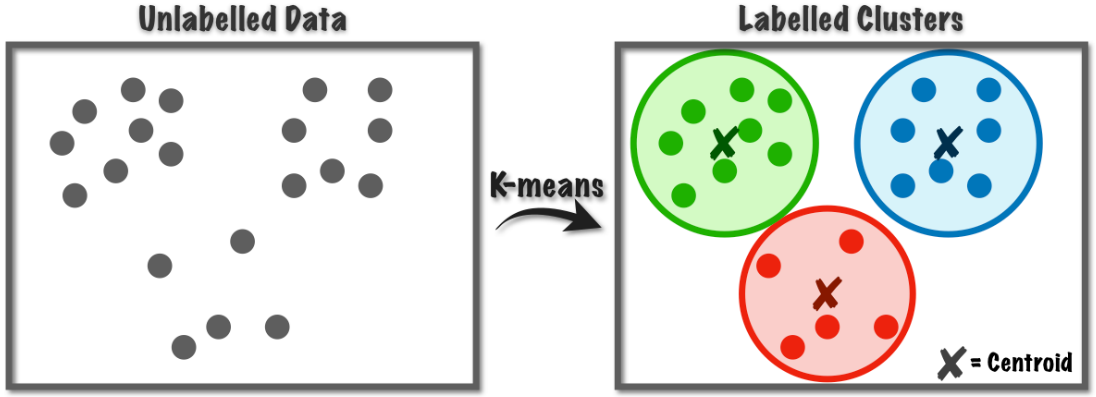
- Find best clustering of **k clusters**
  - Partitional, exclusive, complete and prototype-based;
  - Define clusters by proximity to the mean of the cluster (centroid);
  - The number of clusters is predefined (k).

- **Objective:** find the centroids that **minimize the distance between the examples and the centroids**.



K-Means Clustering: Lloyd Algorithm

- Because the optimal solution for this problem is NP-hard, practical useful solutions can be obtained with simple heuristic algorithms such as the **Lloyd algorithm**.

- **Lloyd algorithm:**
  - Start with random centroids;
  - Assign each example to the closest centroid;
  - Update centroids to mean of respective cluster;
  - Recompute clusters and repeat until convergence.

- **Does not guarantee optimal solutions** as in practical implementations a maximum number of iterations is commonly defined.

K-Means Clustering: Initialization

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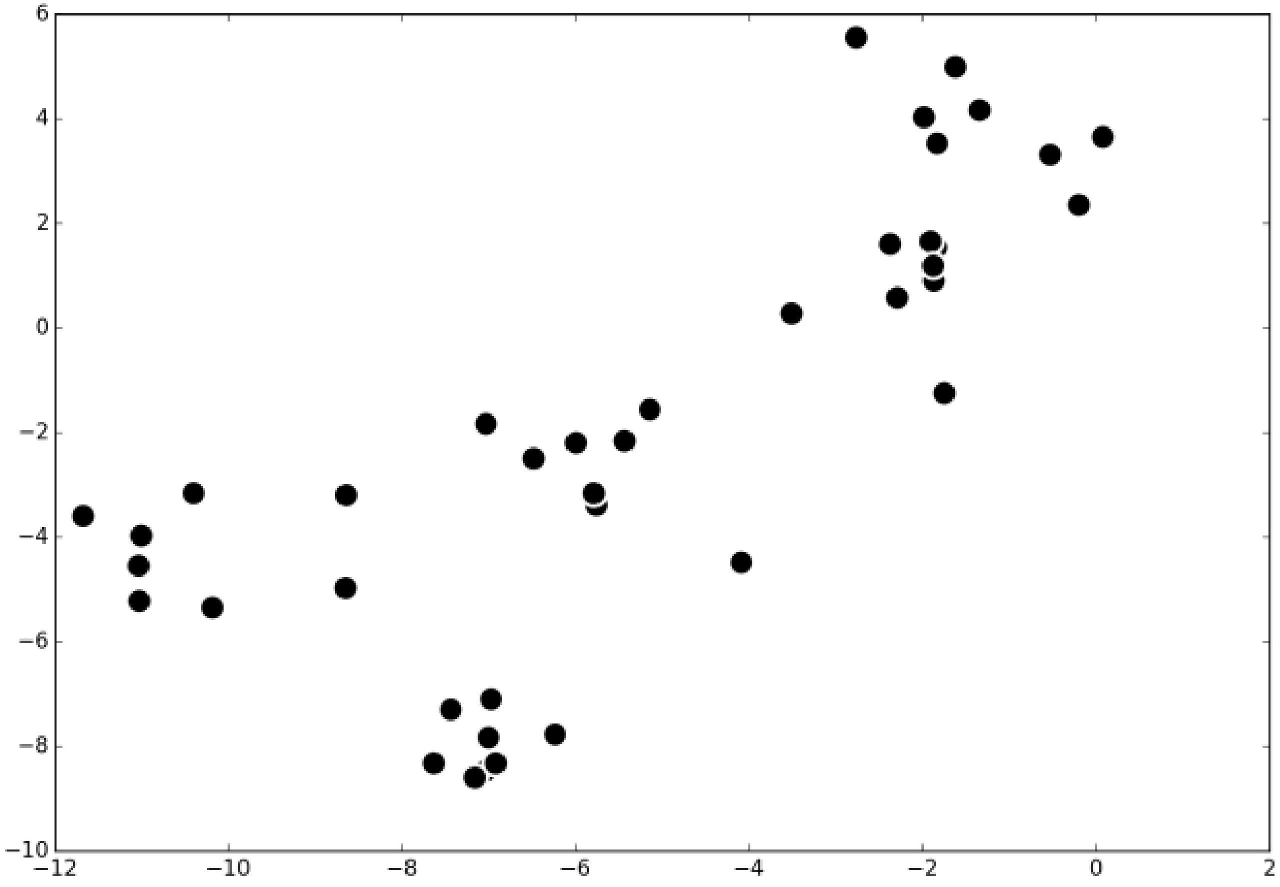
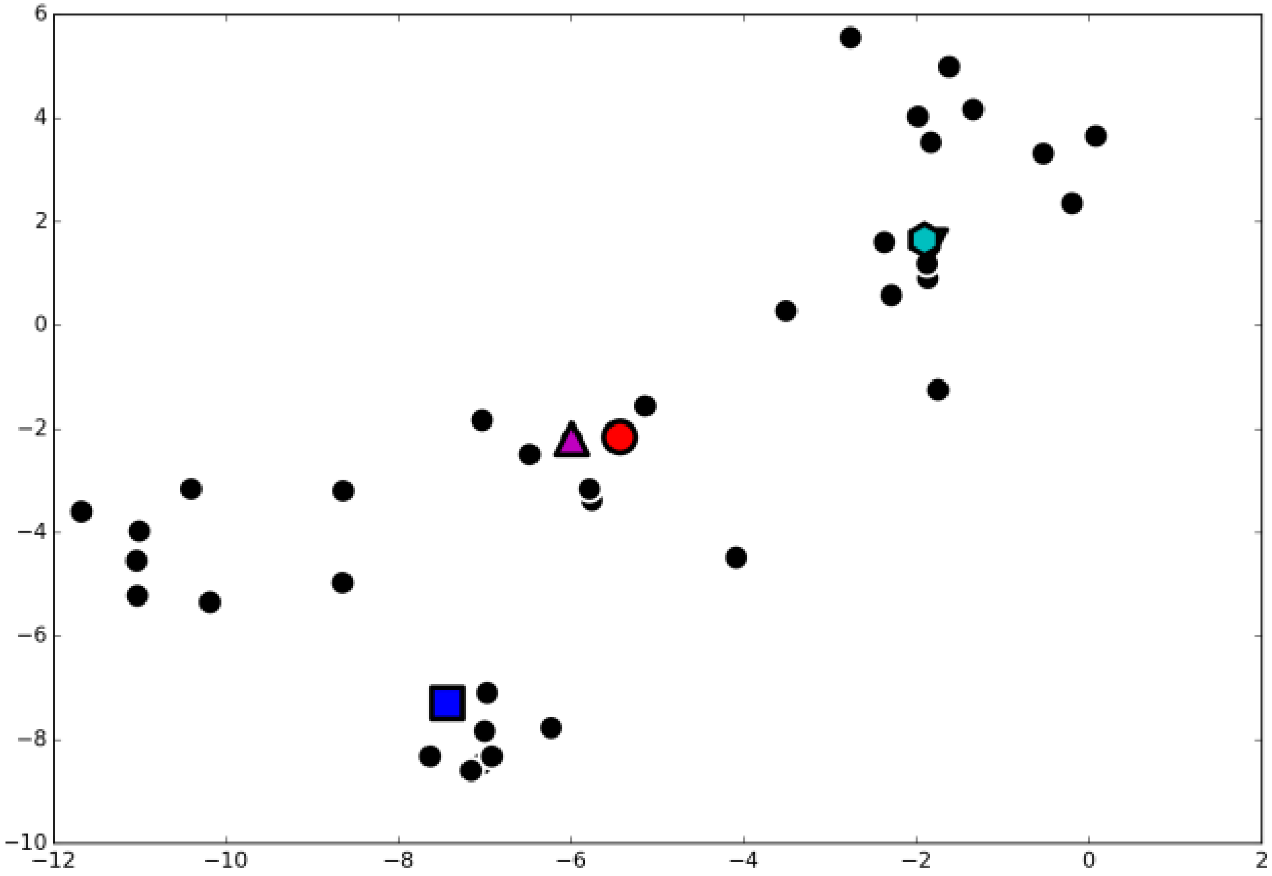
- **Forgy:** start with coordinates of a random set of k examples



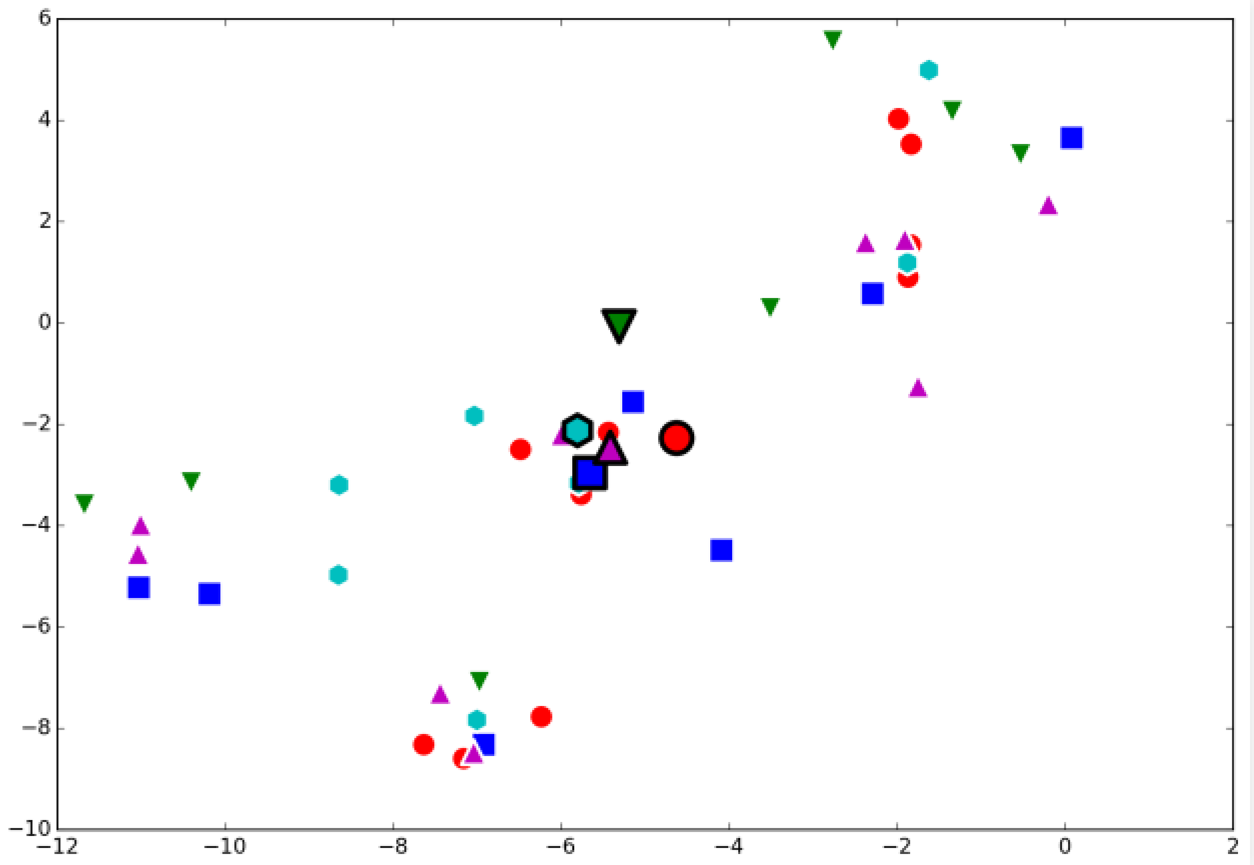
K-Means Clustering: Initialization

- **Forgy:** start with coordinates of a random set of k examples



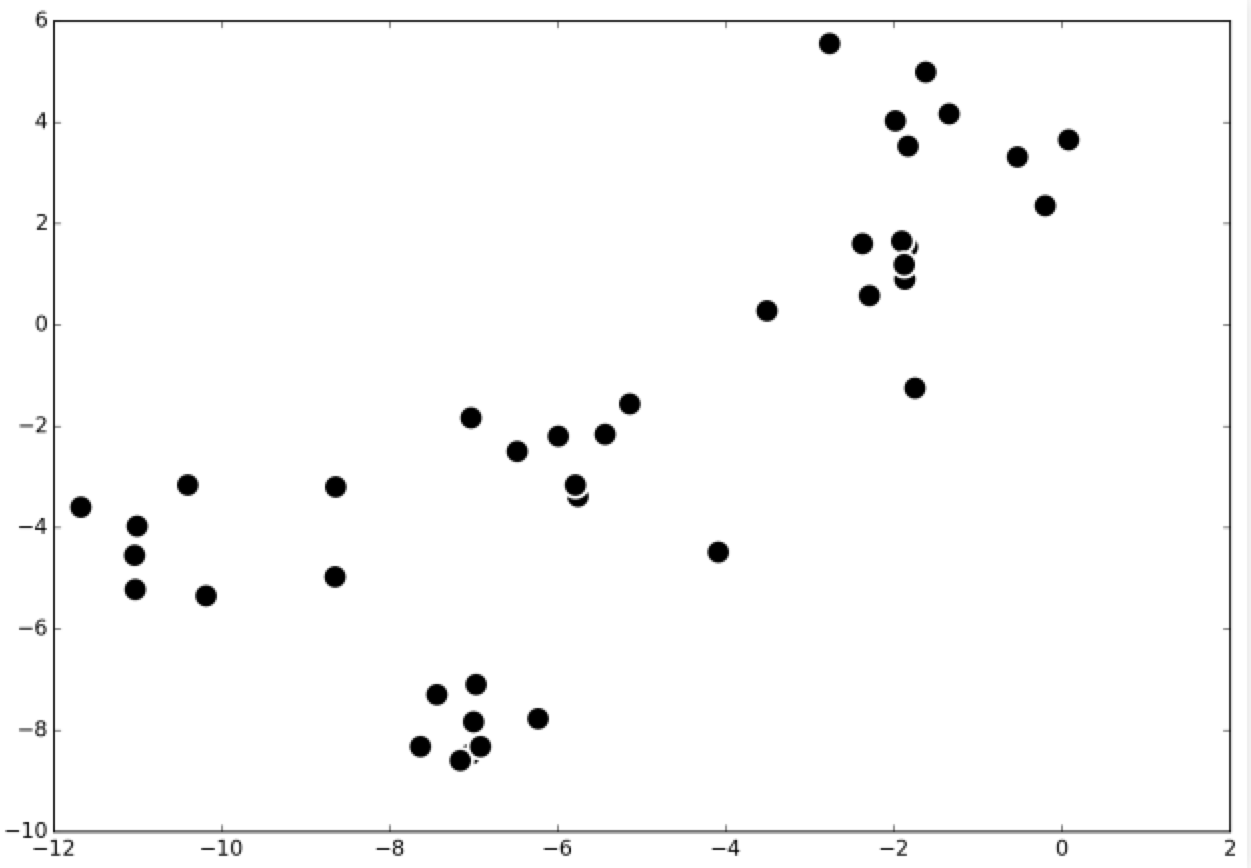
K-Means Clustering: Initialization

- **Random:** random assignment, compute means



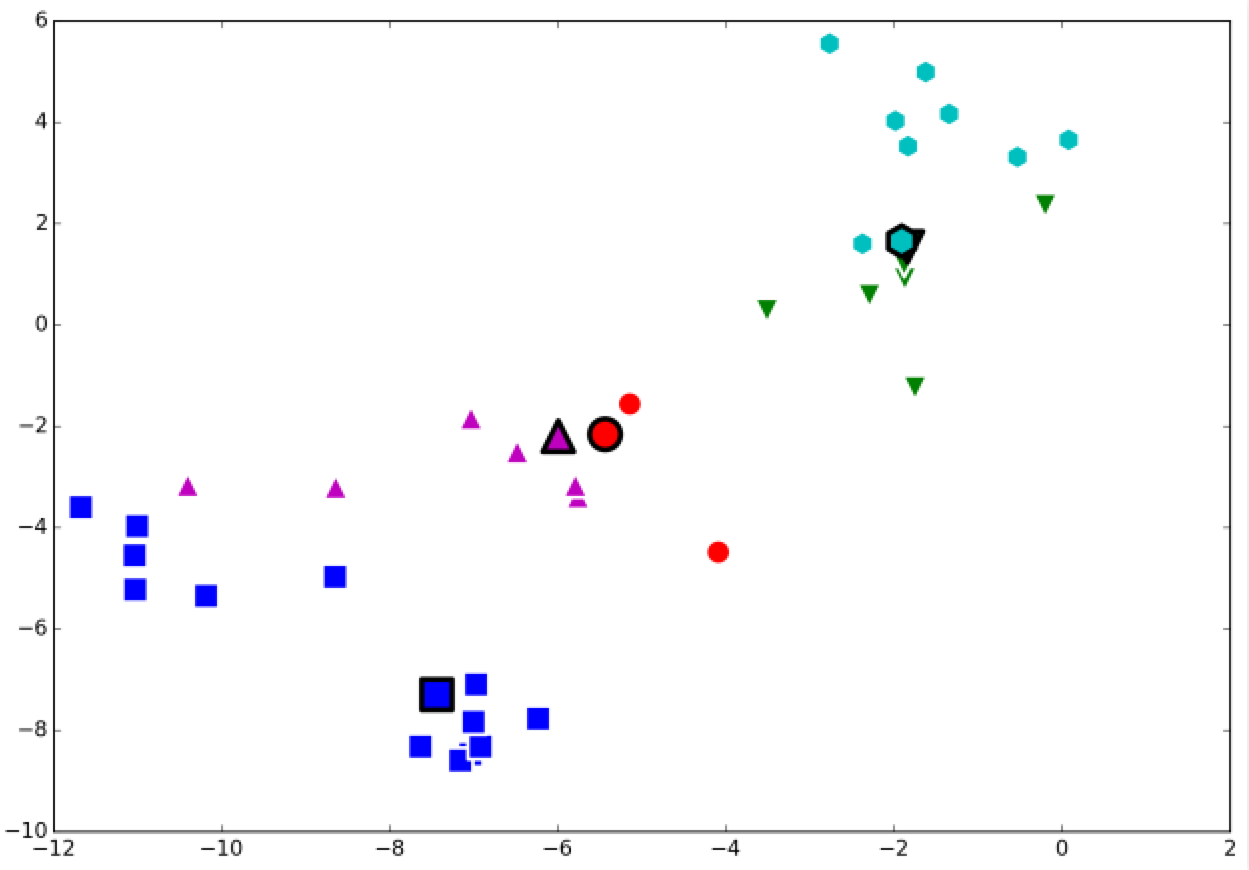
K-Means Clustering: Lloyd Algorithm

- Original data



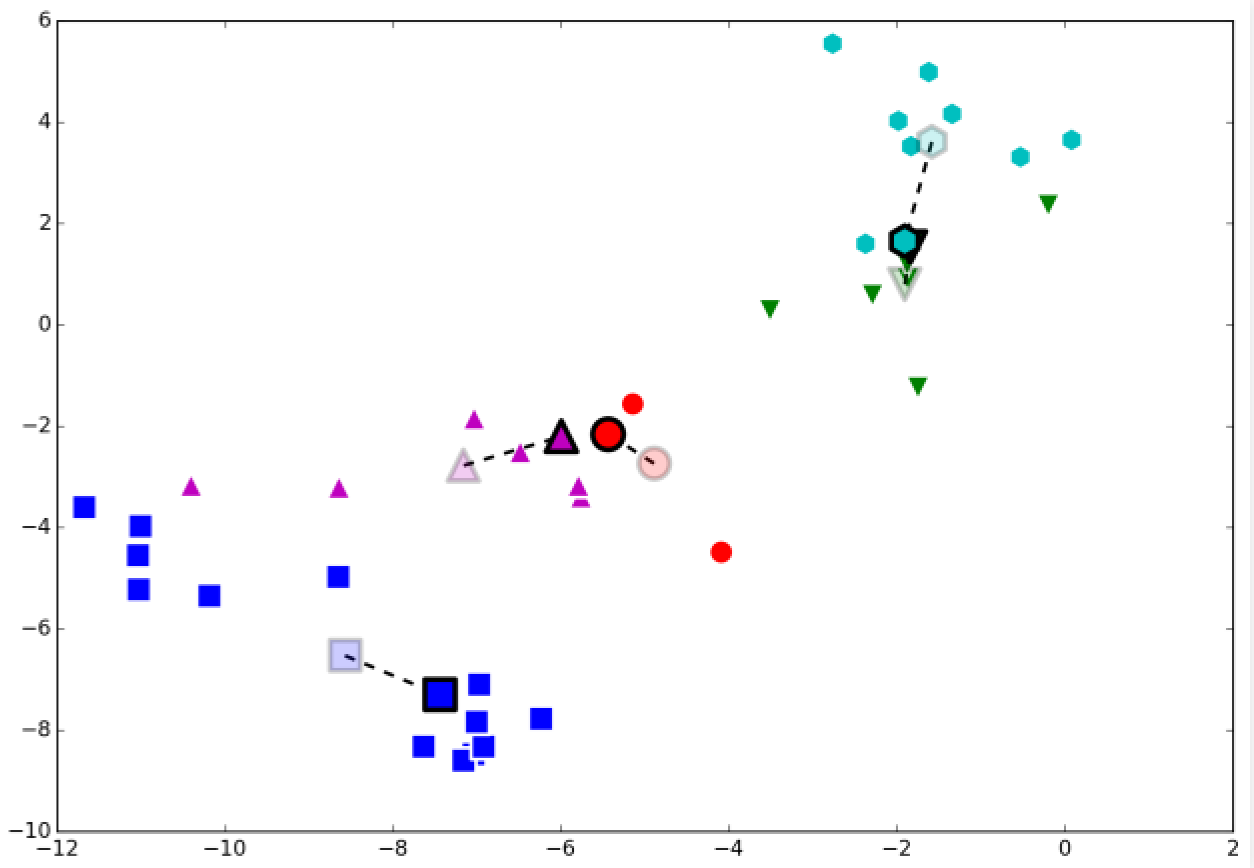
K-Means Clustering: Lloyd Algorithm

- Initialize (Forgy), compute clusters



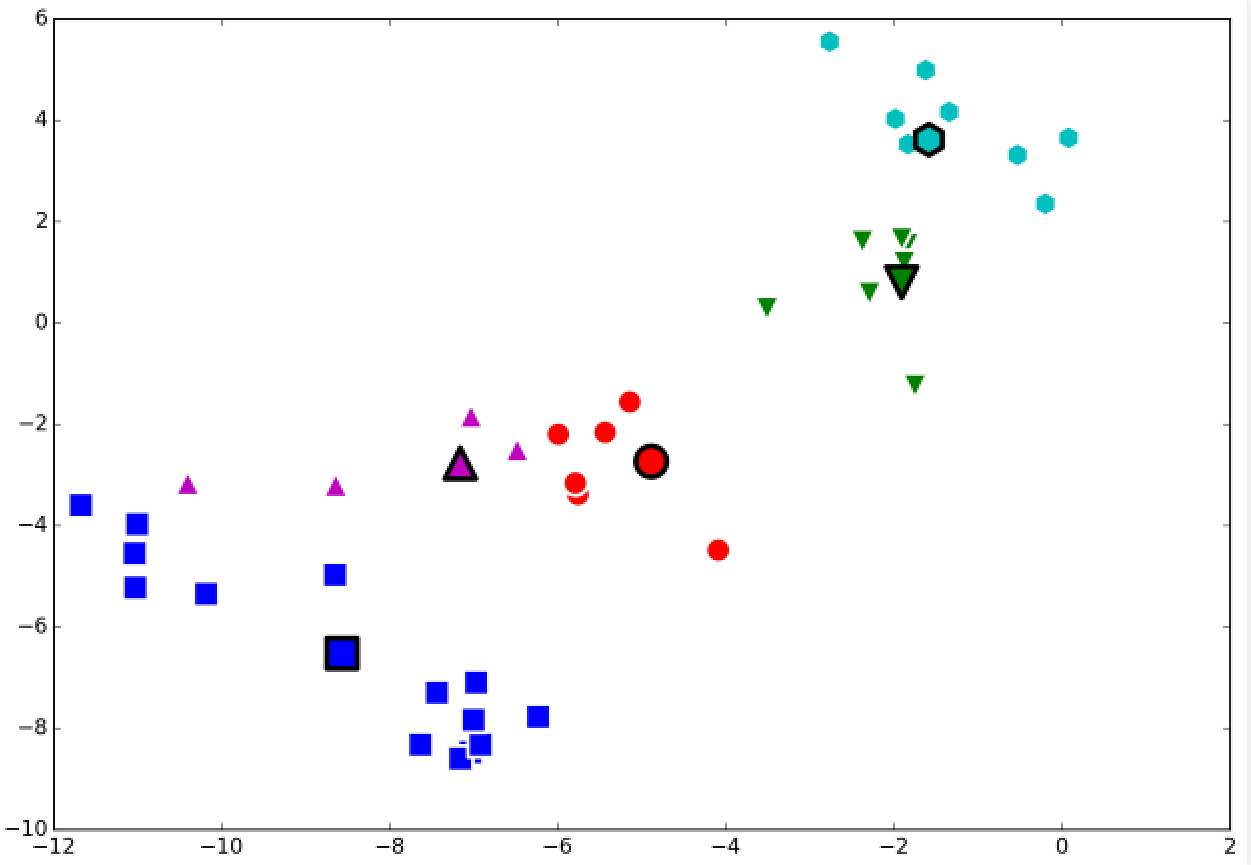
K-Means Clustering: Lloyd Algorithm

• Compute new means, update centroids



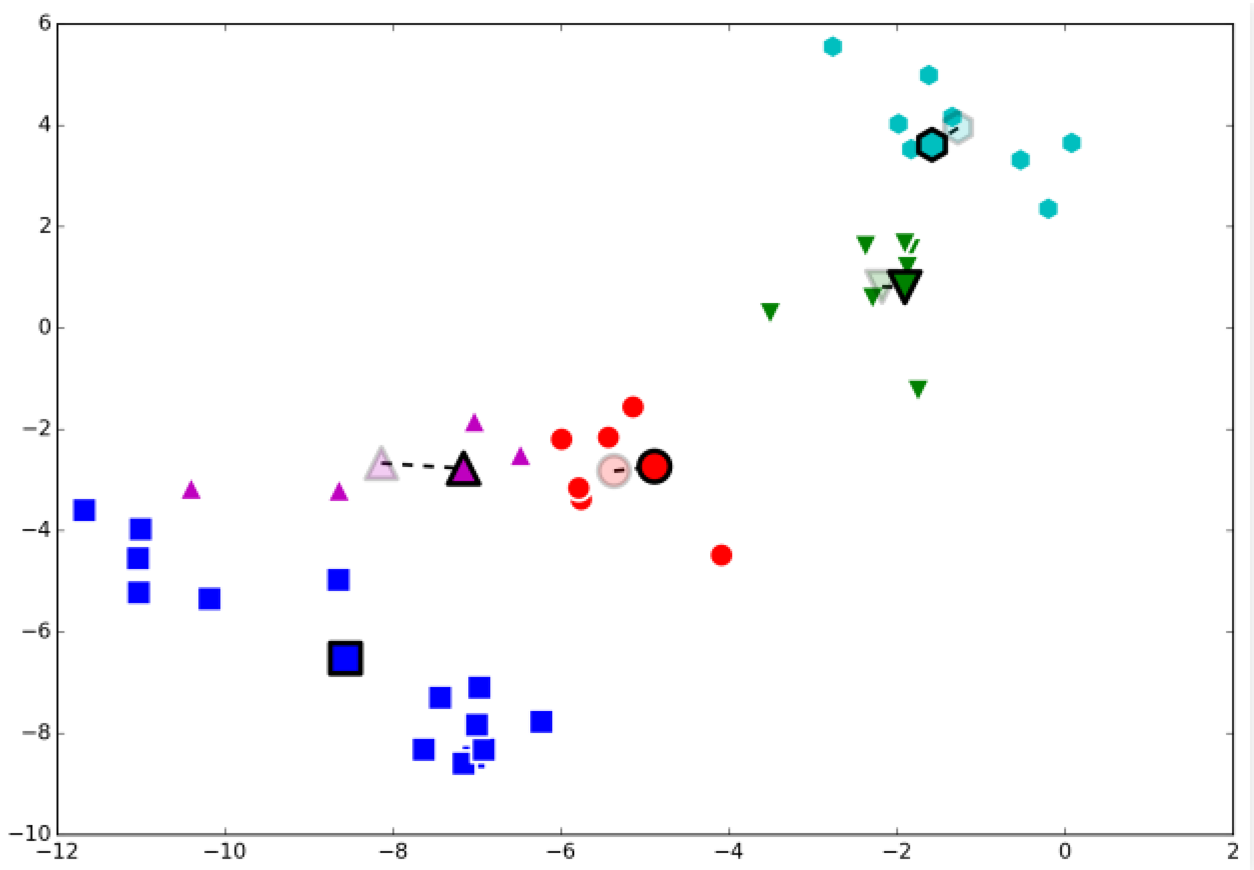
K-Means Clustering: Lloyd Algorithm

- Recompute clusters



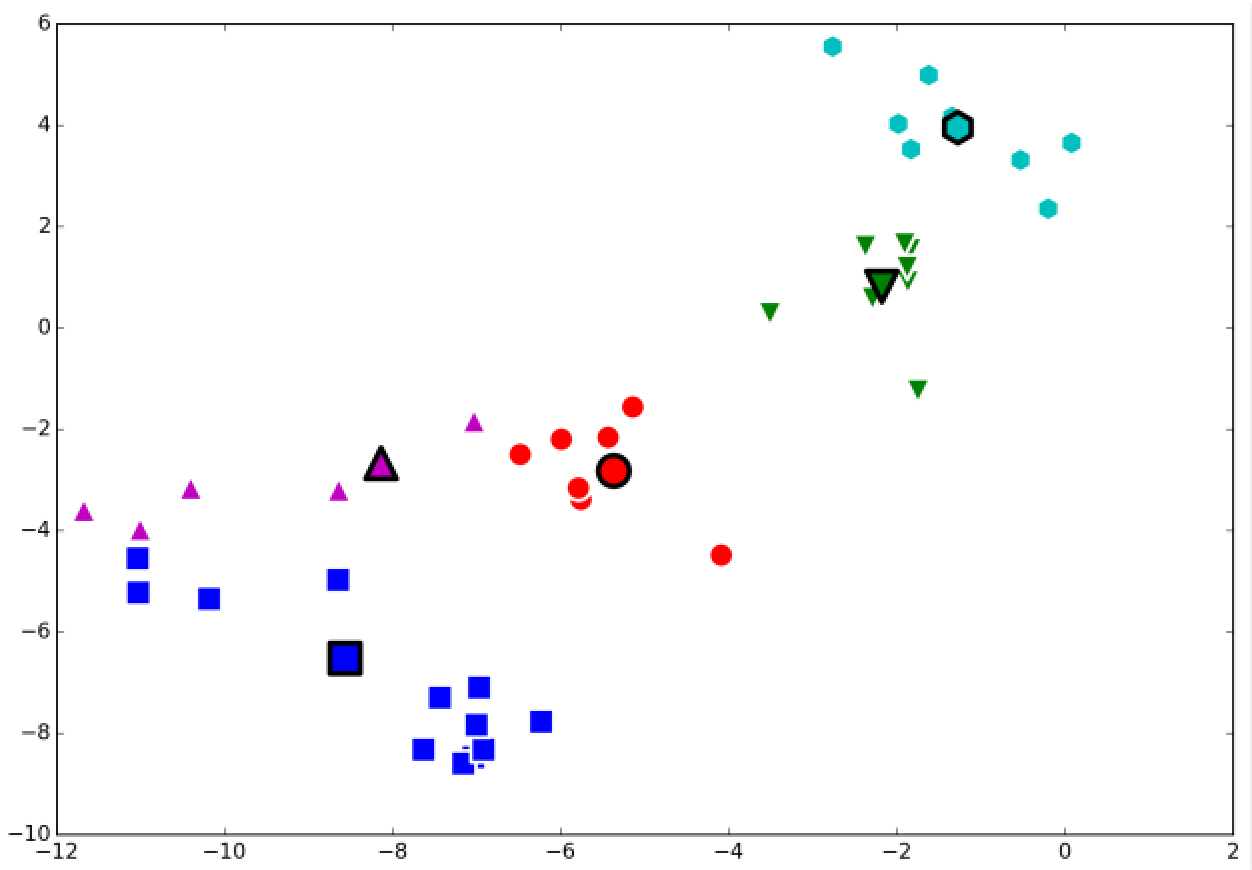
K-Means Clustering: Lloyd Algorithm

- Compute new means, update centroids



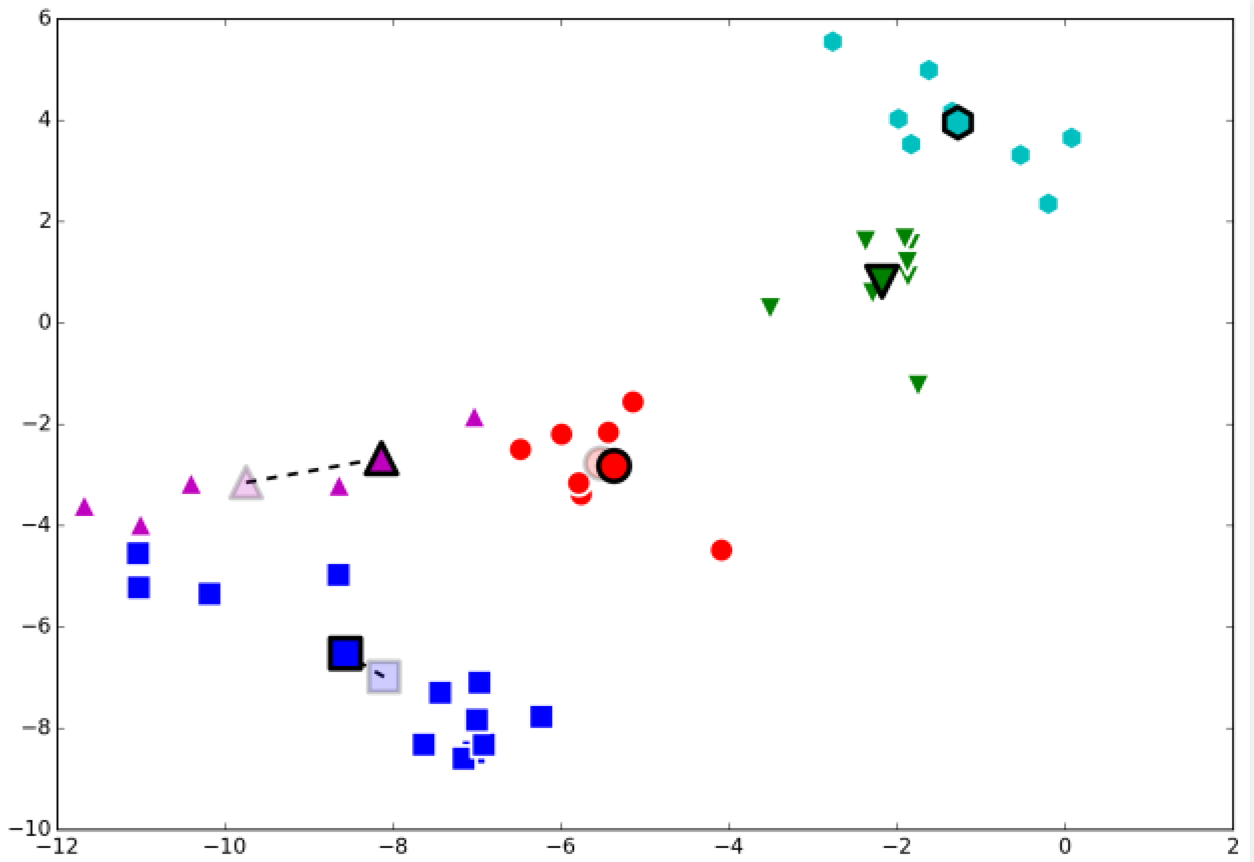
K-Means Clustering: Lloyd Algorithm

- Recompute clusters



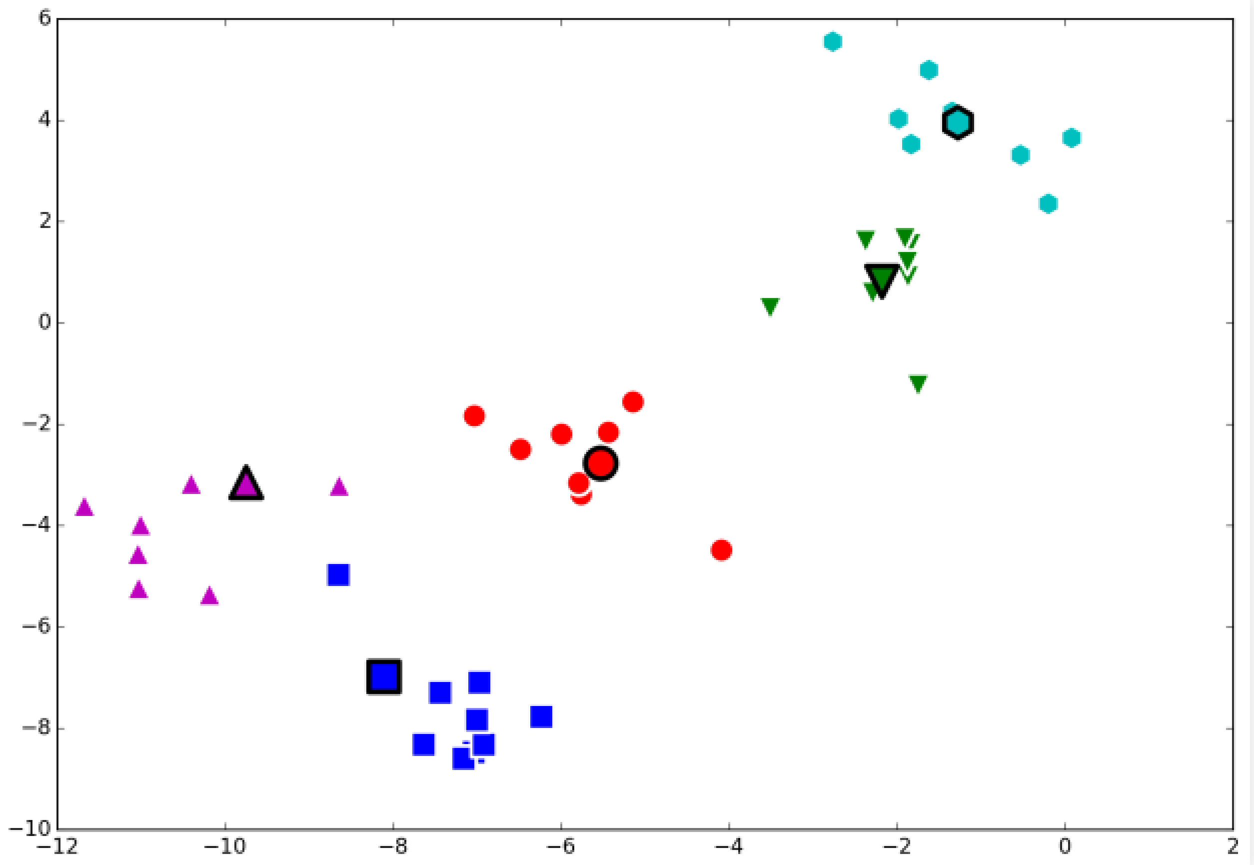
K-Means Clustering: Lloyd Algorithm

- Compute new means, update centroids



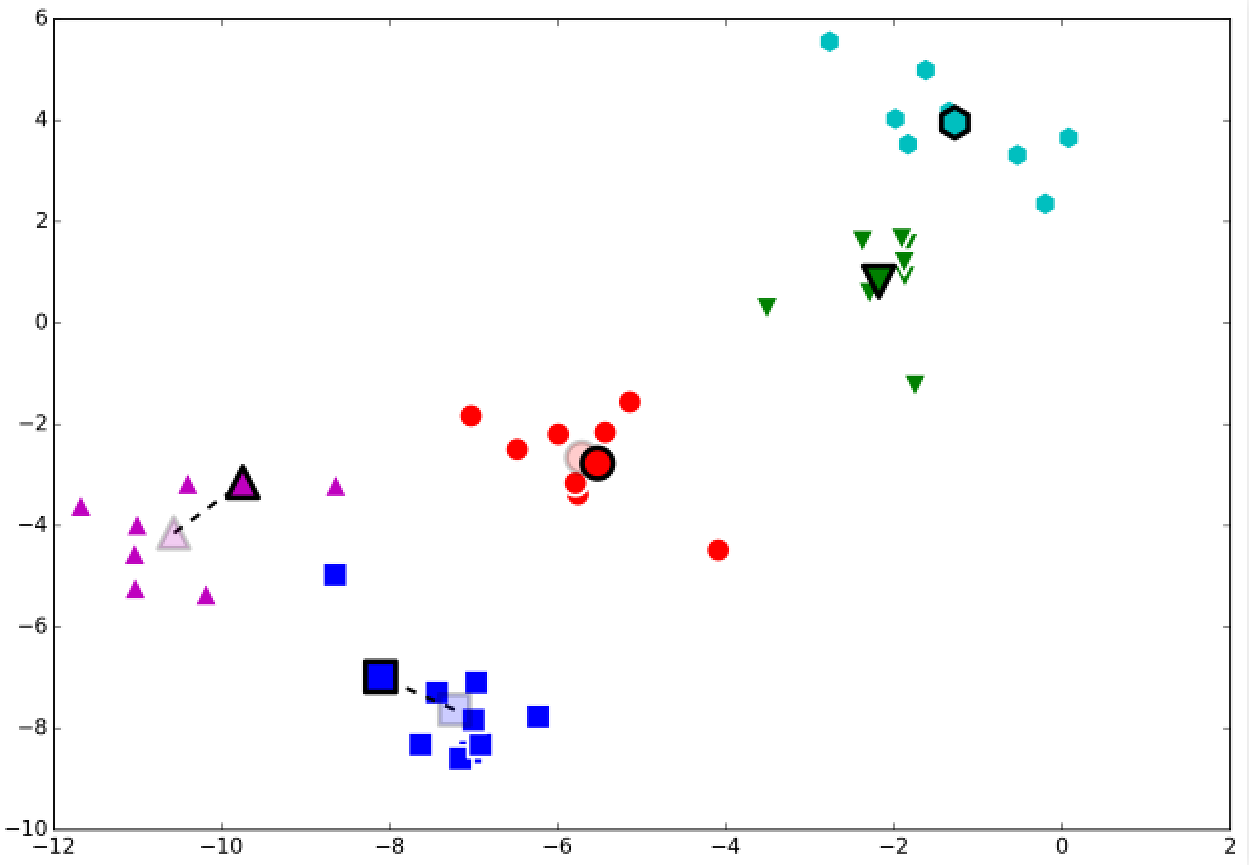
K-Means Clustering: Lloyd Algorithm

- Recompute clusters



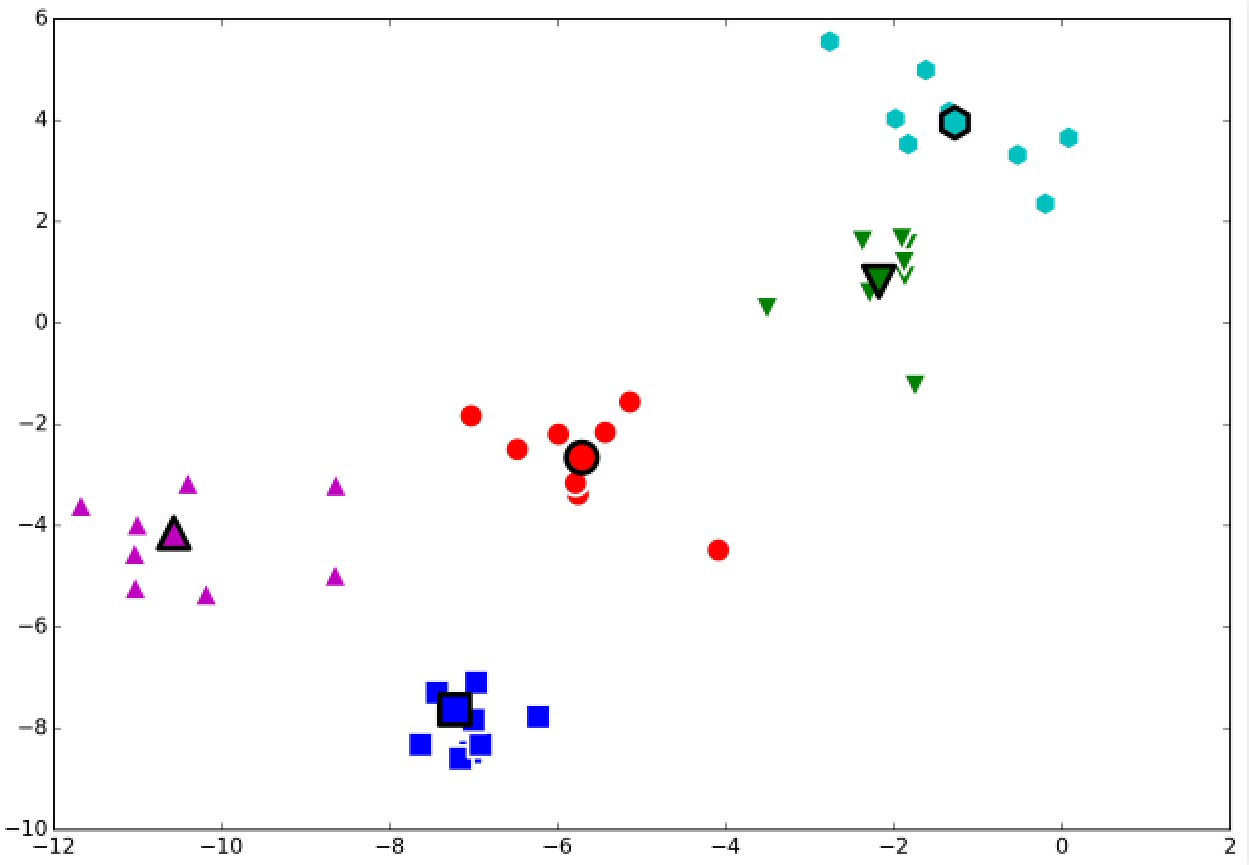
K-Means Clustering: Lloyd Algorithm

- Compute new means, update centroids



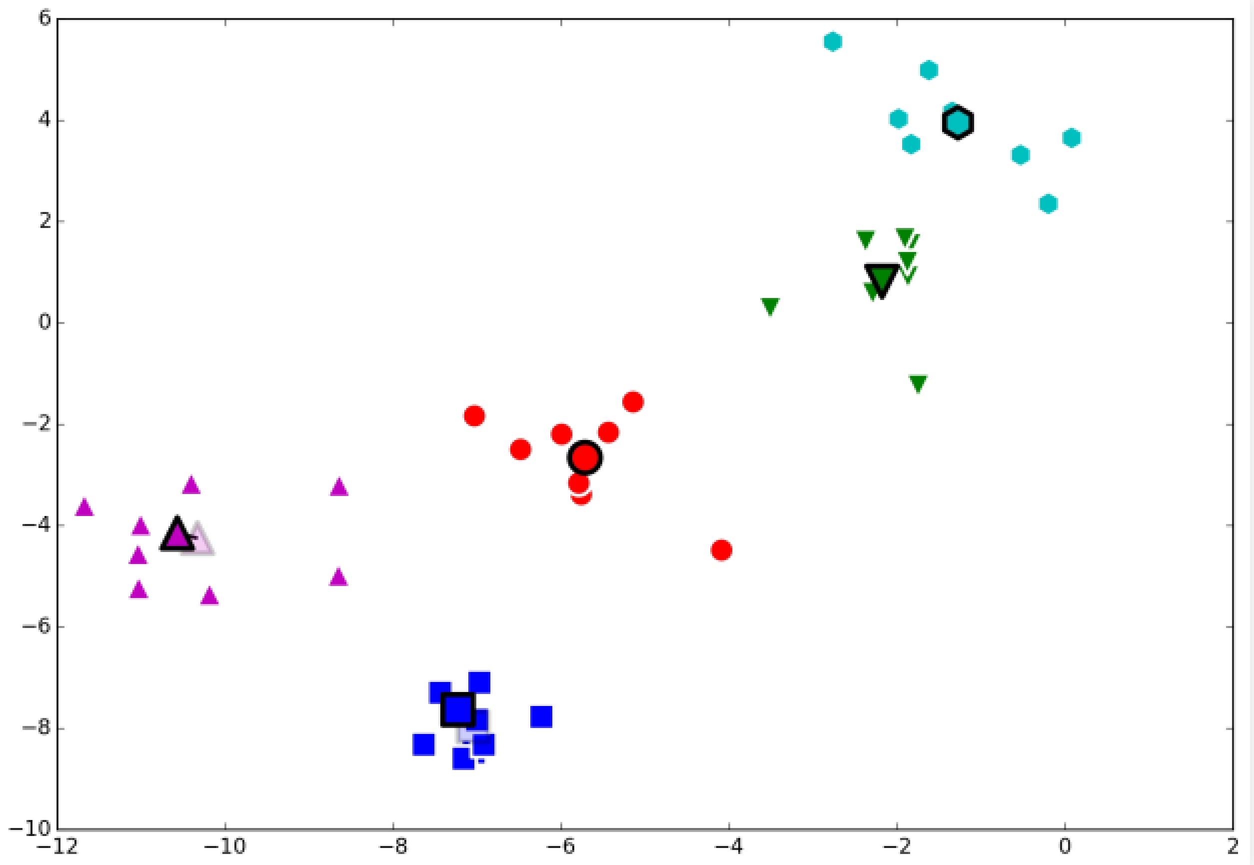
K-Means Clustering: Lloyd Algorithm

- Recompute clusters



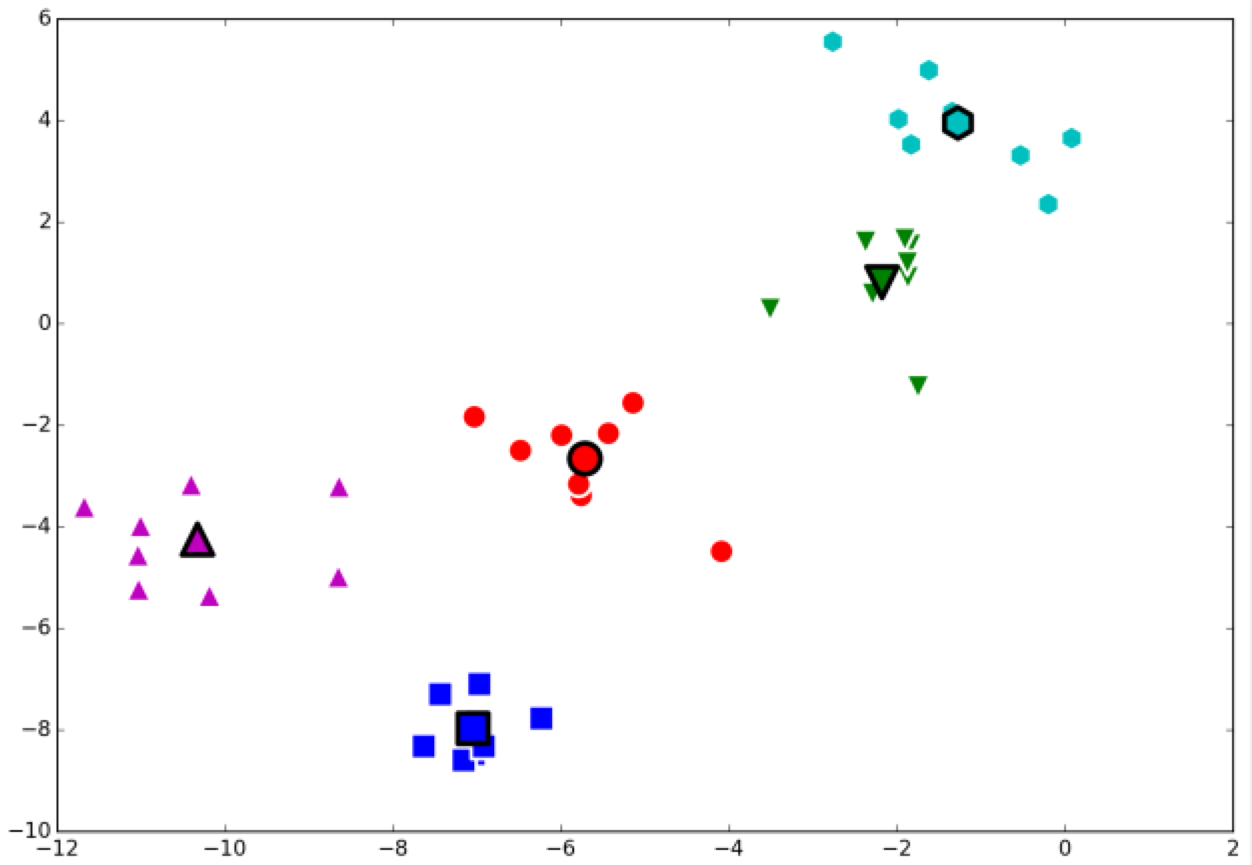
K-Means Clustering: Lloyd Algorithm

- Compute new means, update centroids



K-Means Clustering: Lloyd Algorithm

- Until convergence



K-Means Clustering: Strengths and Limitations

- **Strenghts:**
  - Simple and works well for disjoint clusters;
  - Relatively efficient and scalable (Lloyd algorithm);

- **Limitations:**
  - k needs do be defined in advance;
  - Higly dependent on the initialization;
  - Unable to handle well noisy data and outliers;
  - Not suitable for clusters of different sizes and non-convex shapes.

K-Means Clustering: Choosing k

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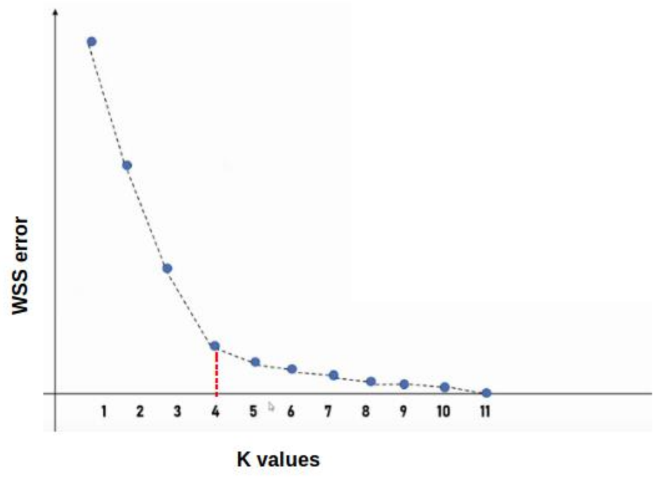
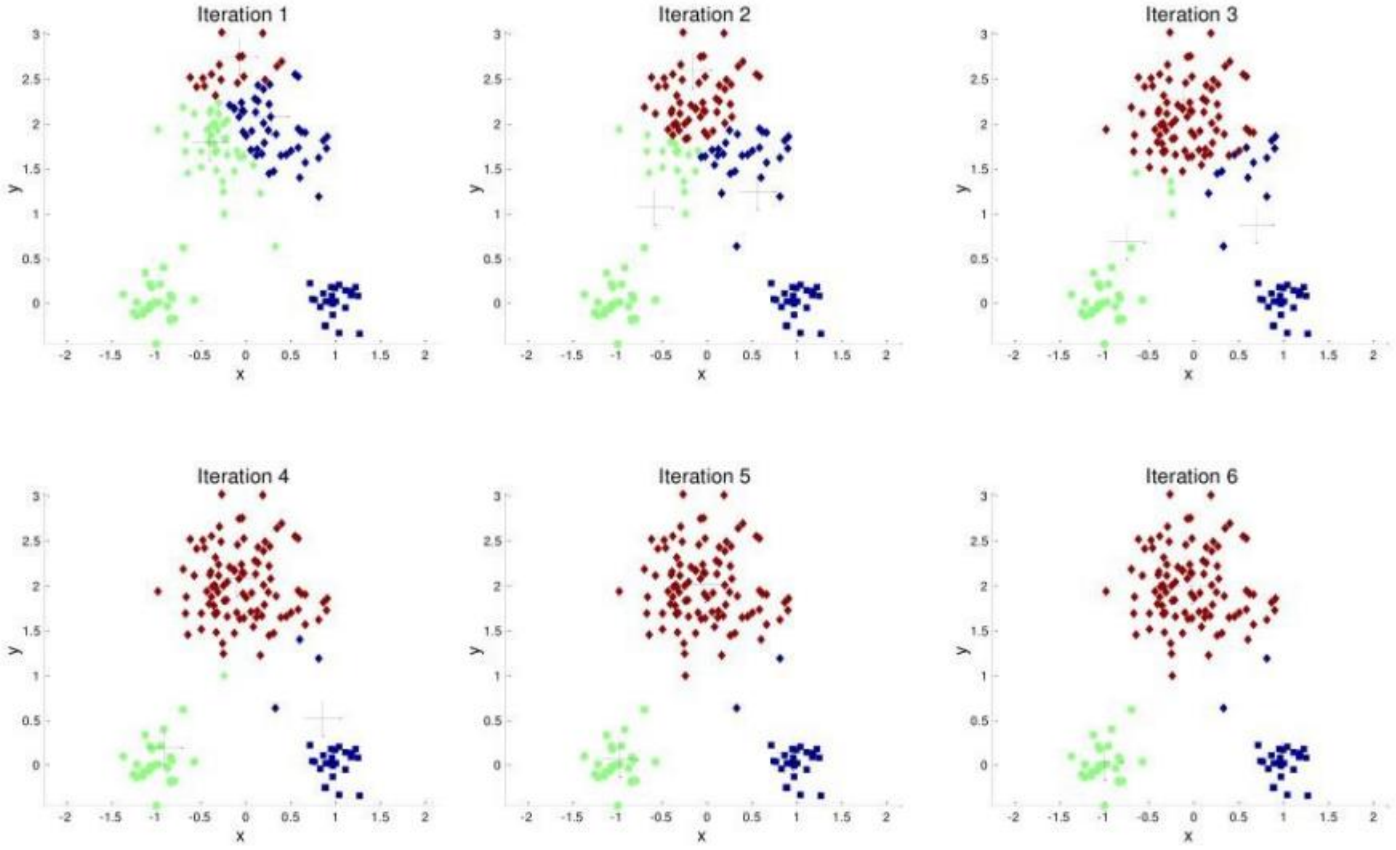
- Chosing the value of k is not a trivial task that heavily affects the outcome of the algorithm.

- **Elbow method:** determine the optimal k
  - Iteratively applies K-means clustering with an increasing number of clusters.
  - Calculates the within-cluster sum of squares (WCSS) for each iteration.
  - WCSS measures the compactness of clusters; lower WCSS indicates better clustering.



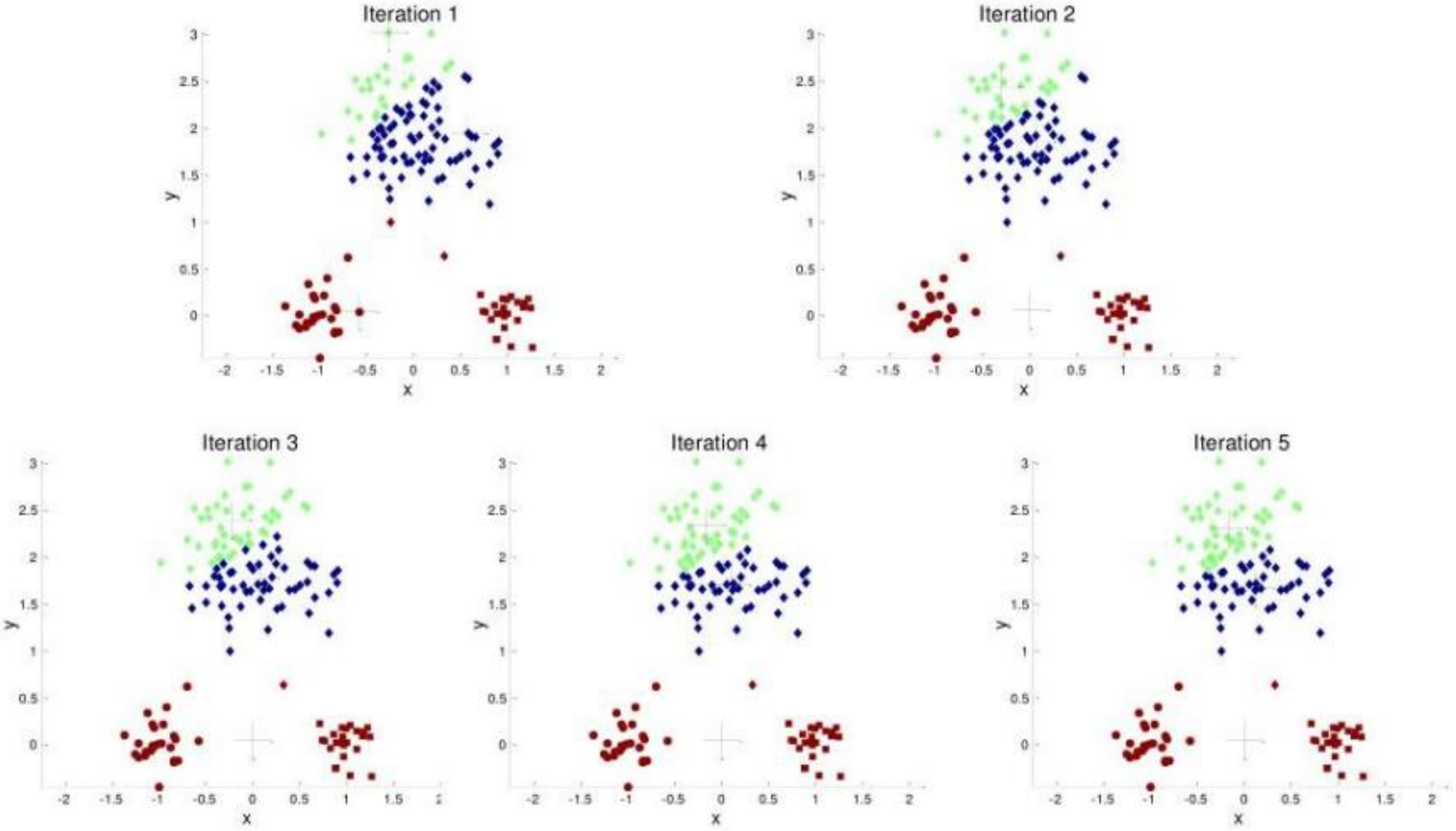
K-Means Clustering: Initialization

- Importance of initialization: case 1

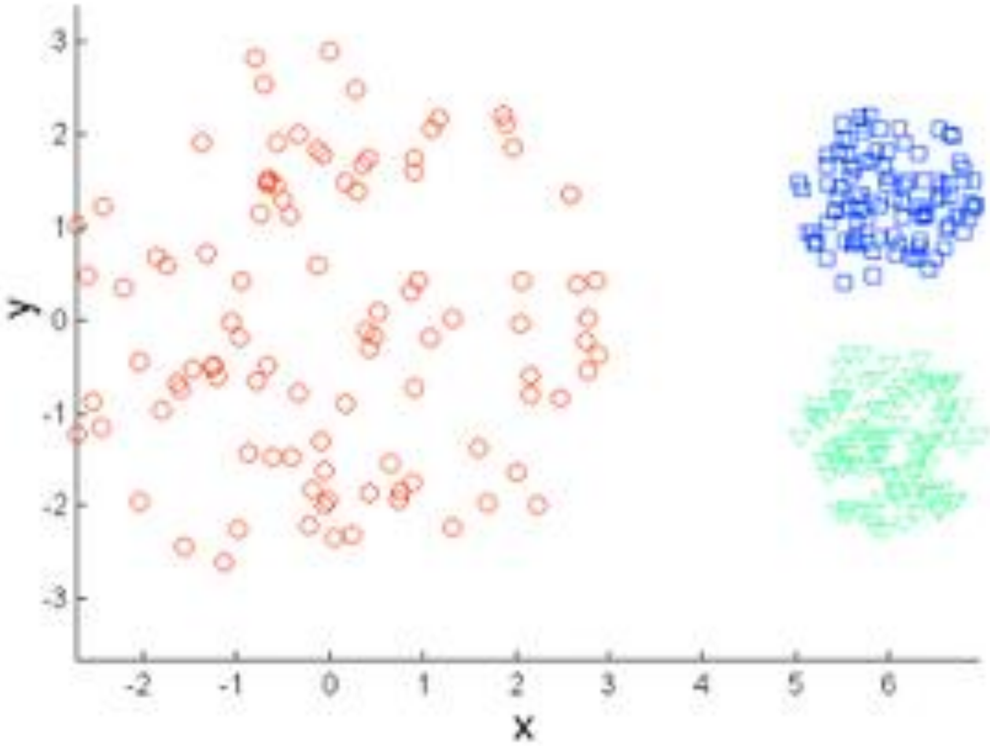


K-Means Clustering: Initialization

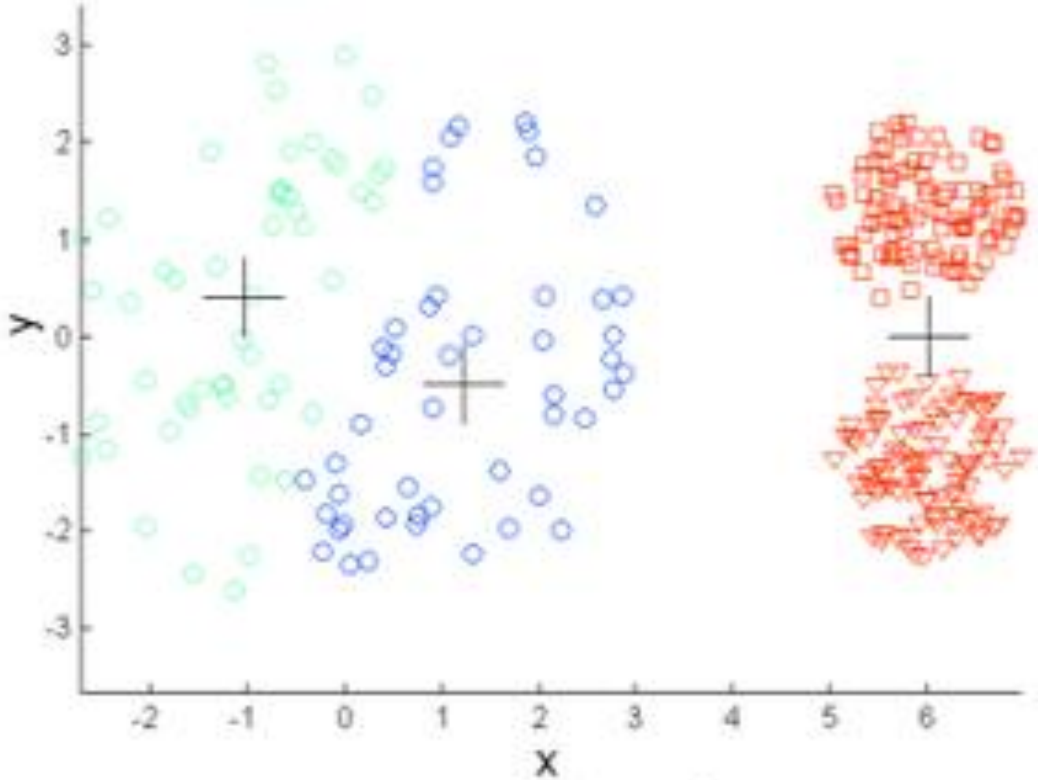
- Importance of initialization: case 2



K-Means Clustering: Different Sizes

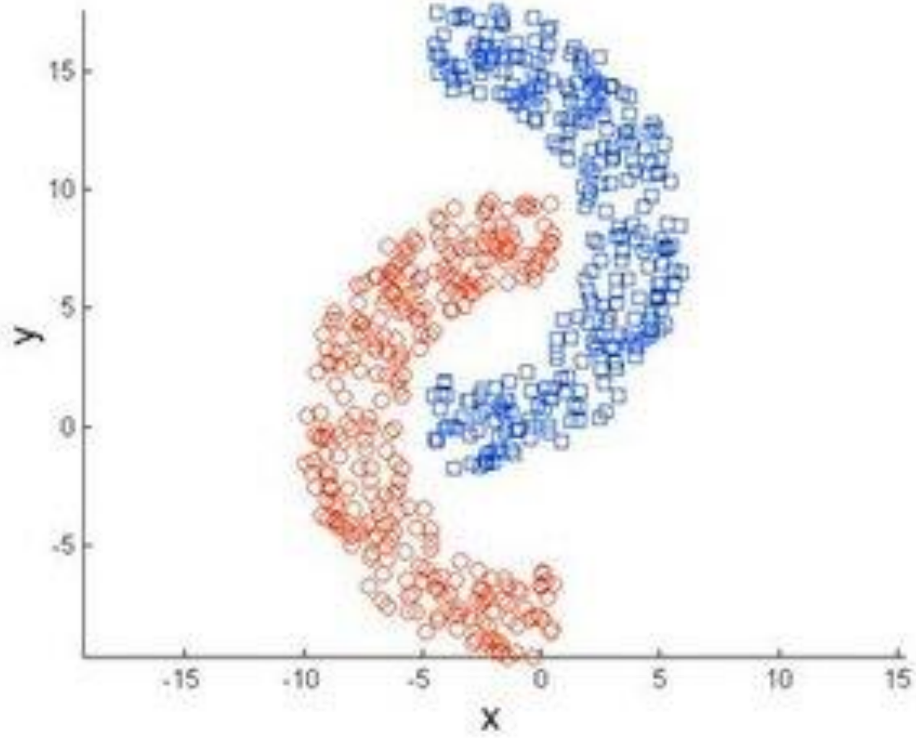


Original Points

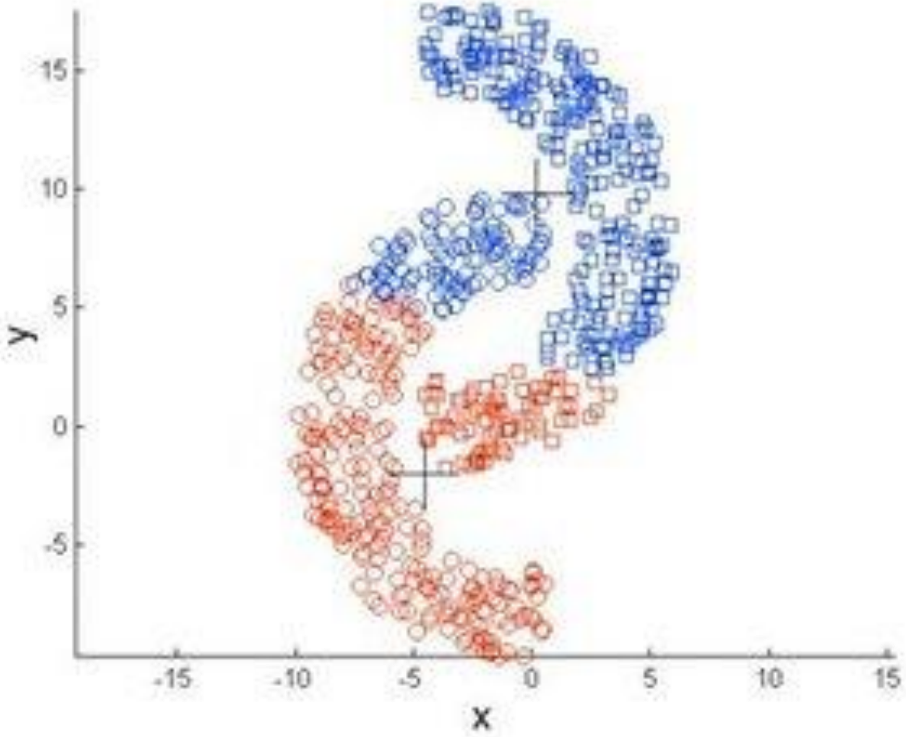


K-means (k = 3)

K-Means Clustering: Non-Convex Shapes



Original Points



K-means (2 Clusters)

K-Means Variants

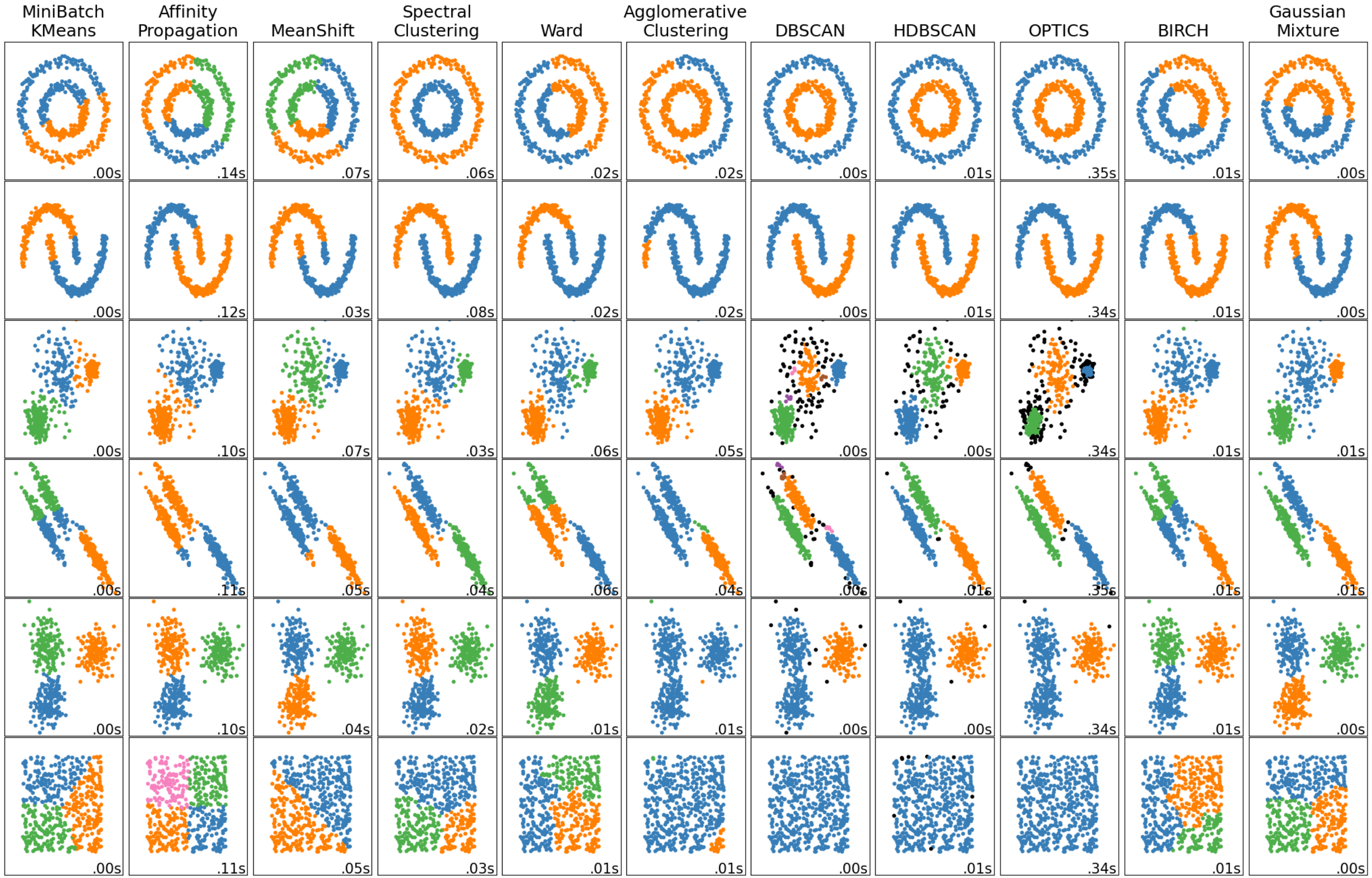
- **K-Medoids**: prototypes are data points (medoids);

- **K-Modes**: for categorical data. Utilizes mode-based distance measures (e.g., Hamming distance)

K-Means - Applications

- **Customer Segmentation:** Identifying groups of customers with similar traits for targeted marketing and personalized services.
- **Image Compression:** Simplifying images by reducing the number of colors, preserving visual quality while saving storage space.
- **Anomaly Detection:** Spotting outliers in datasets, useful for fraud detection and quality control.
- **Document Clustering:** Organizing documents by content similarity for efficient retrieval and topic modeling.
- **Retail Inventory Management:** Optimizing inventory levels and product placement based on sales patterns.
- **Healthcare Data Mining:** Grouping patients with similar medical profiles for diagnosis and treatment planning.
- **Climate Pattern Analysis:** Identifying weather patterns and trends in climate data for forecasting and resource management.

Other Clustering Algorithms



https://scikit-learn.org/stable/modules/clustering.html

Resources

- Berry, M. W., Mohamed, A., & Yap, B. W. (2019). Supervised and unsupervised learning for Data Science. Cham, Switzerland: Springer Nature.

- Patel, A. A. (2019). Hands-on unsupervised learning using python. Sebastopol, CA: O'Reilly Media.