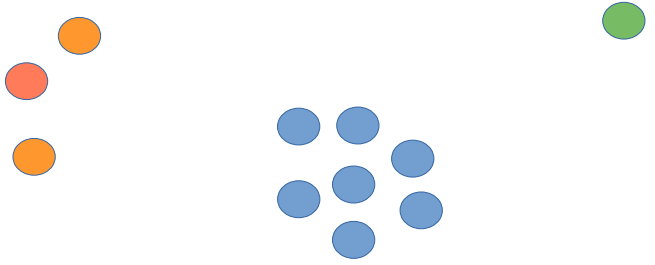
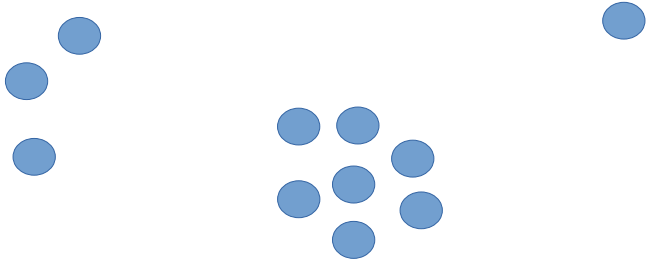
Clustering



Clustering

Group similar data points together, no labels
"unsupervised"



Clustering

Group similar data points together, no labels
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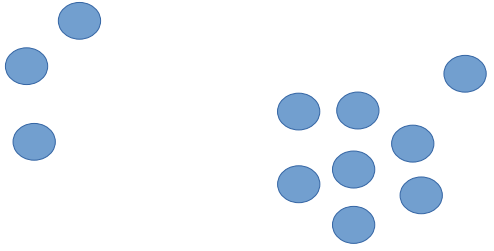
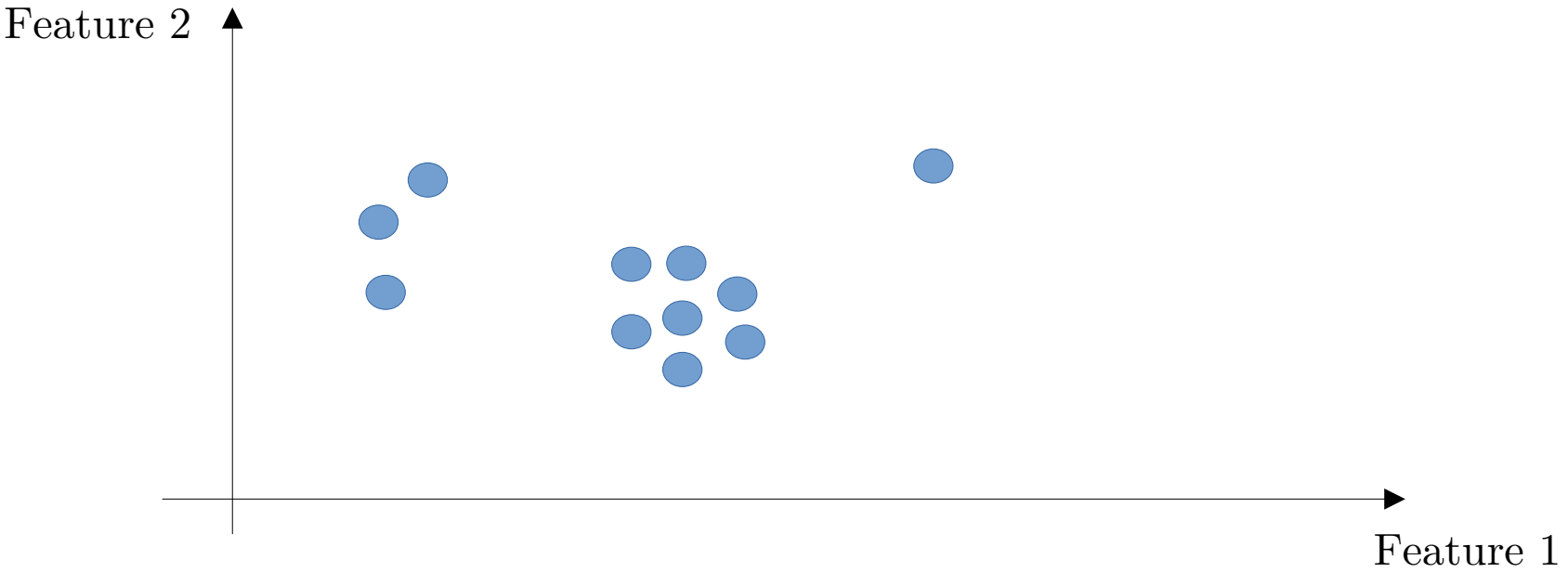
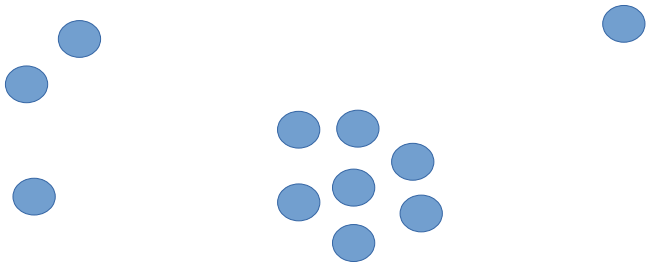


What do we need for clustering?



Group similar data points together, no labels
"unsupervised"



In addition to the data, we need some additional information such as:

- A definition of distance or dissimilarity (how close?)
- Minimal inter-cluster distance (Should I merge?)
- Other measures of separability?
- Number of clusters (find the merging distance automatically)
- ...

Different clustering methods

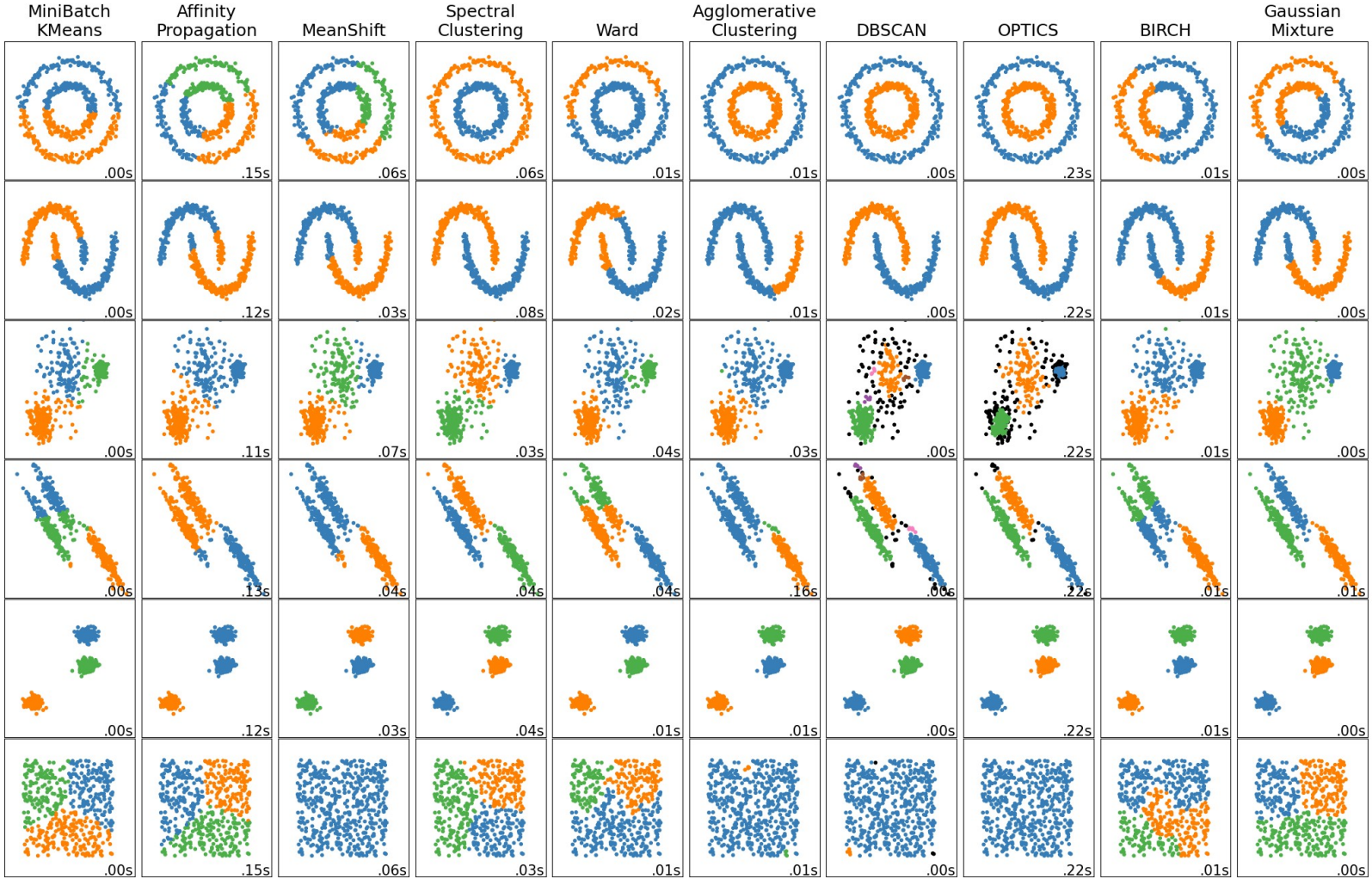
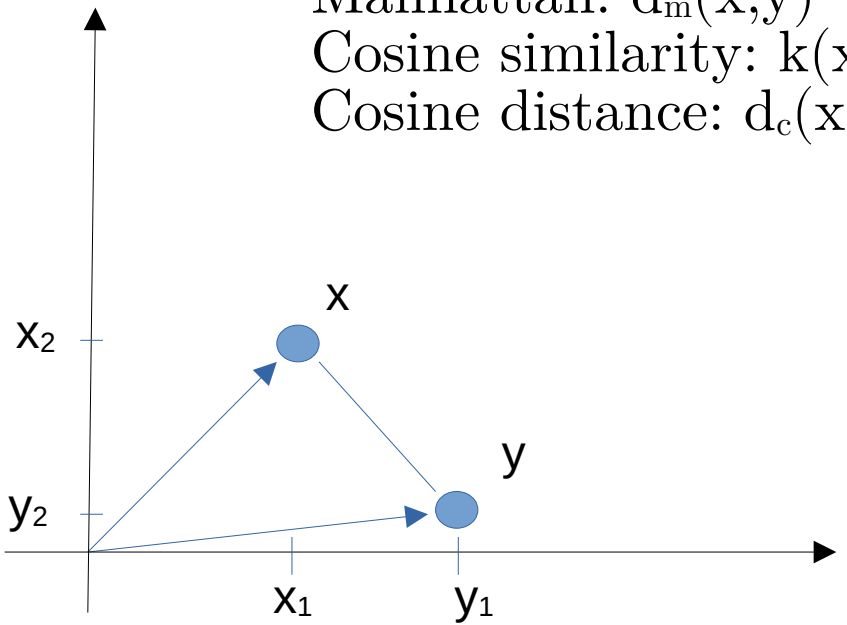


Figure from scikit-learn, clustering

Distance or similarity

Some common distances in dim *n*:
Euclidean: $d_e(x,y)$
Manhattan: $d_m(x,y)$
Cosine similarity: $k(x,y)$
Cosine distance: $d_c(x,y) = 1 - k(x,y)$



$$d_e(x,y) = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}$$

$$d_m(x,y) = \sum_{i=1}^{n}|x_i - y_i|$$

$$k(x,y) = \frac{(x,y)}{\|x\|\,\|y\|} = \cos\theta$$

Sequential clustering

- Datapoints in space
- Distance (or dissimilarity measure) **between a point and a cluster** $d(x_i, C_k)$
- Threshold θ
- Max number of clusters q

Basic Sequential Algorithmic Sequence (BSAS)

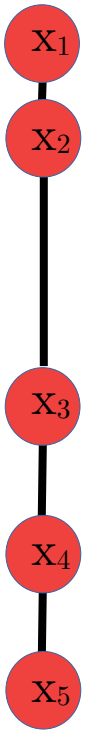
Let m=1
$C_m = x_1$
For i=2 to N,
  Find $C_k : d(x_i, C_k) = \min_{1 \le j \le m} d(x_i, C_j)$
  If $(d(x_i, C_k) > \Theta)$ AND $(m < q)$,
    m=m+1
    $C_m = x_i$
  Else,
    $C_k = C_k \cup x_i$
    Where necessary, update representatives
  end
end

Iterate over the samples

Create a new cluster

Add to closest cluster

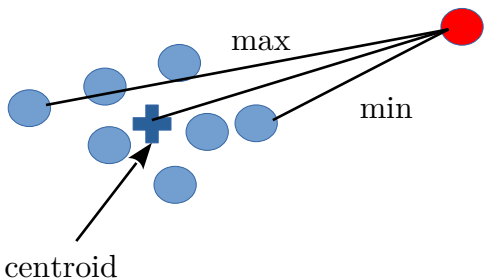
See next slide

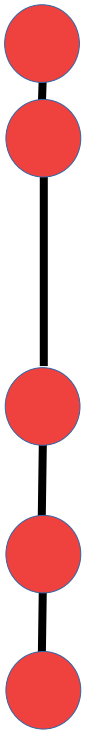


Sequential clustering

Distance between point x_i and cluster C_k: $d(x_i,C_k)$

"update representative": mean point, centroid
Or
Min/max distance between x_i and all the points in C_k

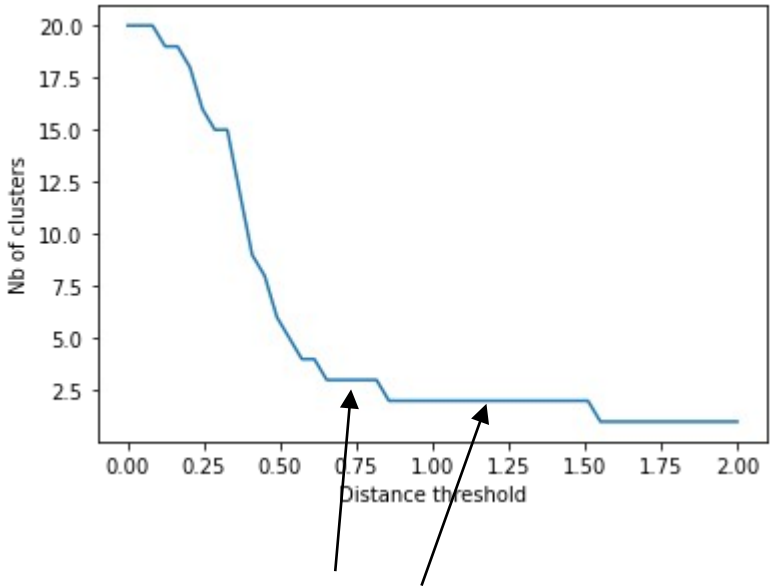




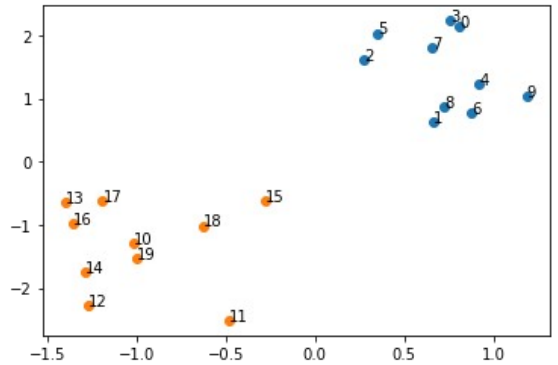
Number of clusters?

Simple way to estimate the best number of clusters

- Run the clustering for different θ



Flat areas where changing the threshold does not affect the nb of clusters → gaps



Select the number associated to the largest flat area

Hierarchical clustering

Keep track of the clustering steps (which sample merged when)
Agglomerative or divisive

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

We focus on agglomerative clustering (the most popular)
- Divisive have a better global view but requires more computation.

This is an introduction, you will get more details in the course Pattern Recognition FYS-3012

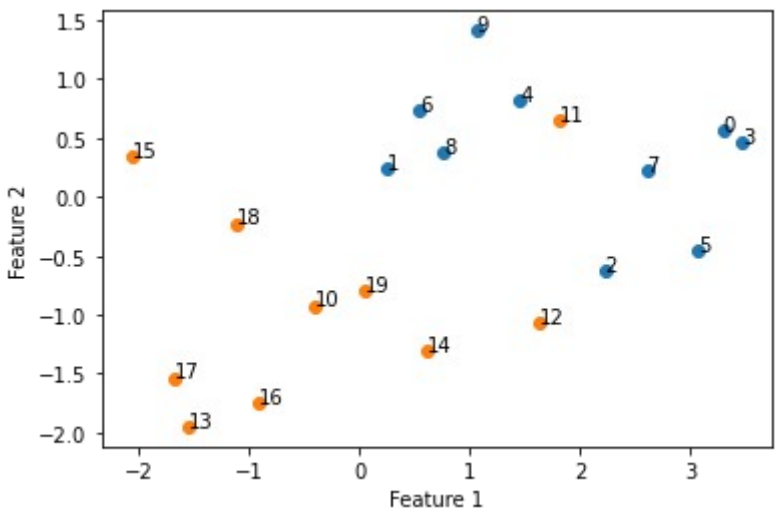
Hierarchical clustering
Dendrogram

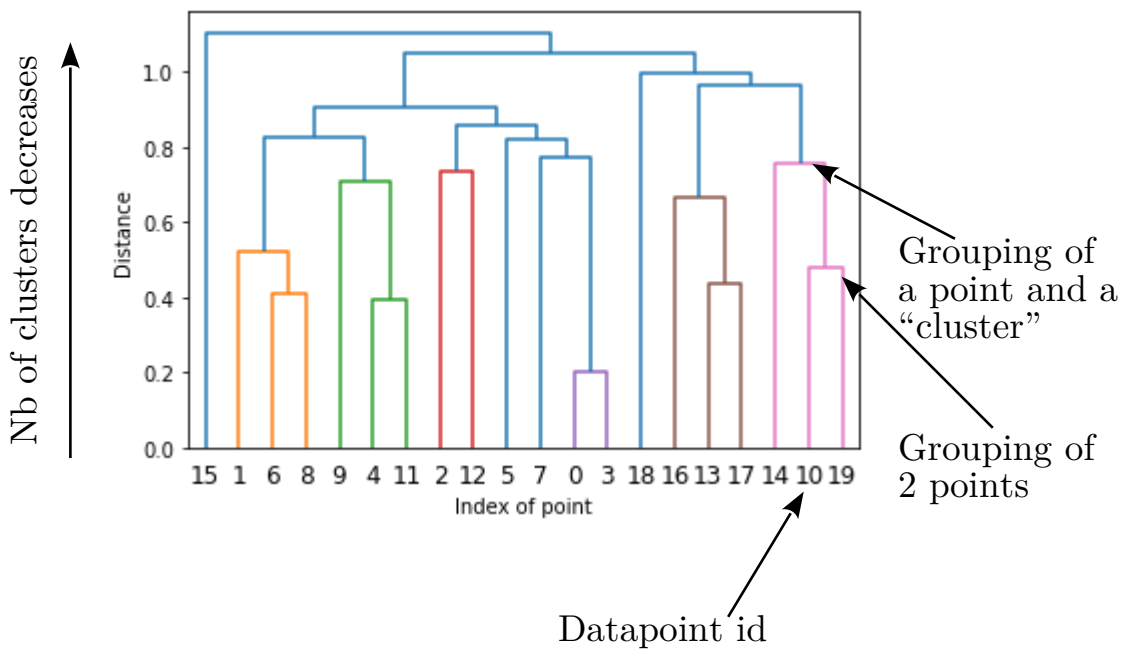
Group the closest datapoints, one by one

Agglomerative scheme:
$R_0 = \{C_i=\{x_i\}, i=1,...,N\}$, each sample is a cluster
$t= 0$
Repeat:
- $t = t+1$
- Find the "closest" 2 clusters C_i and C_j
- Merge them $C_q=C_i \cup C_j$ and update $R_t=(R_{t-1}-\{C_i ,C_j\}) \cup \{C_q\}$
- Until all samples are in a single cluster

Hierarchical clustering
Dendrogram

Group the closest datapoints, one by one



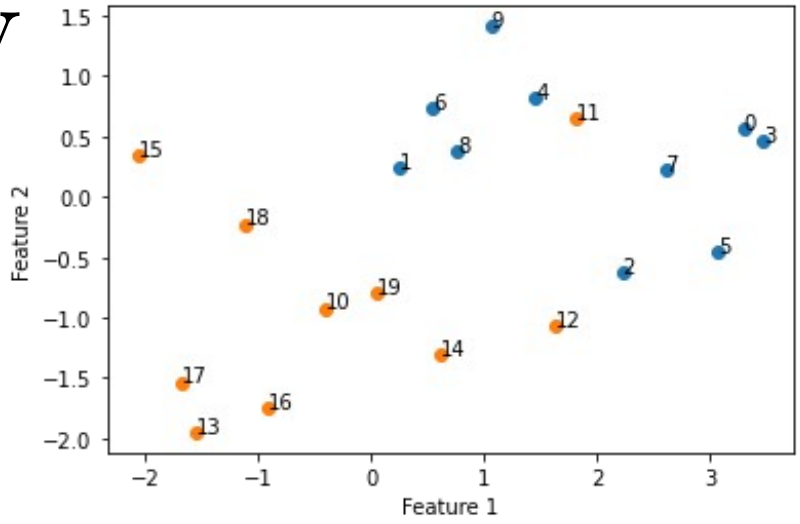


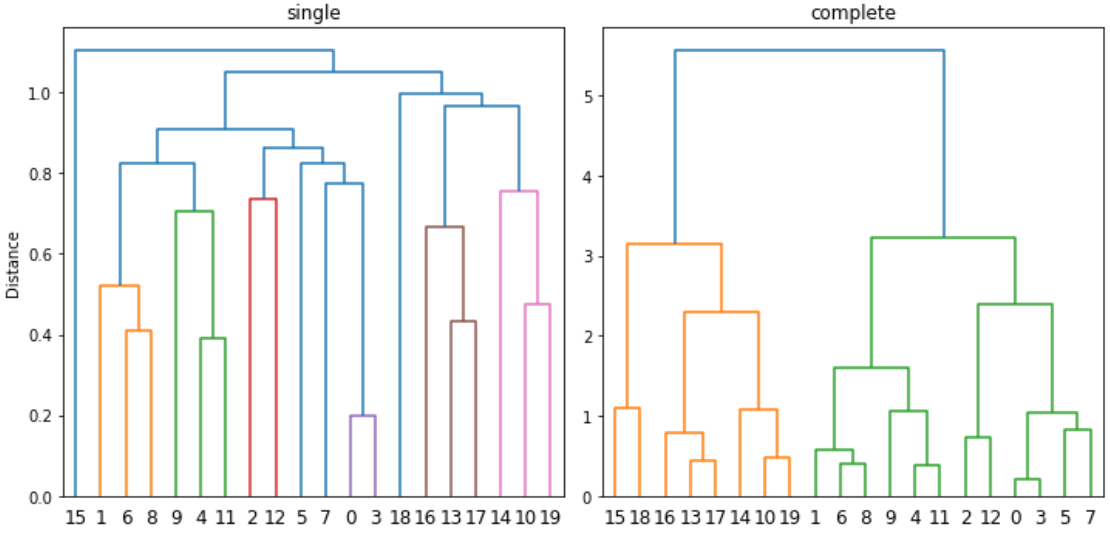
What is the definition of "closest" between a point and a cluster?

Distance or dissimilarity

Cluster C_i and C_j are merged into one (C_i,C_j).
Distance from any C_s to (C_i,C_j) is:

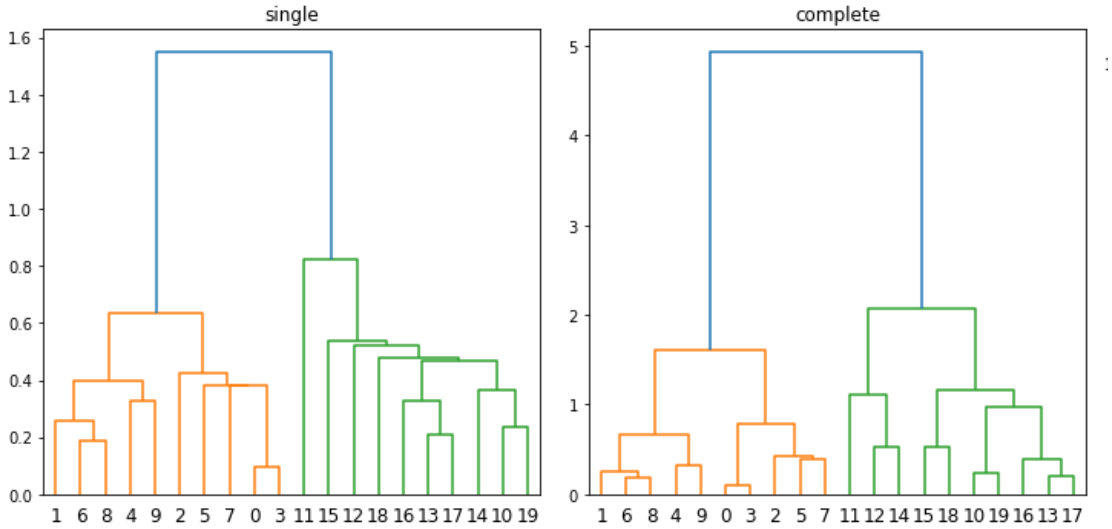
- Single linkage: $\min(d(C_s,C_i), d(C_s,C_j))$
- Average: $[d(C_s,C_i)+d(C_s,C_j)]/2$
- Complete linkage: $\max(d(C_s,C_i), d(C_s,C_j))$

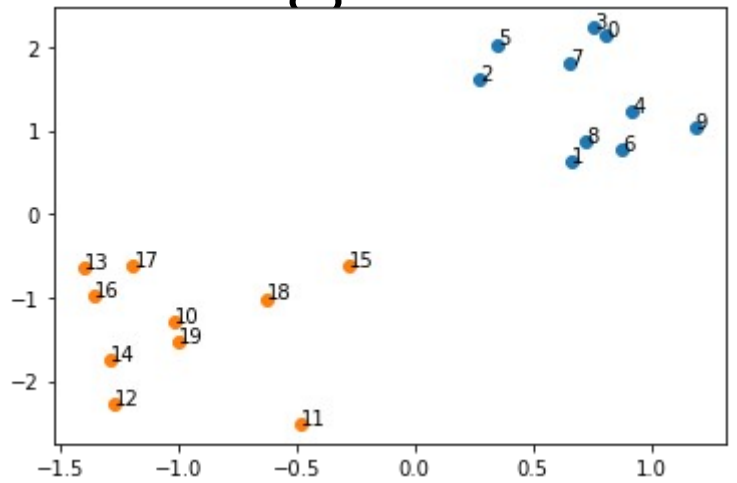


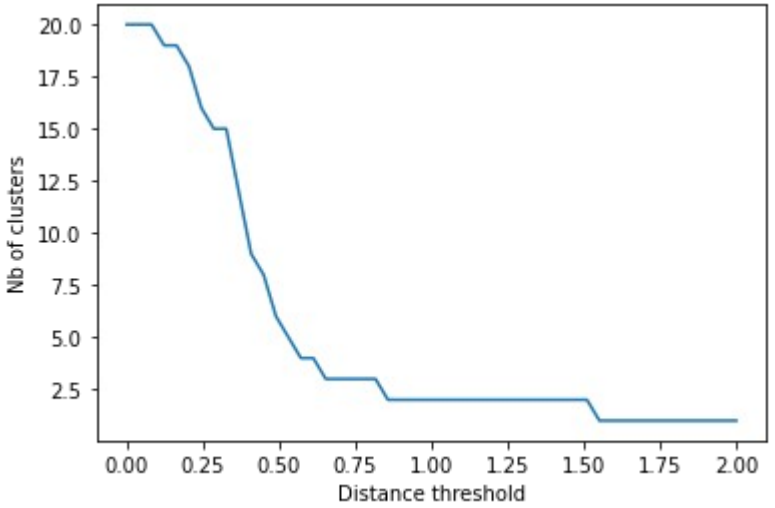


Hierarchical clustering

Best number of clusters?







Conclusion

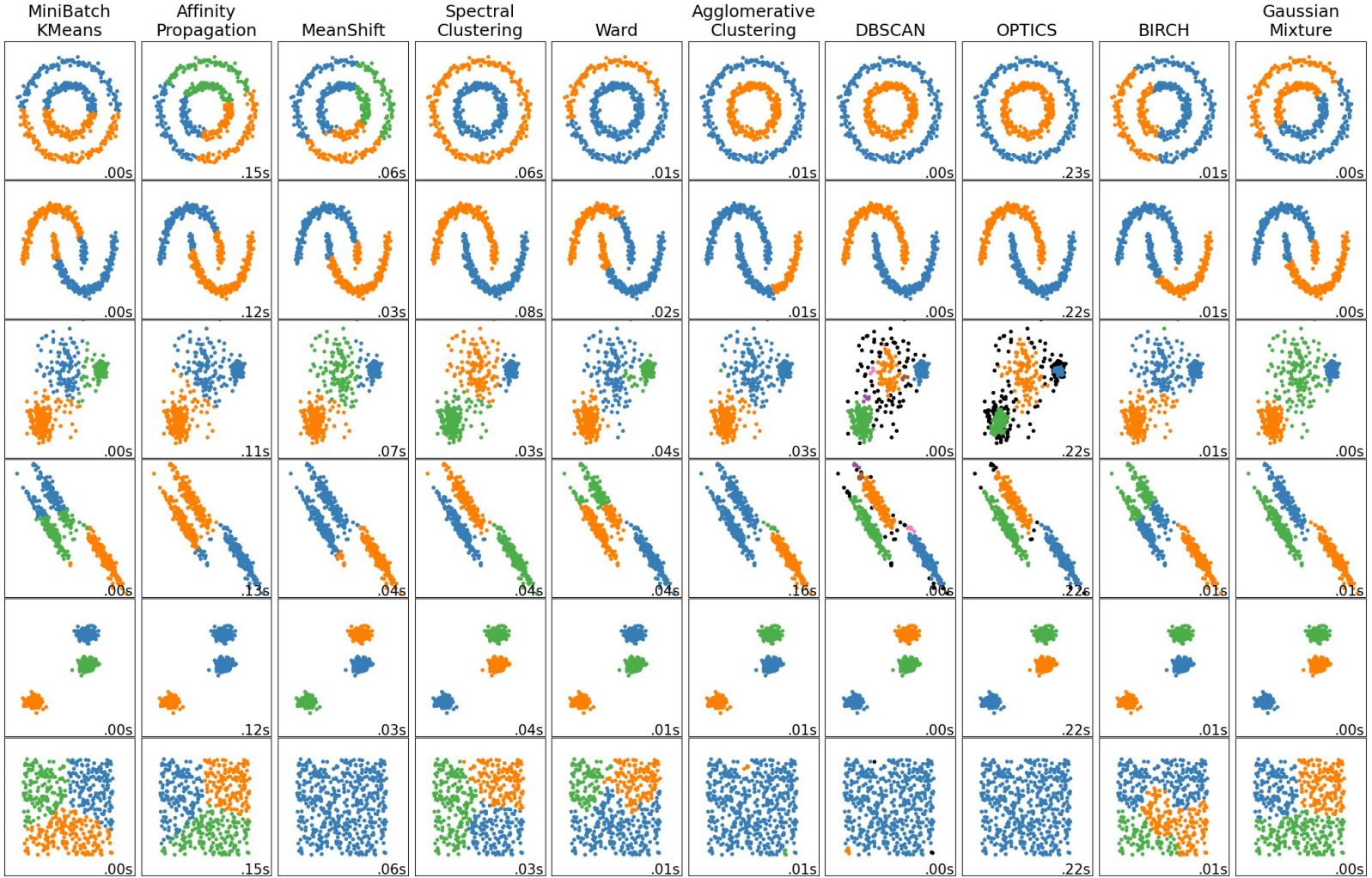


Figure from scikit-learn, clustering