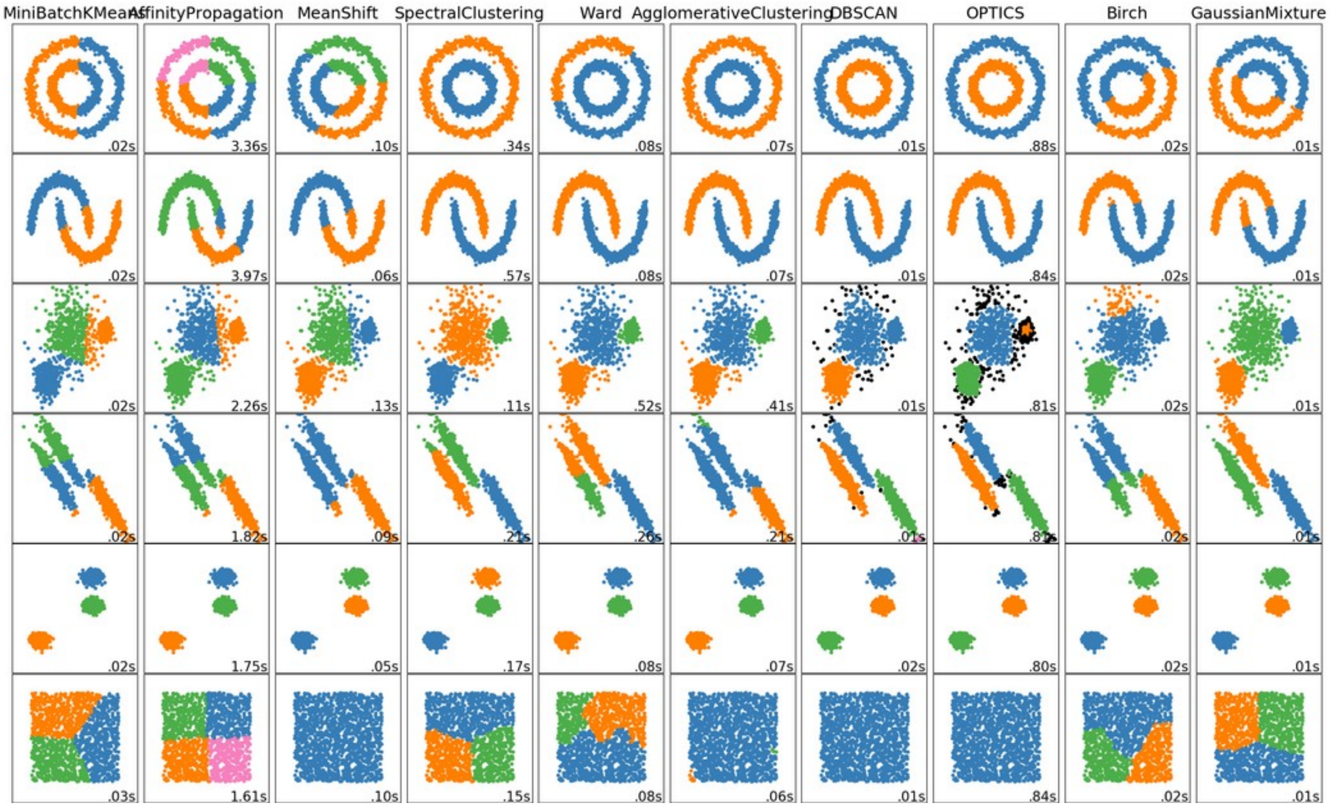
Machine learning
Lecture 9



- Cluster analysis

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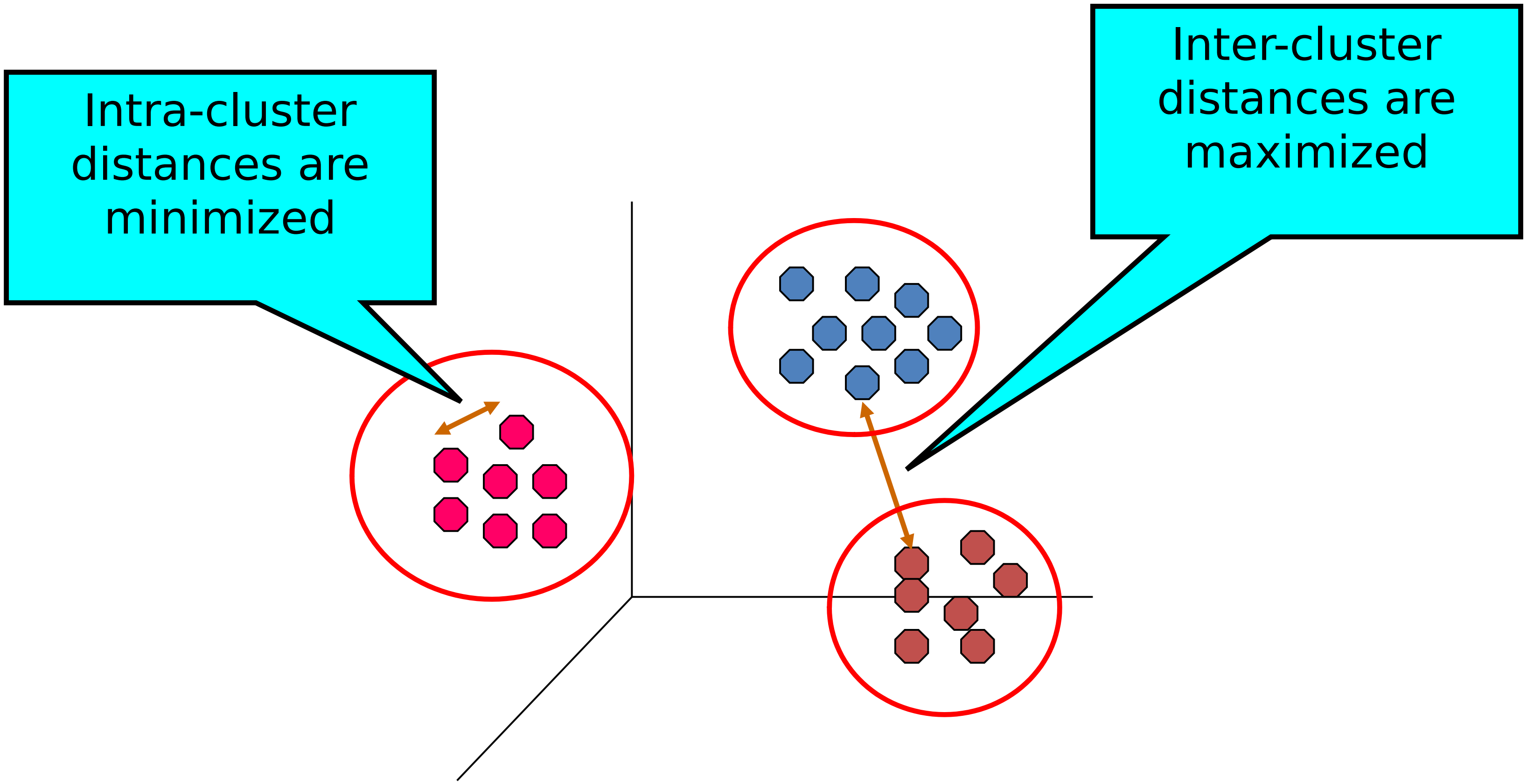
IFJ PAN

16 December 2020

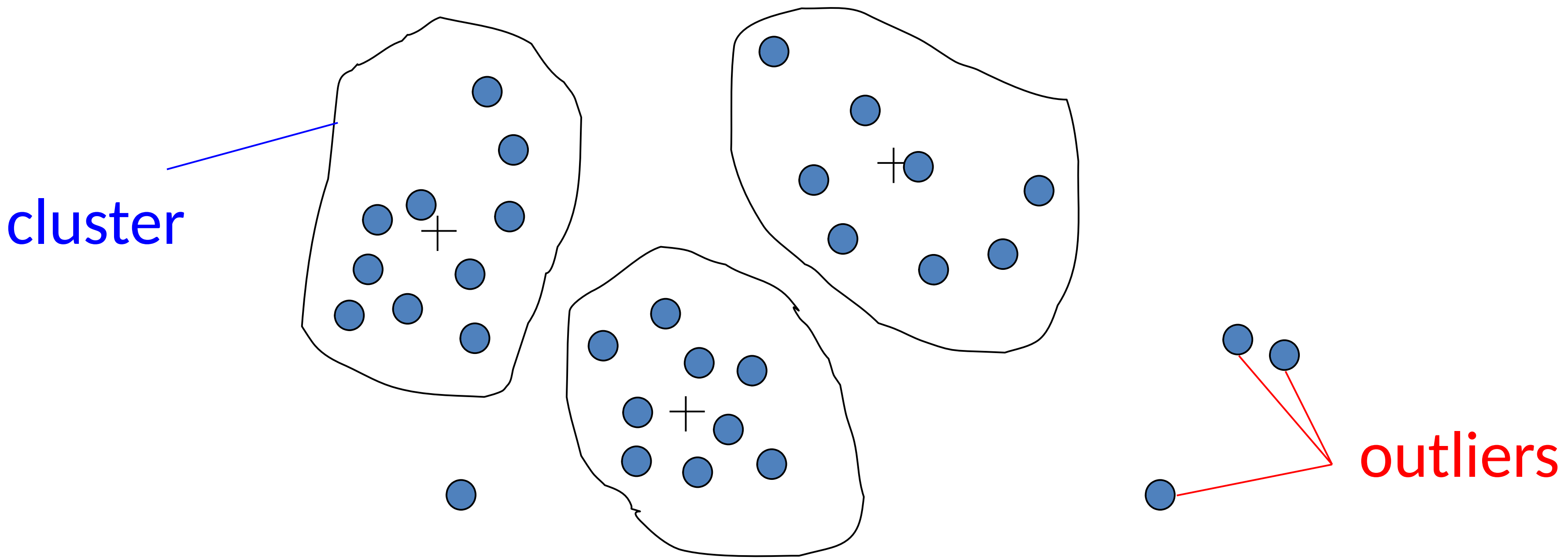
What is clustering?

- A **grouping** of data objects such that the objects **within a group are similar** (or related) to one another **and different from (or unrelated to) the objects in other groups**



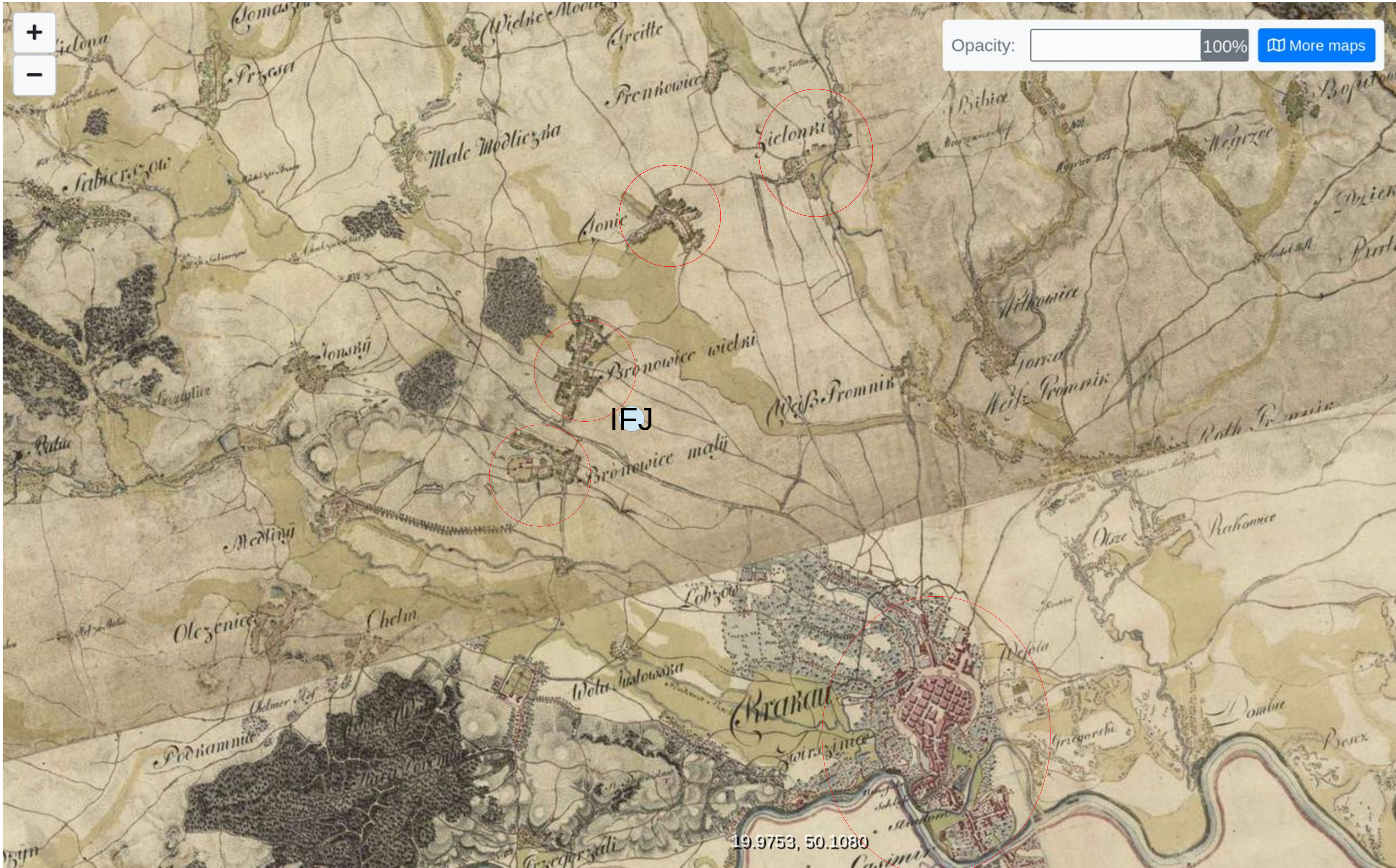
Outliers

- **Outliers** are **objects that do not belong to any cluster** or form clusters of very small cardinality (number of cluster members).



- In some applications we are interested in discovering outliers, not clusters (outlier analysis)

Kraków 1804



Opacity:
100%
More maps
IFJ
Bronowice wielki
Bronowice mały
Krakau
Lobzow
Weiß Promnik
19.9753, 50.1080

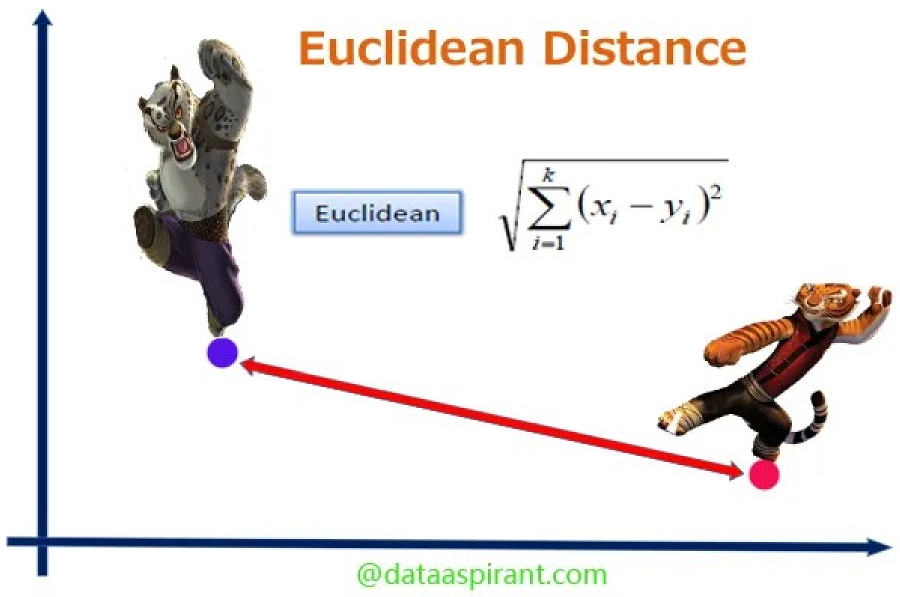
The clustering task

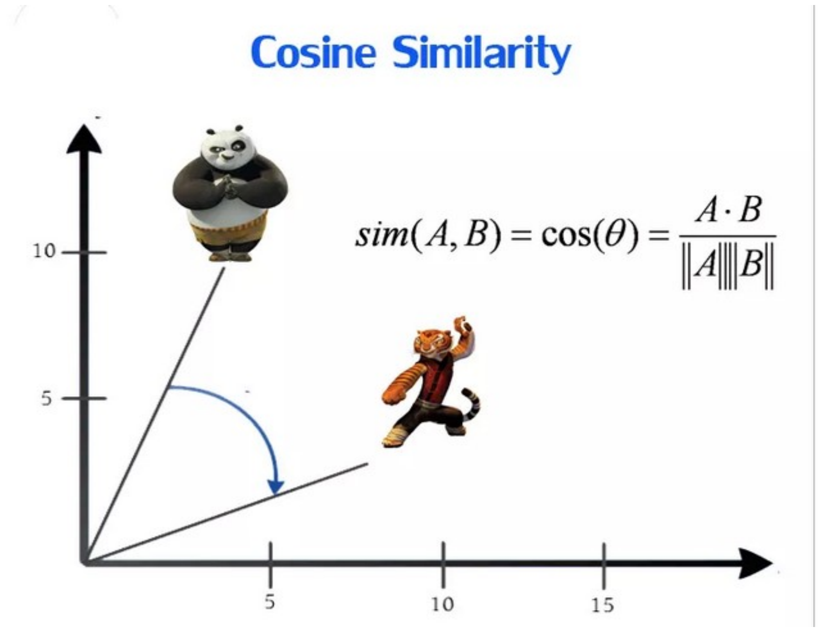
- Assign observations into groups so that the observations belonging in the same group are similar, whereas observations in different groups are different =>
- **We need a distance between points:**

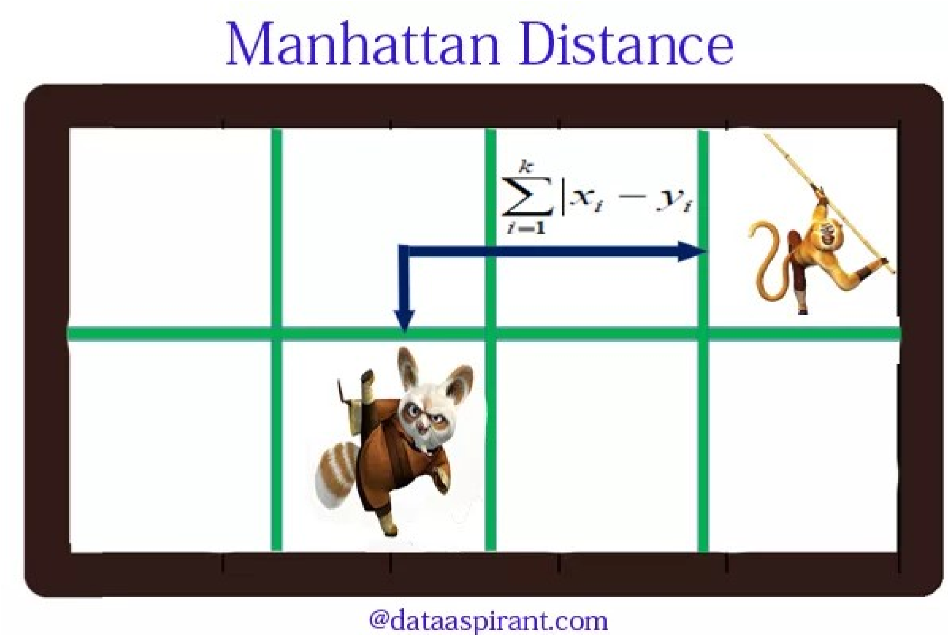
The distance **d(x, y)** between two objects **x** and **y** is a metric if:

- **d(i, j)≥0** (non-negativity)
- **d(i, i)=0** (isolation)
- **d(i, j)= d(j, i)** (symmetry)
- **d(i, j) ≤ d(i, h)+d(h, j)** (triangular inequality)

Distance







- Euclidian
- Manhattan
- Cosine similarity
- …. many other

Data Structures

- *data* matrix

$$\text{tuples/objects}\left\{\overbrace{\begin{bmatrix} x_{11} & \cdots & x_{1\ell} & \cdots & x_{1d} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{i1} & \cdots & x_{i\ell} & \cdots & x_{id} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{n1} & \cdots & x_{n\ell} & \cdots & x_{nd} \end{bmatrix}}^{\text{attributes/dimensions}}\right.$$

- *Distance* matrix

$$\text{objects}\left\{\overbrace{\begin{bmatrix} 0 & & & & \\ d(2,1) & 0 & & & \\ d(3,1) & d(3,2) & 0 & & \\ \vdots & \vdots & \vdots & & \\ d(n,1) & d(n,2) & \cdots & \cdots & 0 \end{bmatrix}}^{\text{objects}}\right.$$

Non-hierarchical methods
the k-means algorithm

- Given a set **X** of **n** points in a **d**-dimensional space and an integer **k**

- **Task:** choose a set of **k** points (cluster centers) $\{c_1, c_2, \ldots, c_k\}$ in the **d**-dimensional space to form clusters $\{C_1, C_2, \ldots, C_k\}$ such that

$$Cost(C) = \sum_{i=1}^{k} \sum_{x \in C_i} L_2^{\,2}(x - c_i)$$

  is minimized

- Some special cases: k = 1, k = n

The k-means algorithm

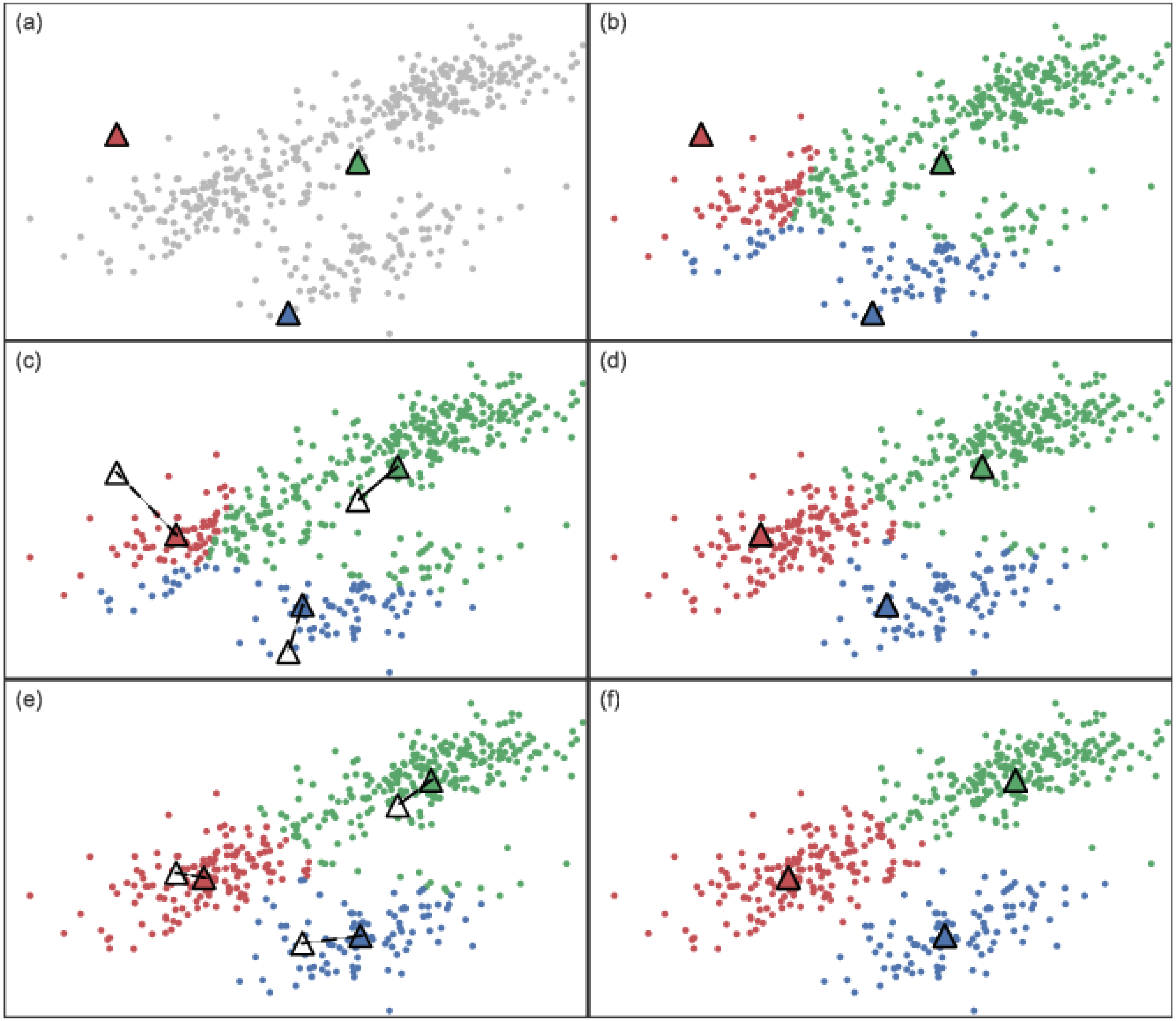
- Randomly pick **k** cluster centers $\{c_1,\ldots,c_k\}$

- For each **i**, set the cluster C_i to be the set of points in **X** that are closer to c_i than they are to c_j for all $i \neq j$

- For each **i** let c_i be the center of cluster C_i (mean of the vectors in C_i)

- Repeat until convergence

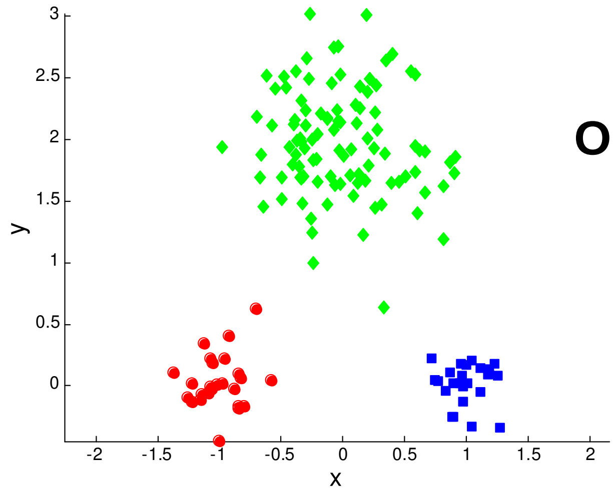
K-means algorithm



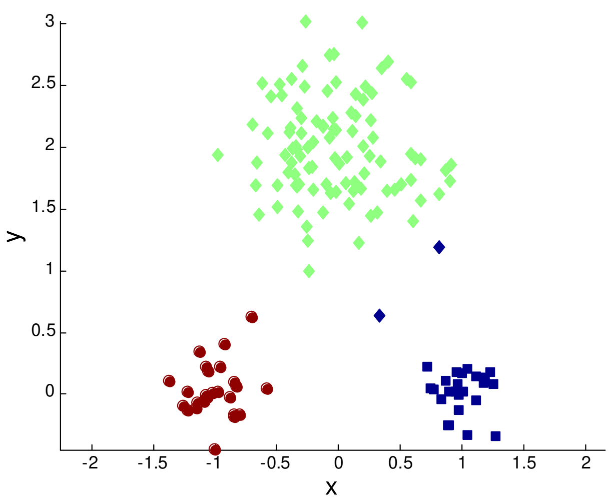
Properties of the k-means algorithm

- Finds a local optimum
- Converges often quickly (but not always)
- The choice of initial points can have large influence in the result

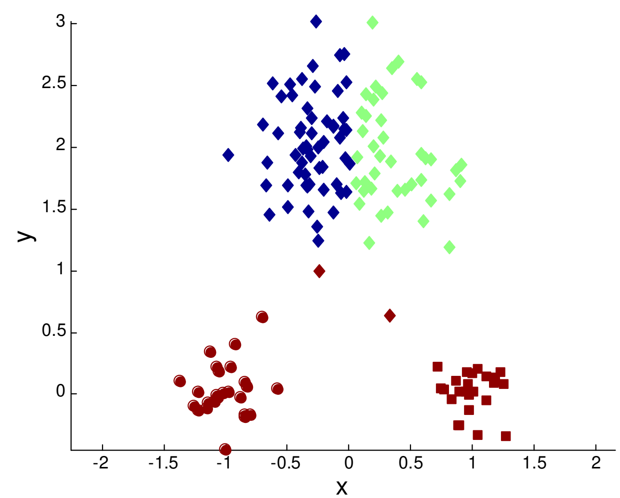
Two different K-means clusterings



Original Points



Optimal Clustering



Sub-optimal Clustering

Some alternatives to random initialization of the central points

- Multiple runs
  - Helps, but probability is not on your side

- Select original set of points by methods other than random. E.g., pick the most distant (from each other) points as cluster centers (kmeans++ algorithm in Scikit Learn)

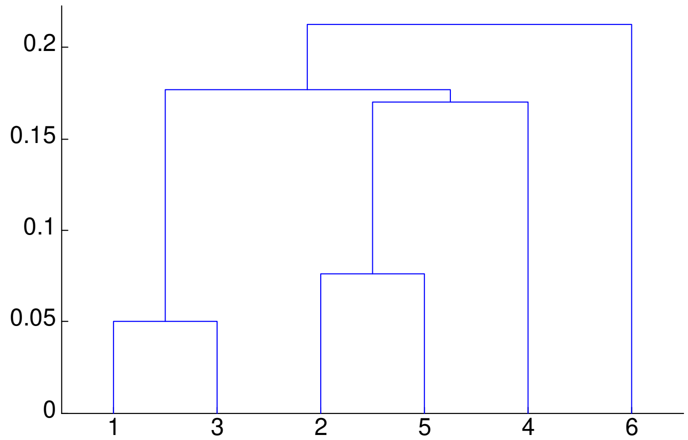
Example of k-means algorithm

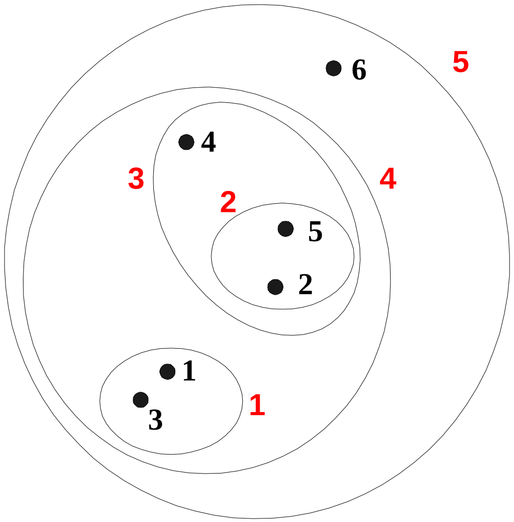
- https://github.com/marcinwolter/MachineLearning2020/blob/main/plot_kmeans_assumptions.ipynb

- The KMeans algorithm clusters data by trying to separate samples in n groups of equal variance, minimizing a criterion known as the inertia or within-cluster sum-of-squares (see below). This algorithm requires the number of clusters to be specified. It scales well to large number of samples and has been used across a large range of application areas in many different fields.

Hierarchical Clustering

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

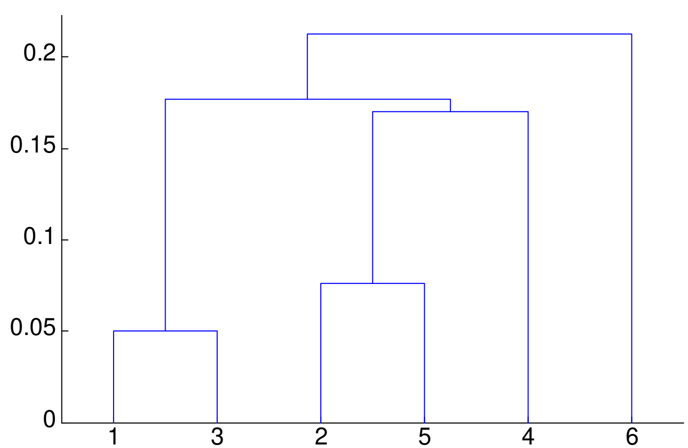


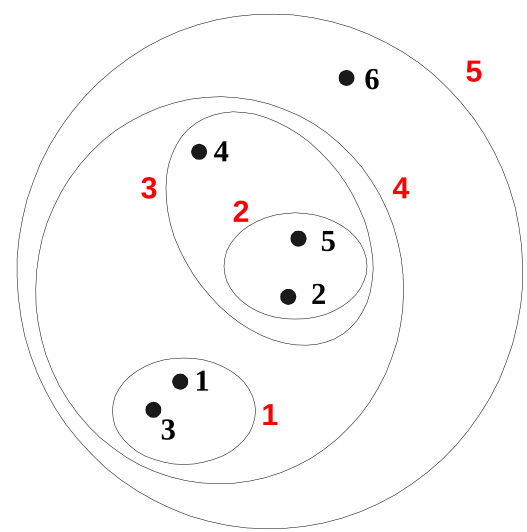


Strengths of Hierarchical Clustering

- No assumptions on the number of clusters
  - Any desired number of clusters can be obtained by ‘cutting’ the dendrogram at the proper level

- Hierarchical clustering may correspond to some meaningful features





Hierarchical Clustering

- Two main types of hierarchical clustering
  - **Agglomerative:**
    - Start with the points as individual clusters
    - At each step, merge the closest pair of clusters until only one cluster (or **k** clusters) left
  - **Divisive:**
    - Start with one, all-inclusive cluster
    - At each step, split a cluster until each cluster contains a point (or there are **k** clusters)

Complexity of hierarchical clustering

- Distance matrix is used for deciding which clusters to merge/split
- At least quadratic in the number of data points
- Not usable for large datasets

Agglomerative clustering algorithm

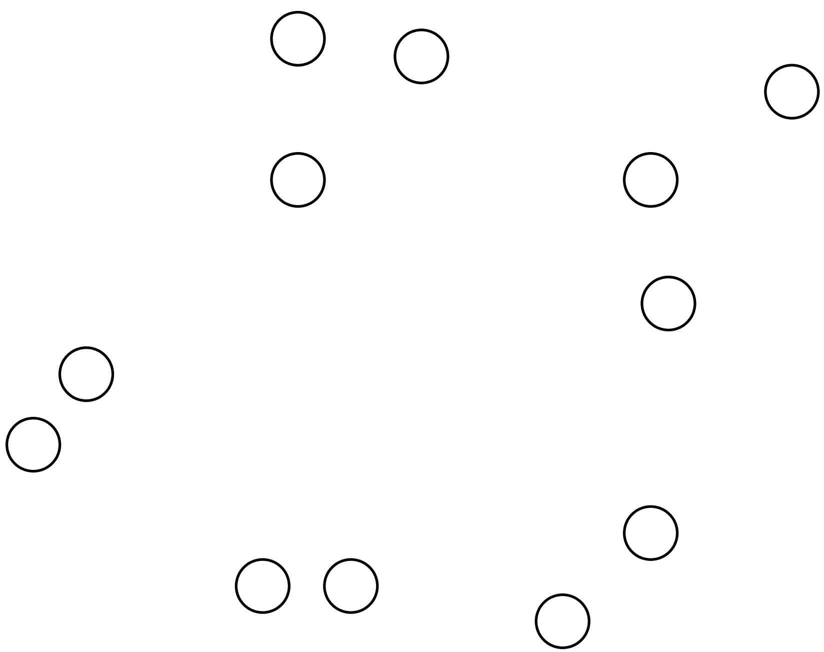
- **Most popular hierarchical clustering technique**

- Basic algorithm
  1. Compute the distance matrix between the input data points
  2. Let each data point be a cluster
  3. **Repeat**
  4. Merge the two closest clusters
  5. Update the distance matrix
  6. **Until** only a single cluster remains

- Key operation is the computation of the distance between two clusters
  – Different definitions of the distance between clusters lead to different algorithms

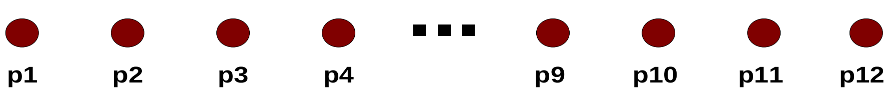
Input / Initial setting

- Start with clusters of individual points and a distance/proximity matrix



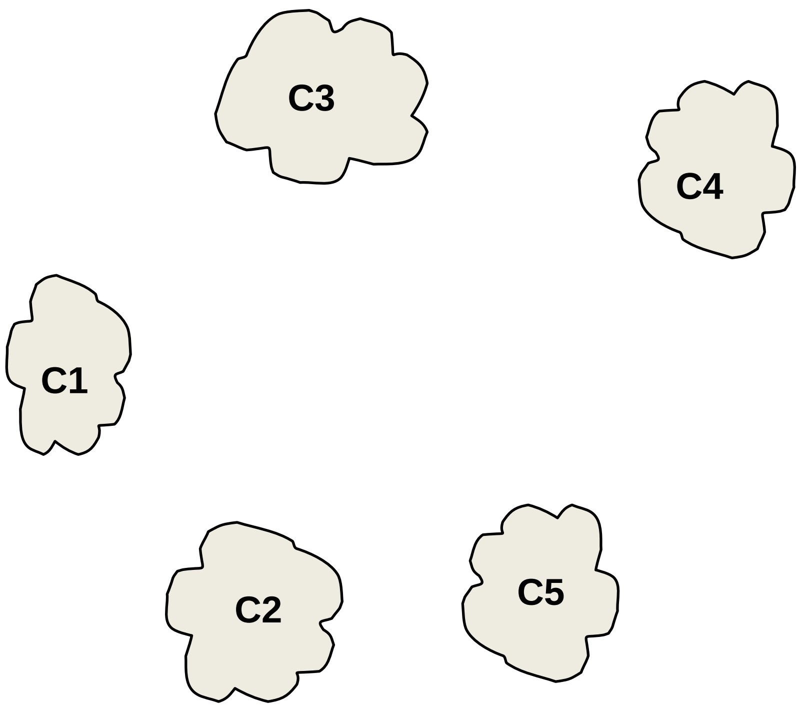
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
. . .						

Distance/Proximity Matrix



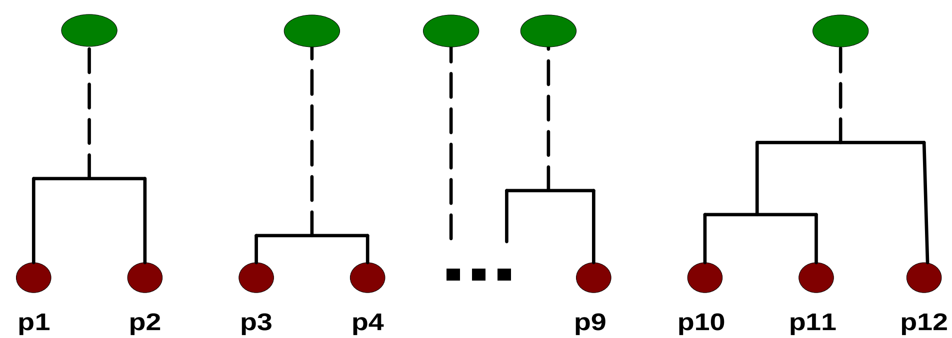
Intermediate State

- After some merging steps, we have some clusters



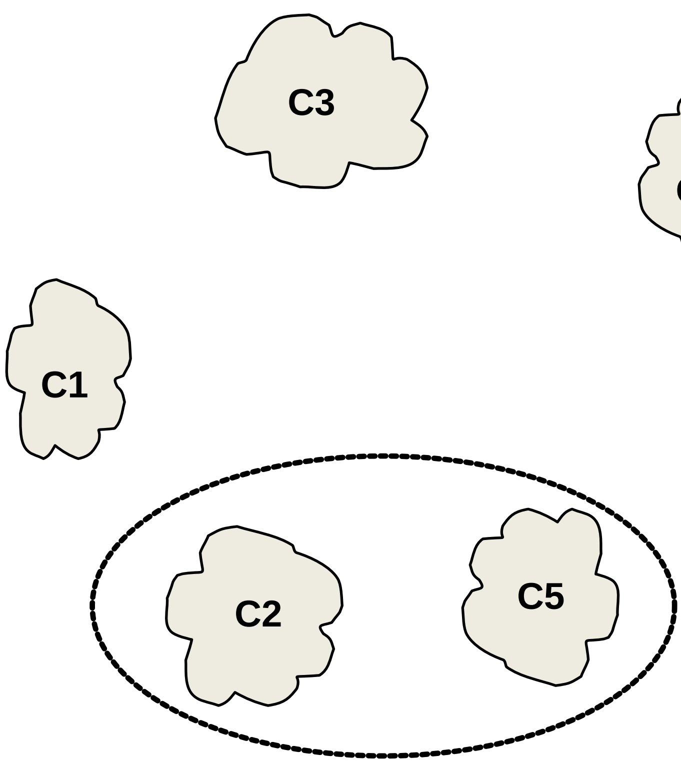
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

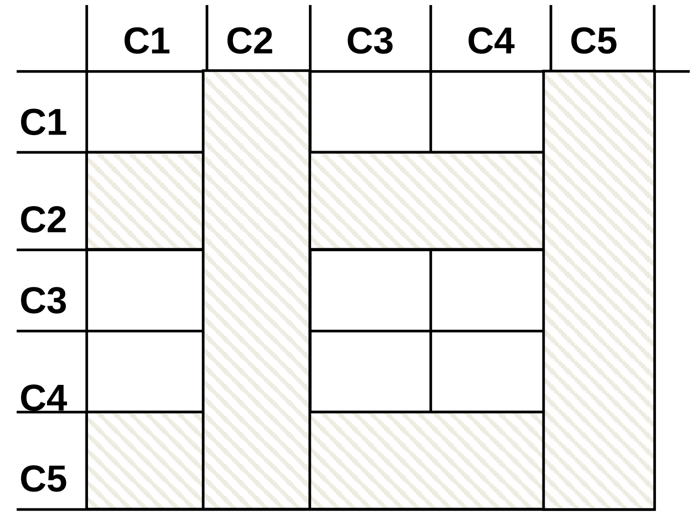
Distance/Proximity Matrix



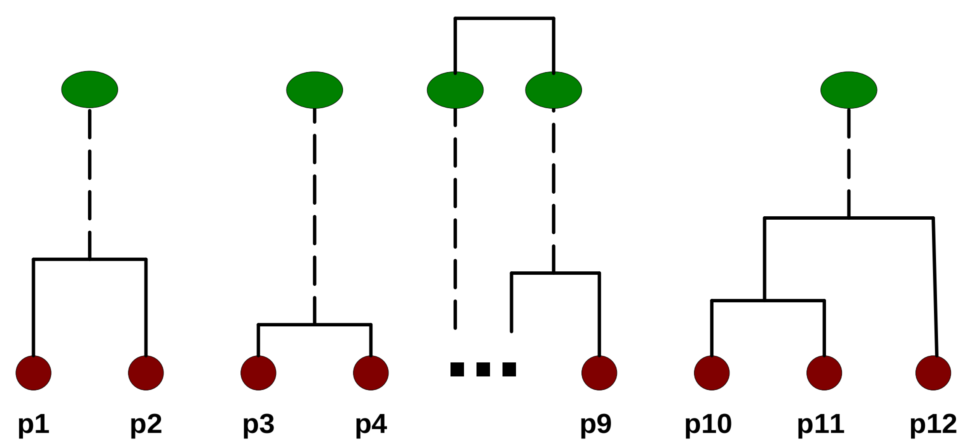
Intermediate State

- Merge the two closest clusters (C2 and C5) and update the distance matrix.



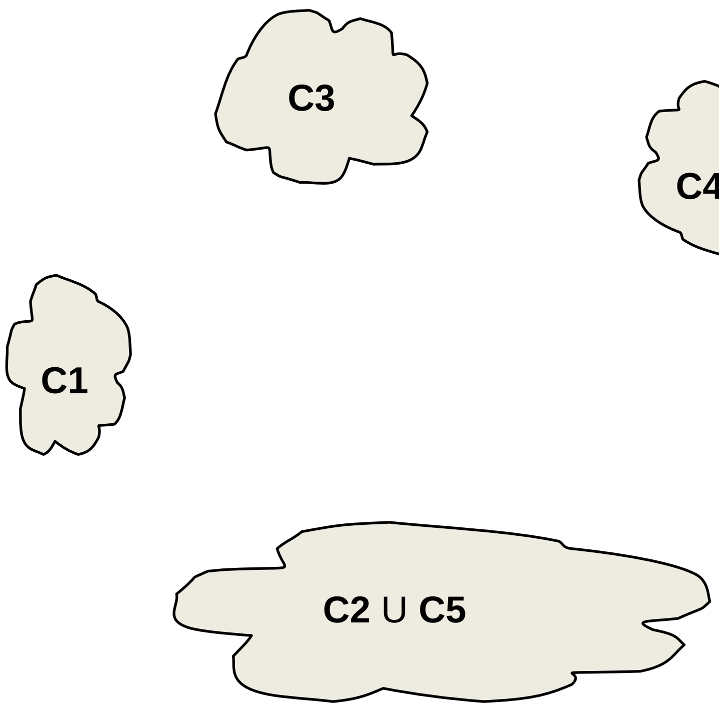


Distance/Proximity Matrix

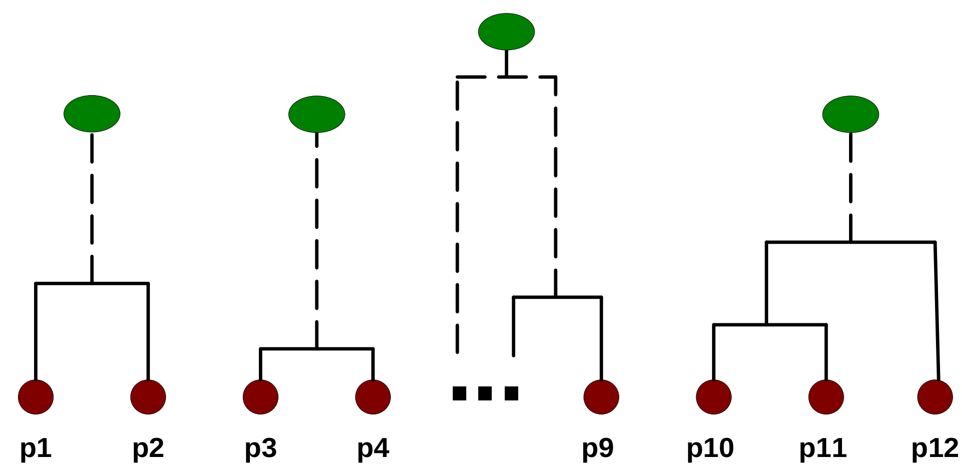


After Merging

- “How do we update the distance matrix?”



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



Distance between two clusters

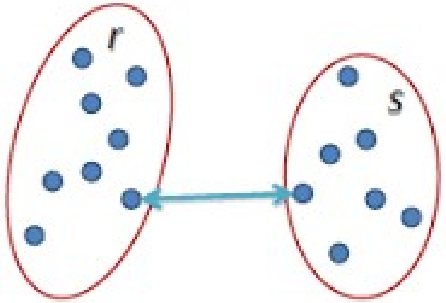
- Each cluster is a set of points
- How do we define distance between two sets of points?
  - Lots of alternatives
  - Not an easy task

Distance between two clusters

- **Single-link distance** between clusters C_i and C_j is the ***minimum distance*** between any object in C_i and any object in C_j

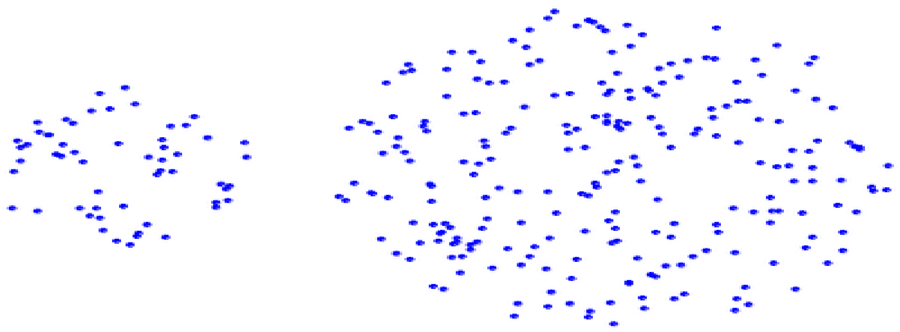
- The distance is **defined by the two most similar objects**

$$D_{sl}(C_i, C_j) = \min_{x,y} \{ d(x,y) \mid x \in C_i, y \in C_j \}$$

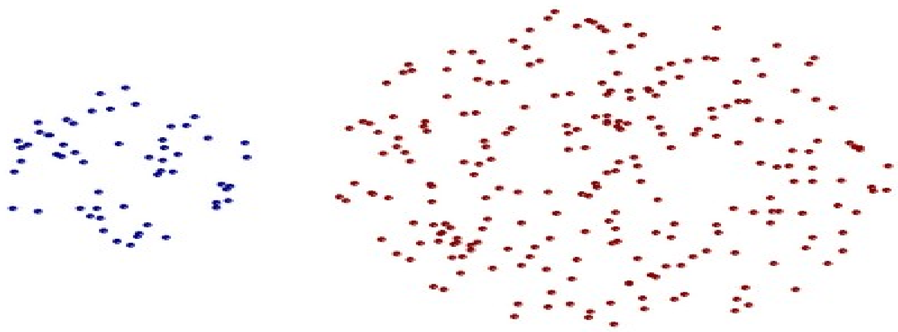


$$L(r,s) = \min(D(x_{ri}, x_{sj}))$$

Strengths of single-link clustering



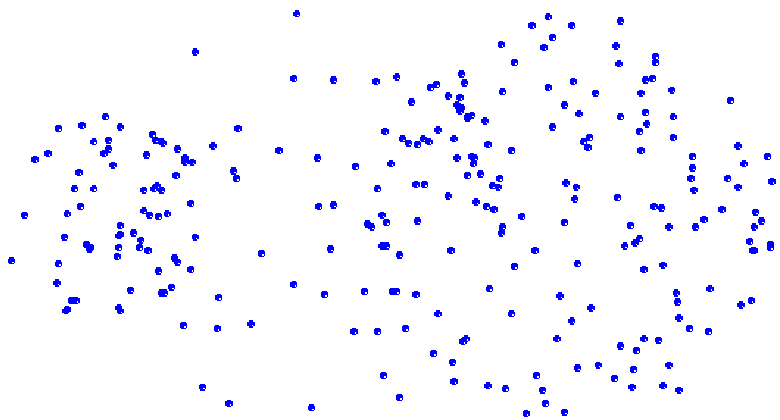
Original Points



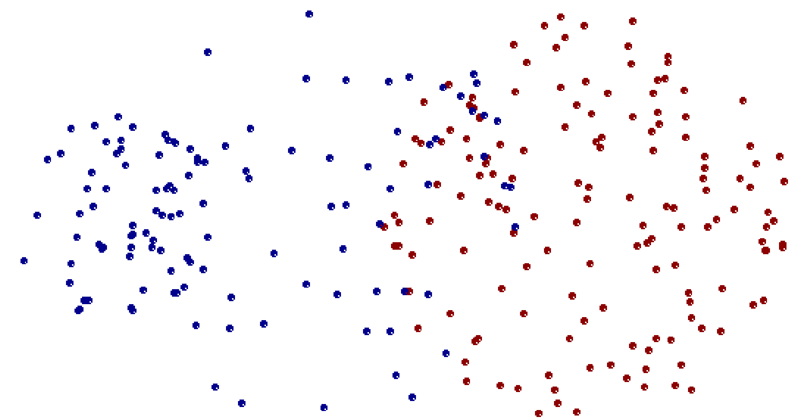
Two Clusters

- Can handle non-elliptical shapes

Limitations of single-link clustering



Original Points



Two Clusters

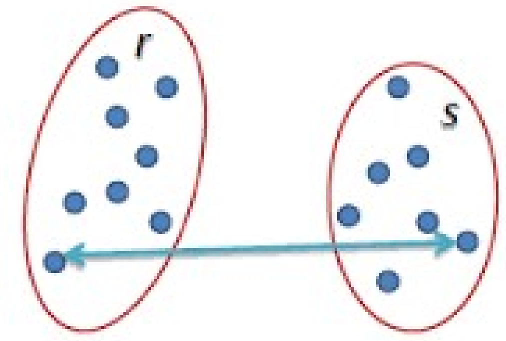
- Sensitive to noise and outliers
- Produces long, elongated clusters

Distance between two clusters

- **Complete-link distance** between clusters C_i and C_j is the ***maximum distance*** between any object in C_i and any object in C_j

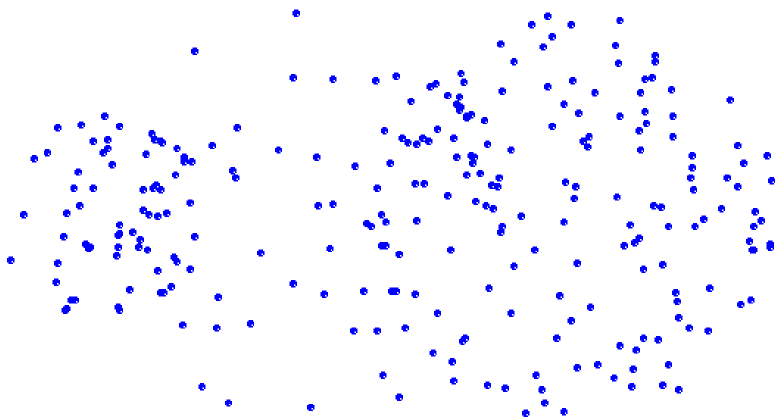
- The distance is **defined by the two most dissimilar objects**

$$D_{cl}(C_i, C_j) = \max_{x,y}\{d(x,y) \mid x \in C_i, y \in C_j\}$$

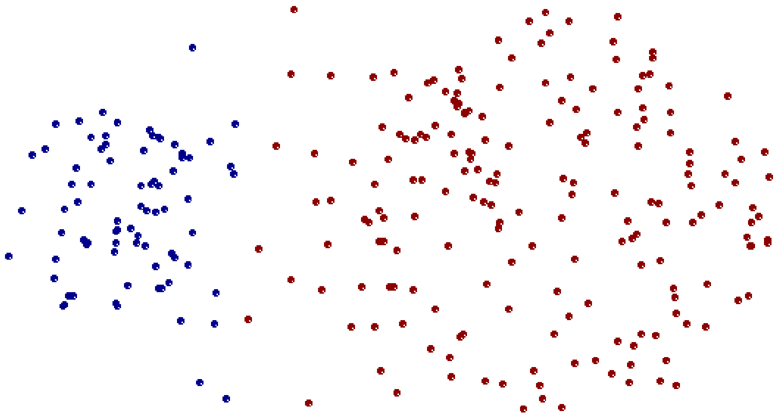


$$L(r,s) = \max(D(x_{ri}, x_{sj}))$$

Strengths of complete-link clustering



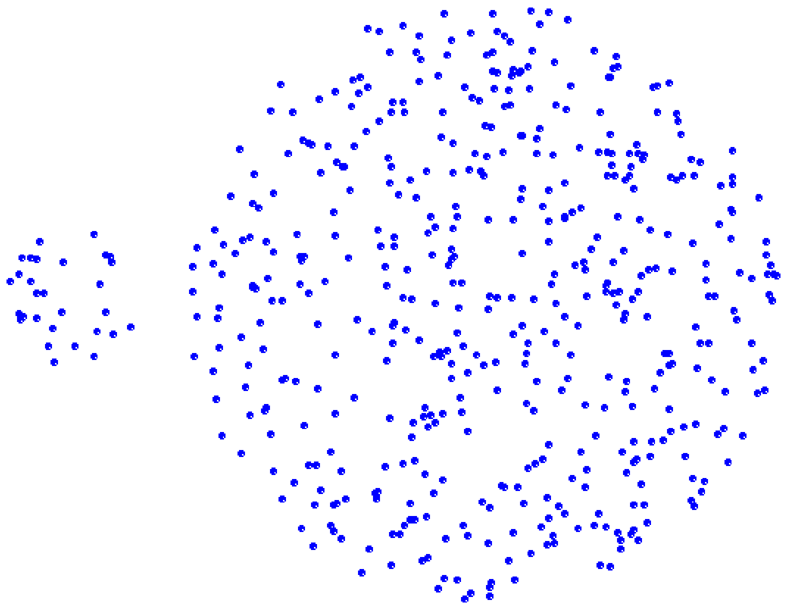
Original Points



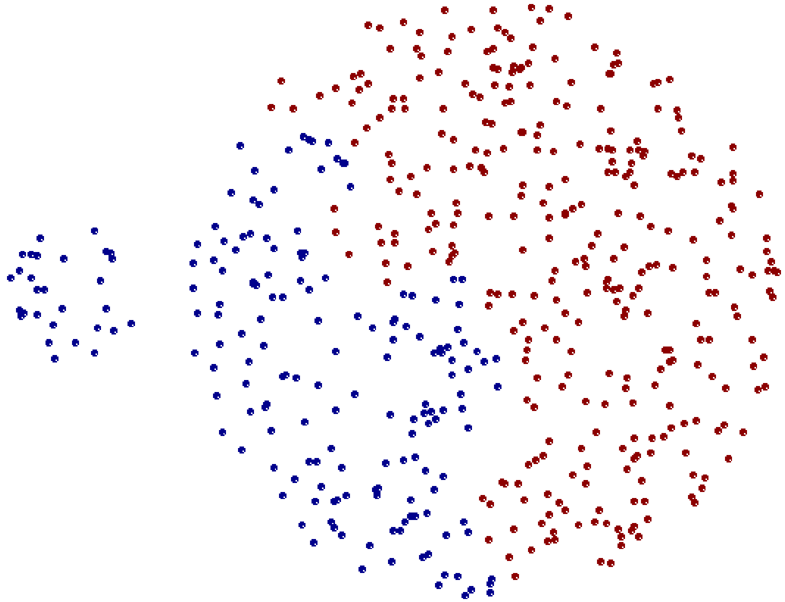
Two Clusters

- More balanced clusters (with equal diameter)
- Less susceptible to noise

Limitations of complete-link clustering



Original Points



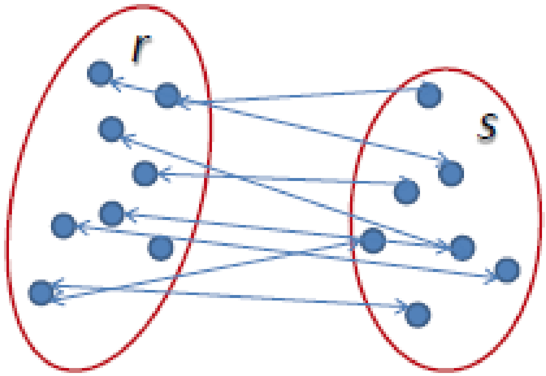
Two Clusters

- Tends to break large clusters
- All clusters tend to have the same diameter – small clusters are merged with larger ones

Distance between two clusters

- **Group average distance** between clusters C_i and C_j is the ***average distance*** between any object in C_i and any object in C_j

$$D_{avg}(C_i, C_j) = \frac{1}{|C_i| \times |C_j|} \sum_{x \in C_i, y \in C_j} d(x, y)$$



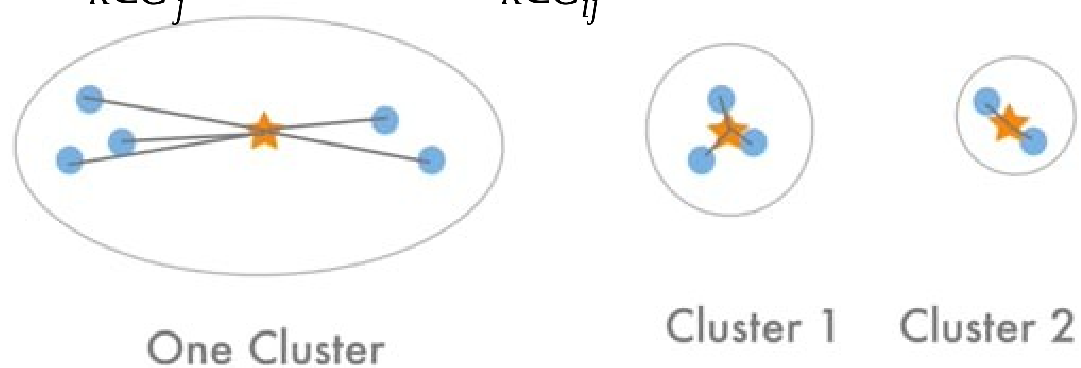
$$L(r,s) = \frac{1}{n_r n_s} \sum_{i=1}^{n_r} \sum_{j=1}^{n_s} D(x_{ri}, x_{sj})$$

Distance between two clusters

- **Ward's distance** between clusters C_i and C_j is the ***difference*** between the ***total within cluster sum of squares for the two clusters separately***, and the ***within cluster sum of squares resulting from merging the two clusters*** in cluster C_{ij}

$$D_w\left(C_i, C_j\right) = \sum_{x \in C_i} \left(x - r_i\right)^2 + \sum_{x \in C_j} \left(x - r_j\right)^2 - \sum_{x \in C_{ij}} \left(x - r_{ij}\right)^2$$

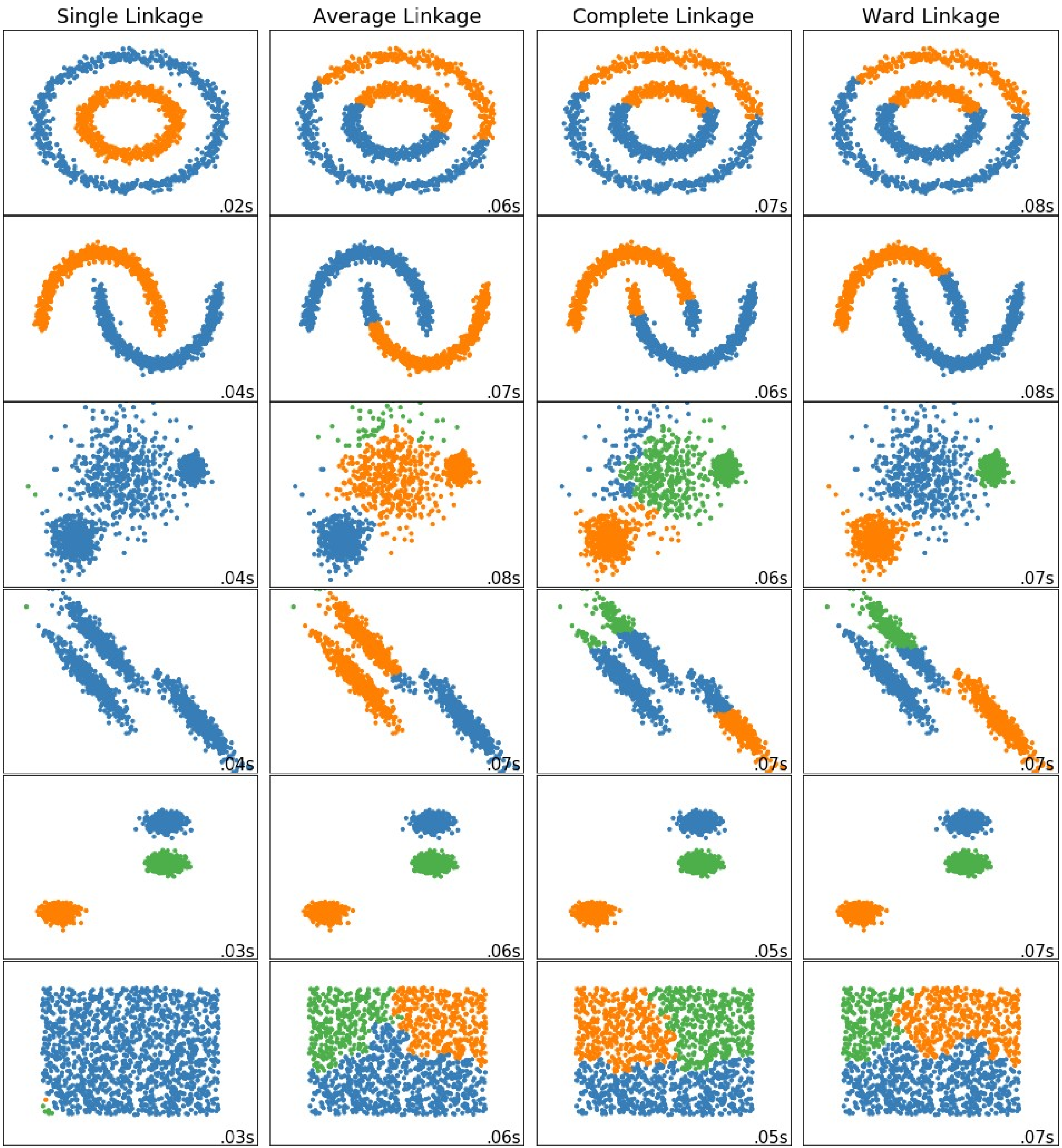
- r_i: centroid of C_i
- r_j: centroid of C_j
- r_{ij}: centroid of C_{ij}



Ratio of sum of squared distance from means, between one cluster, and the two clusters defines the intercluster distance

Ward’s distance for clusters

- Similar to group average and centroid distance
- Less susceptible to noise and outliers
- Hierarchical analogue of k-means
  - Can be used to initialize k-means


Single Linkage
Average Linkage
Complete Linkage
Ward Linkage
.02s
.06s
.07s
.08s
.04s
.07s
.06s
.08s
.04s
.08s
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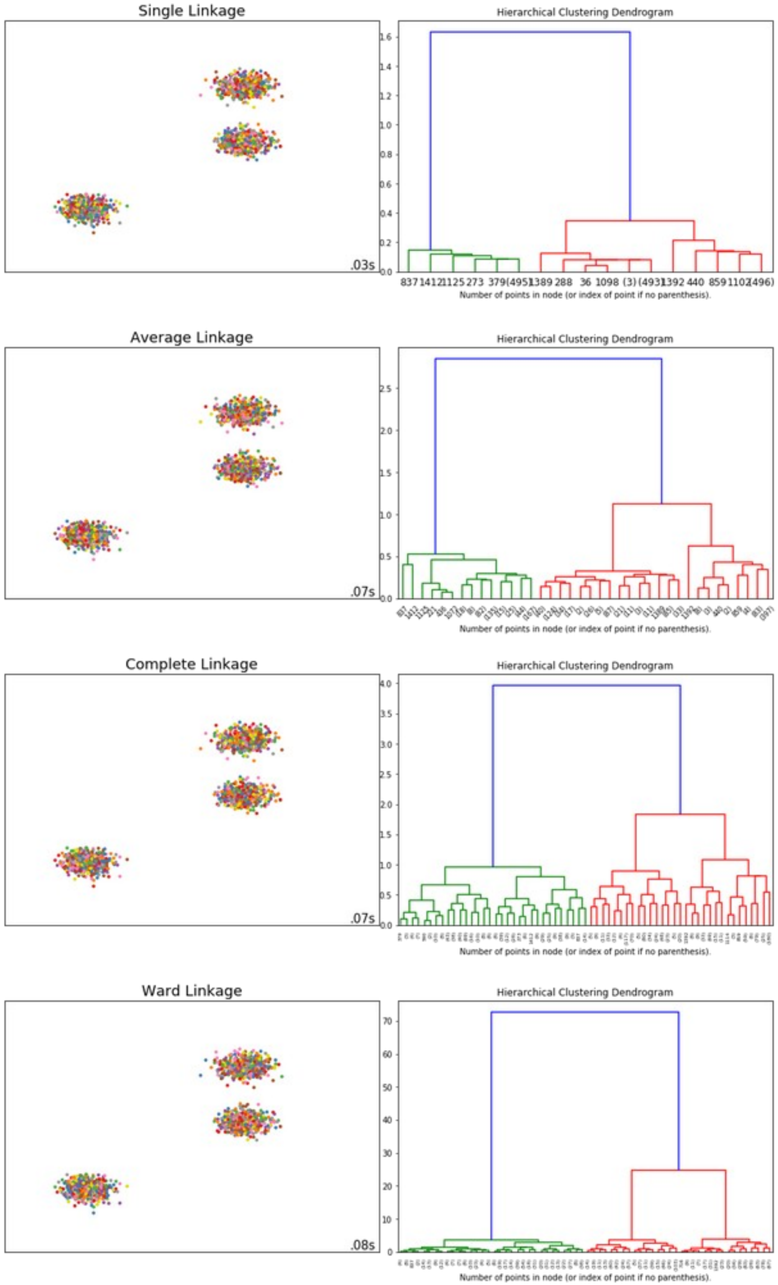
Comparison of distance measurements

https://github.com/marcinwolter/MachineLearning2020/blob/main/plot_linkage_comparison.ipynb



Cluster analysis

- Clustering analysis is broadly used in many applications such as market research, pattern recognition, data analysis, and image processing.
- As a data mining function, cluster analysis serves as a tool to gain insight into the distribution of data to observe characteristics of each cluster.