JSC 270 - Lecture 7
Clustering

https://jsc270.github.io/

ANNOUNCEMENTS

Perusall will be available at 2pm today

Next lecture is a guest lecture on NLP by Alistair Johnson

Supervised vs Unsupervised Learning

Supervised learning:

Data: (x_1,y_1), (x_2,y_2),...,(x_N,y_N)

Goal: find f(x), such that f minimizes a loss, eg $L(y, \hat{y}) = (y - \hat{y})^2$

Examples: classification, regression

Supervised vs Unsupervised Learning

Supervised learning:

Data: (x_1,y_1), (x_2,y_2),...,(x_N,y_N)

Goal: find f(x), such that f minimizes a loss, eg $L(y,\hat{y}) = (y-\hat{y})^2$

Examples: classification, regression

Unsupervised:

Data: $(x_1, x_2,..., x_N)$

Goal: P(X) or characteristics of the set of data

Examples: clustering

Clustering

How would you define clustering intuitively?

Clustering

Identifying subsets of similar items, where similar can be defined in a variety of ways

Examples of clustering

What applications of clustering can you think of?

Examples of clustering

Healthcare: identifying sets of similar patients (called *subphenotyping*)

Marketing: identifying groups of clients that could be targeted with the same messaging

Text: grouping together emails/documents by topic

What clustering methods do you know?

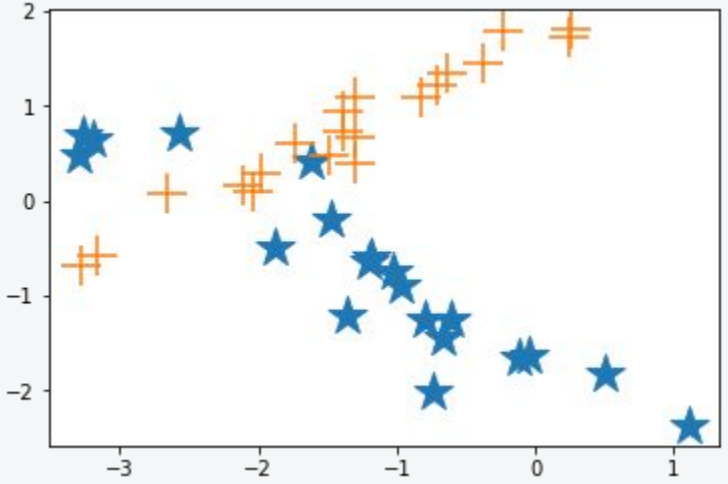
Clustering methods out there...

- Hierarchical clustering
  - Agglomerative
- K-means (X-means)
- Model based (e.g. Mixture of Gaussians)
- Affinity propagation
- Spectral
- LDA (Latent Dirichlet Allocation)
- Network/Graph clustering
  - Graph cuts (e.g. min cut - cut min # of edges)
  - Highly connected subgraphs

many more....

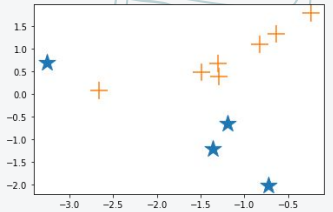
DATA

DATA

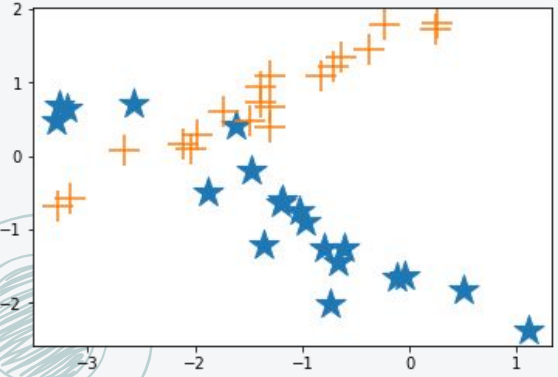


40 points
2 features
2 clusters

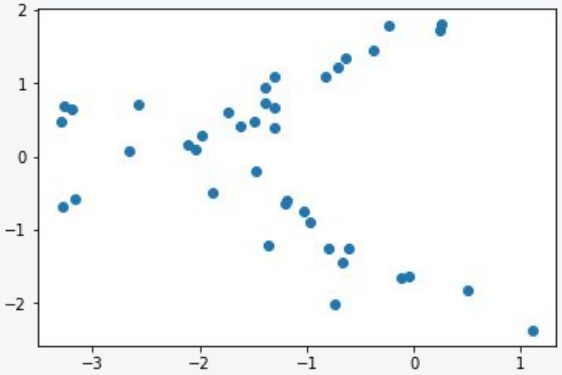
DATA



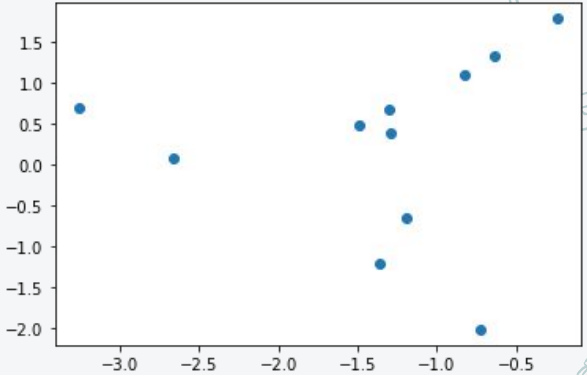
Original data



What we see



A subsample of 11 points



Clustering methods out there...

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  - **Agglomerative**
- **K-means (X-means)**
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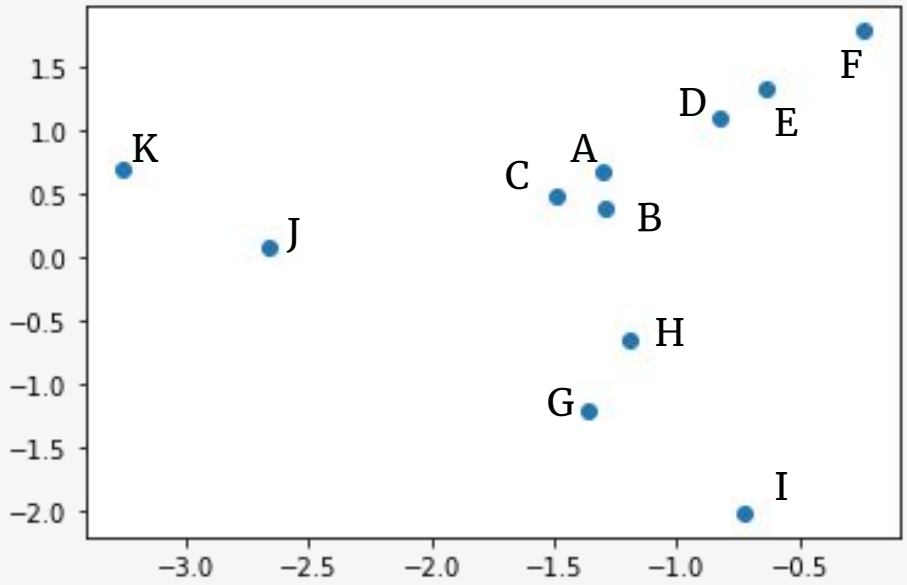
many more....

Agglomerative hierarchical clustering

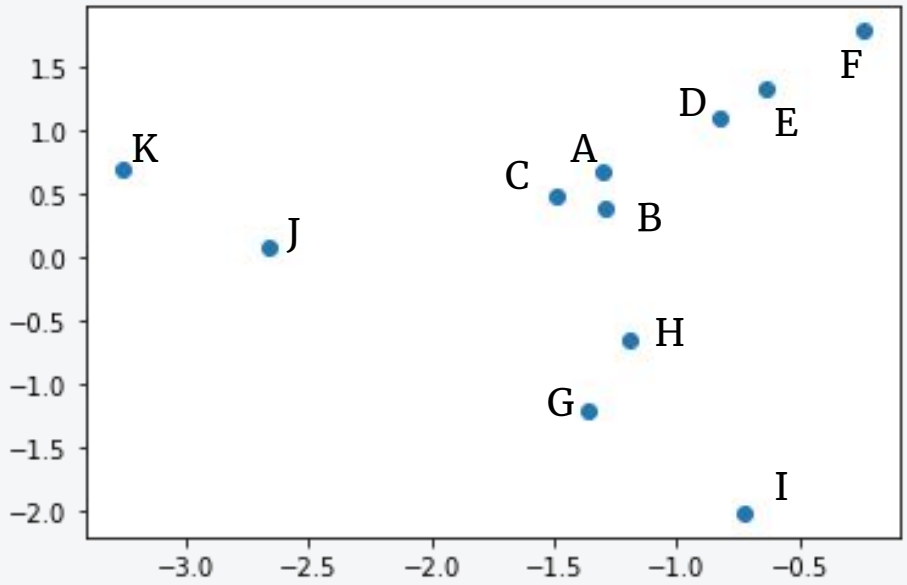
- Start with each point being each own cluster

- Compute similarity between all current clusters
- Use linkage function to combine the closest ones
- Repeat until desired number of clusters or all merged

Agglomerative hierarchical clustering

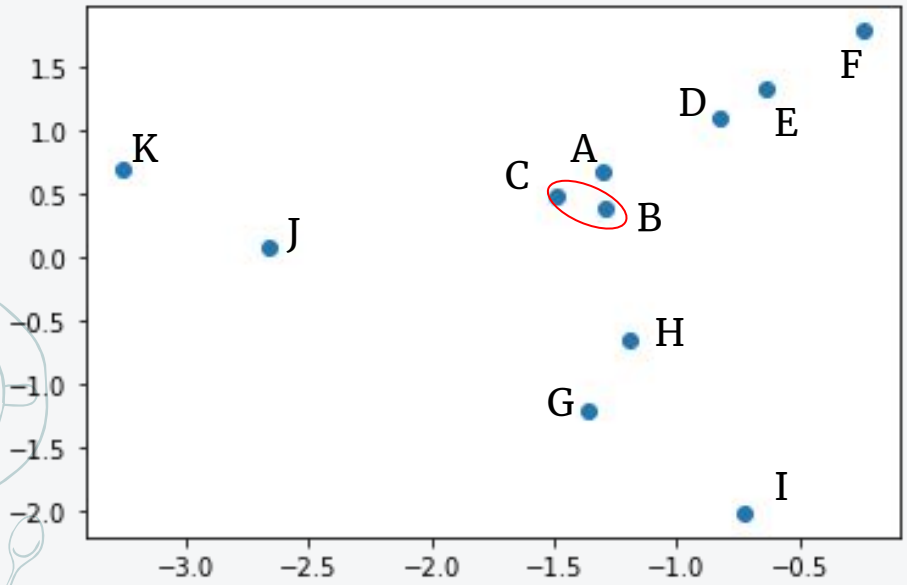


Agglomerative Hierarchical Clustering

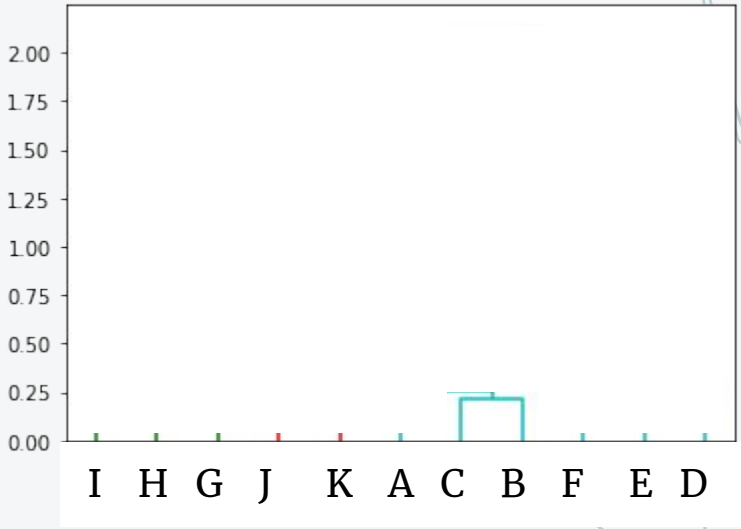


Distance: Euclidean
Linkage: Centroid

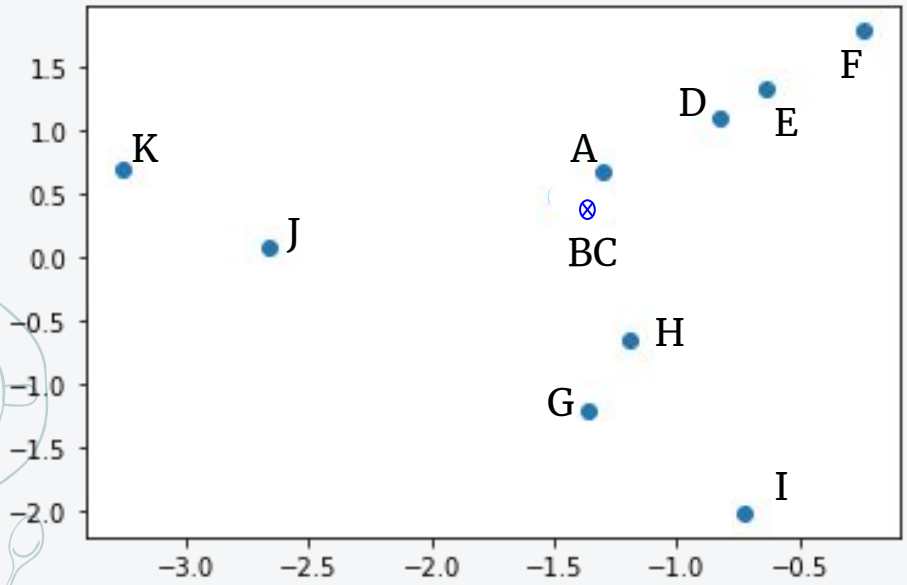
Agglomerative Hierarchical Clustering



Dendrogram



Agglomerative Hierarchical Clustering



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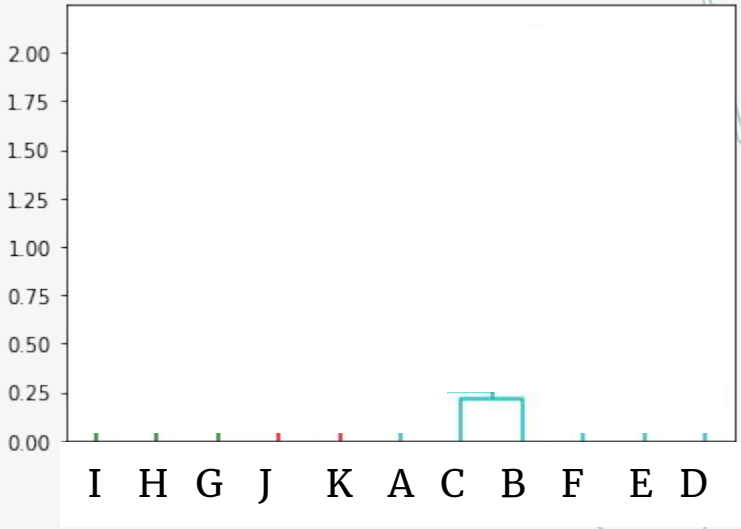
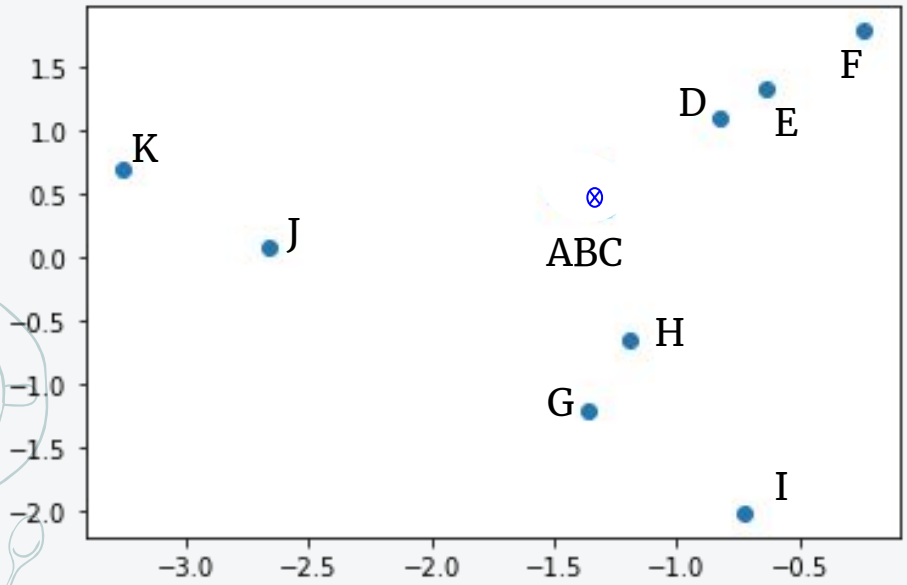


Agglomerative Hierarchical Clustering



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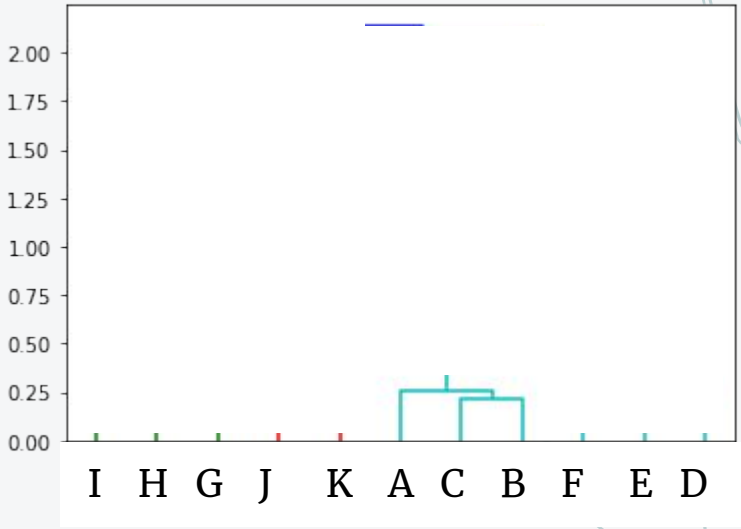
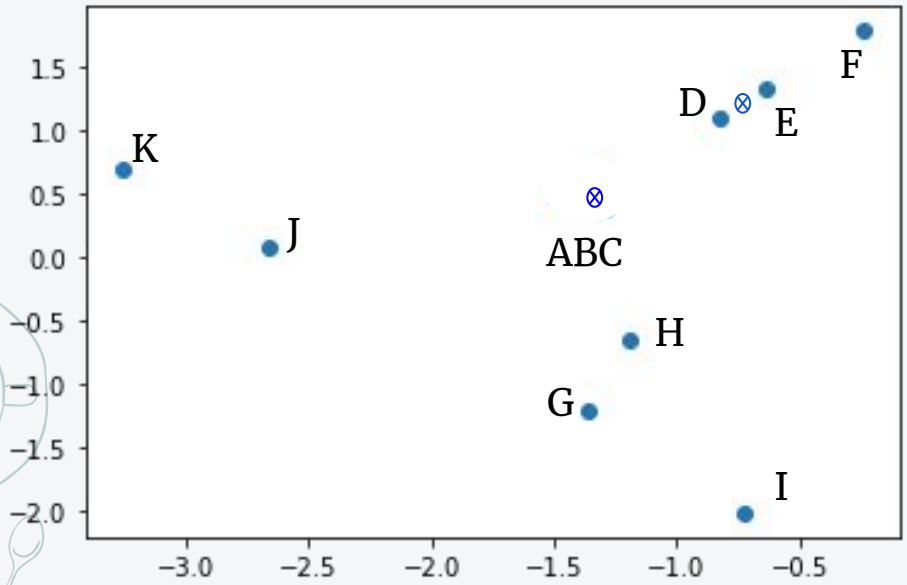
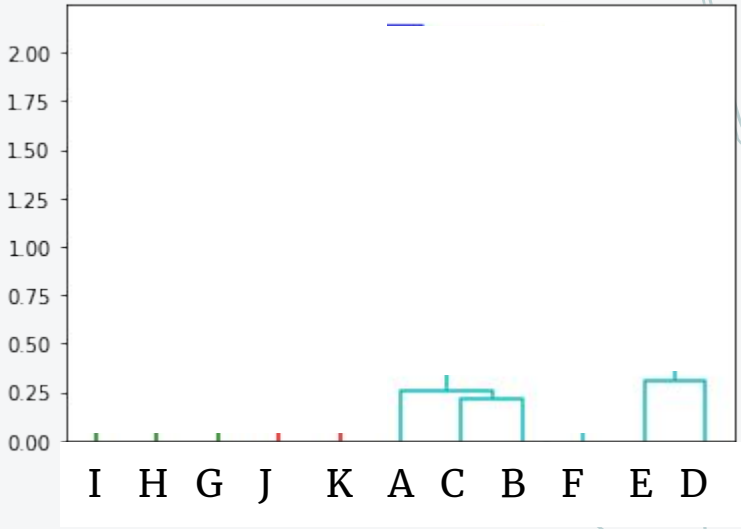


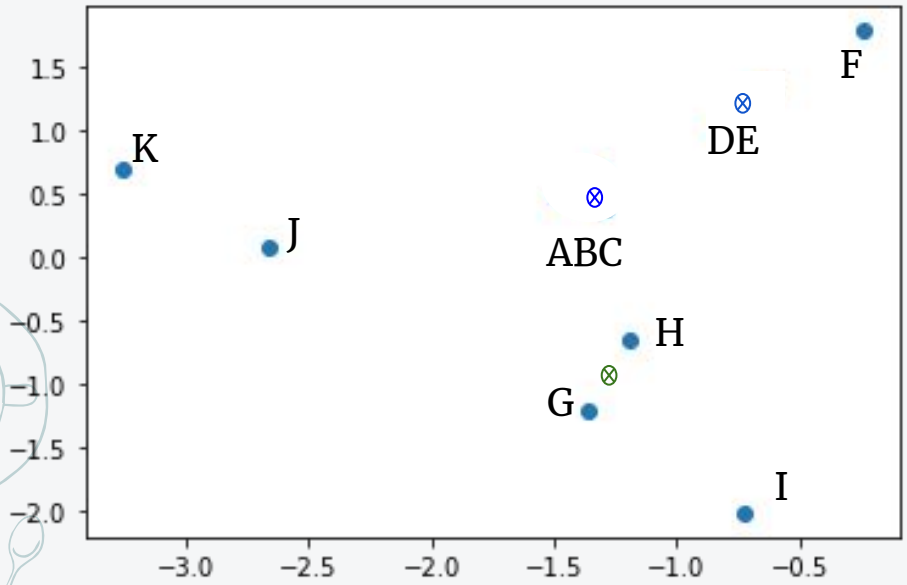
Agglomerative Hierarchical Clustering



Dendrogram



Agglomerative Hierarchical Clustering



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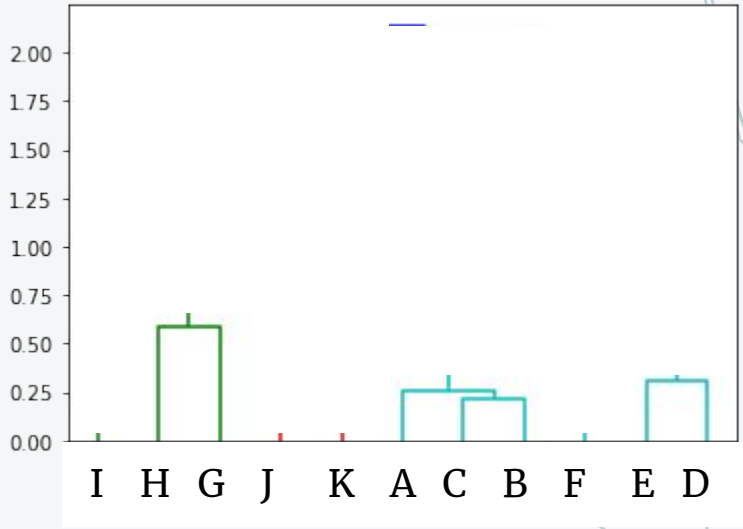
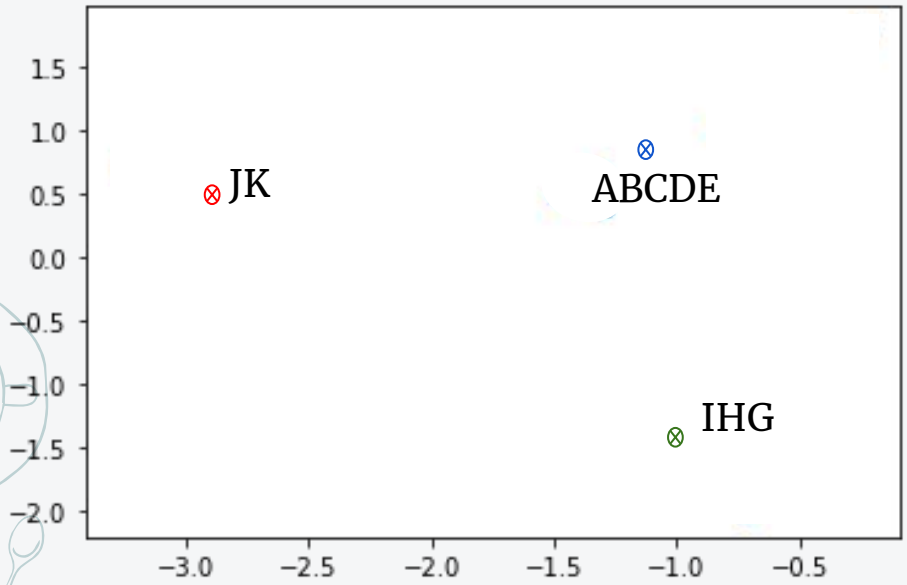


Agglomerative Hierarchical Clustering



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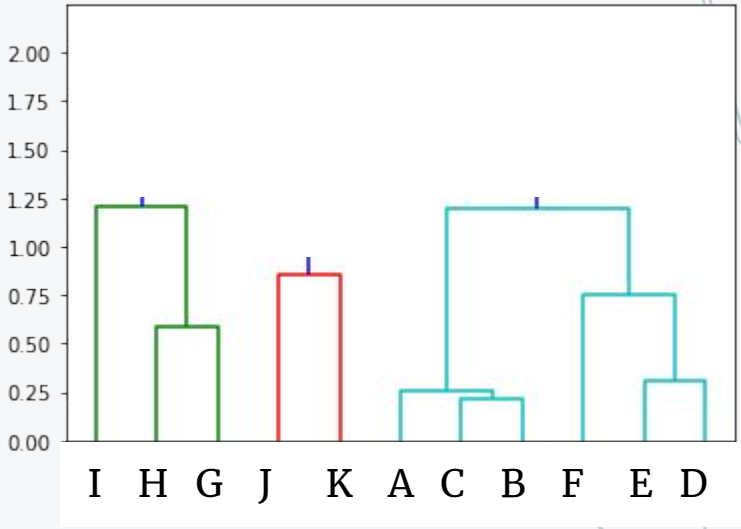

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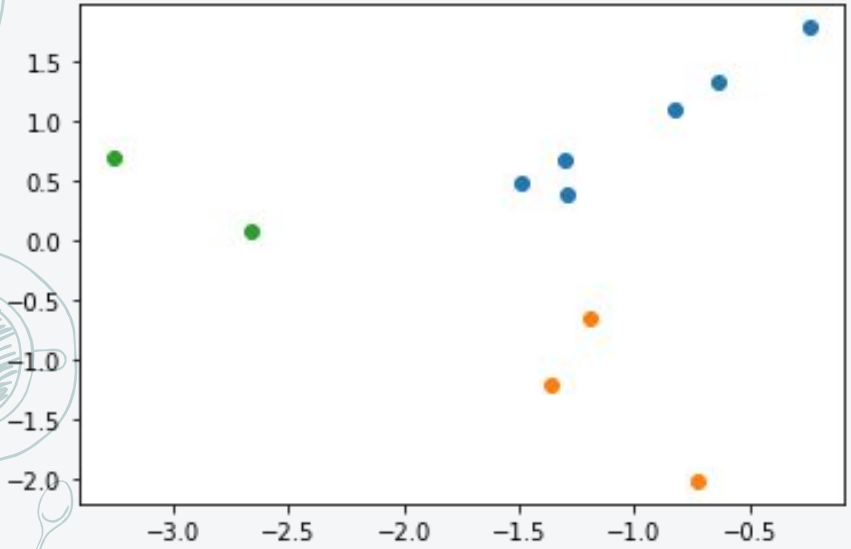

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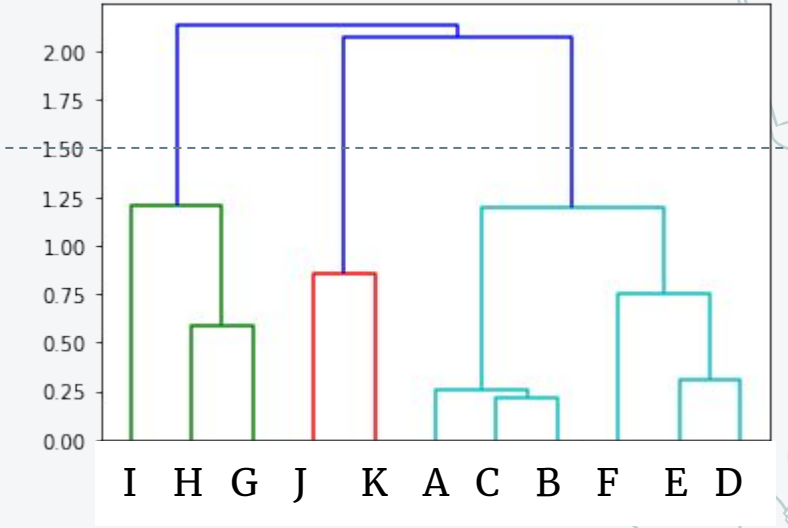
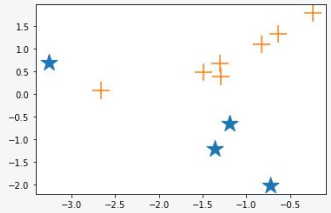
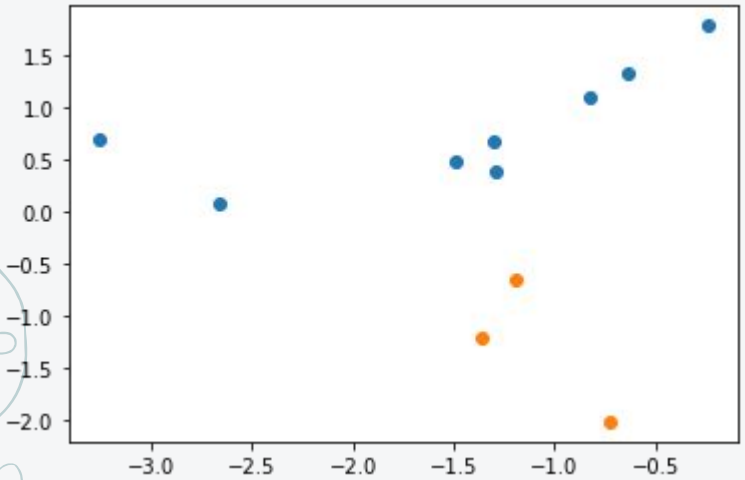


Agglomerative Hierarchical Clustering

K = 2





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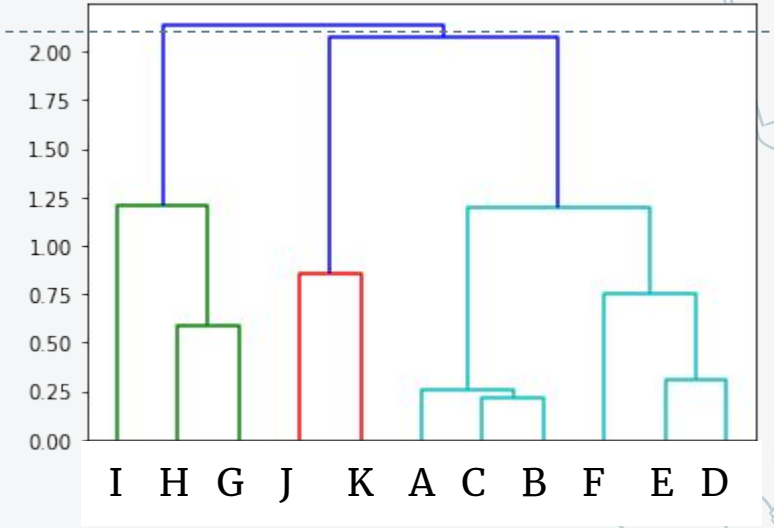

What parameters does it take?

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Distance - computing how close points are

Linkage - deciding what to merge

Settings: distance

$\vec{x}=\{x_1,x_2,\ldots x_P\}$
$\vec{y}=\{y_1,y_2,\ldots,y_P\}$

- Euclidean (usually default, same as L2 norm) - shortest distance between 2 points $\sqrt{\sum_{i=1}^{P}(x_i-y_i)^2}$

https://towardsdatascience.com/machine-learning-algorithms-part-12-hierarchical-agglomerative-clustering-example-in-python-1e18e0075019

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- Cosine $\frac{\sum_{i=1}^{P}x_iy_i}{\sqrt{\sum_{i=1}^{P}x_i^2}\sqrt{\sum_{i=1}^{P}y_i^2}}$

note: euclidean distance applied to unit normalized vectors will provide the same ordering

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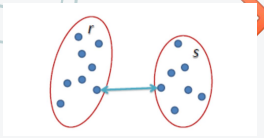
  note: euclidean distance applied to unit normalized vectors will provide the same ordering
- Mahalanobis distance: $d(\vec{x},\vec{y})=\sqrt{(\vec{x}-\vec{y})^T S^{-1}(\vec{x}-\vec{y})}$, where S is covariance

note: if S is an identity matrix, then Mahalanobis reduces to euclidean
If S is diagonal, then Mahalanobis is standardized euclidean

https://towardsdatascience.com/machine-learning-algorithms-part-12-hierarchical-agglomerative-clustering-example-in-python-1e18e0075019

Settings: Linkage

Linkage - takes distance information and groups pairs of objects into clusters based on their similarity



- single - min. of all pairwise distances between the elements in cluster 1 and the elements in cluster 2. Tends to produce long, “loose” clusters.

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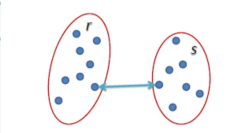

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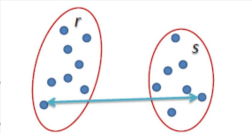

- complete - max. of all pairwise distances “. Tends to produce more compact clusters.

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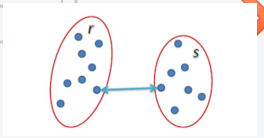

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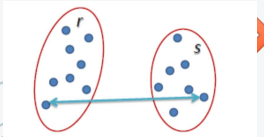

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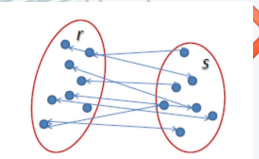

- average - avg. of all pairwise distances

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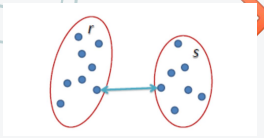

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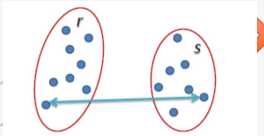

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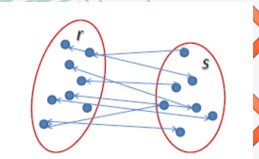
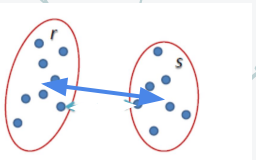


- average - avg. of all pairwise distances
- centroid - distance between cluster centroids



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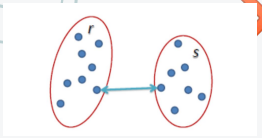

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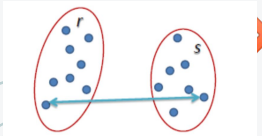

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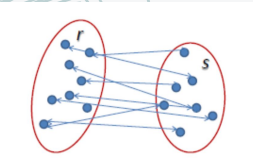
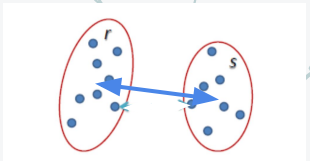
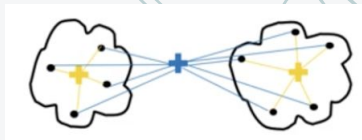


- average - avg. of all pairwise distances
- centroid - distance between cluster centroids
- Ward - minimizes within cluster variance

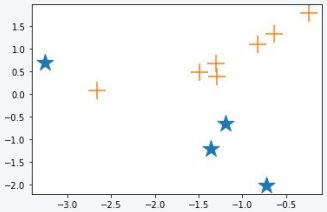




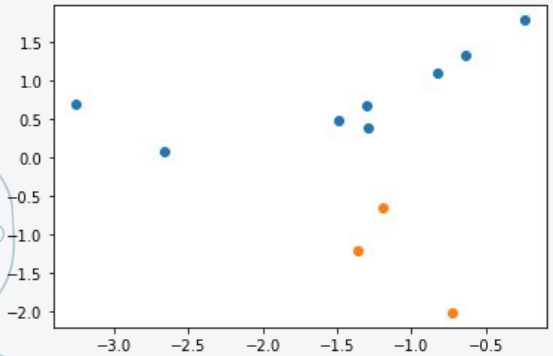
https://towardsdatascience.com/machine-learning-algorithms-part-12-hierarchical-agglomerative-clustering-example-in-python-1e18e0075019

Agglomerative Hierarchical Clustering

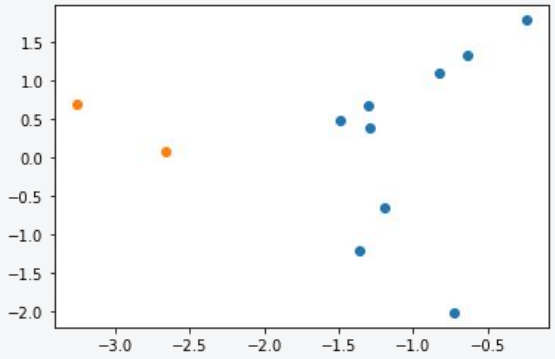
K = 2,
distance= Euclidean



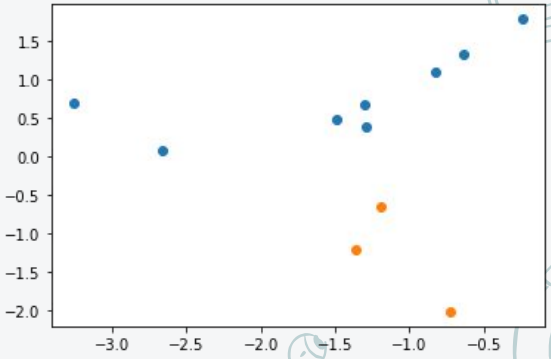
linkage = centroid

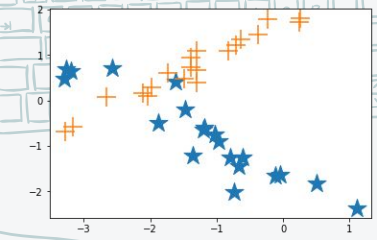


linkage = single



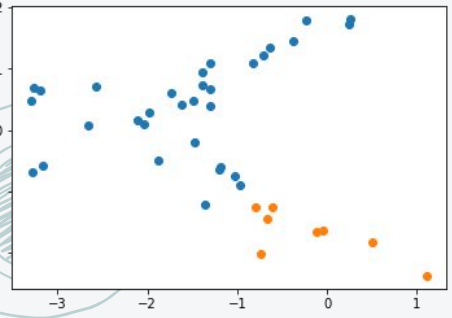
linkage = Ward



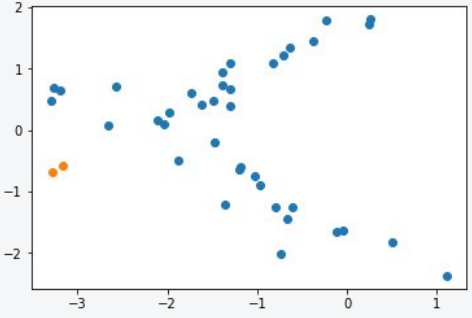


How are we doing on the original bigger dataset?

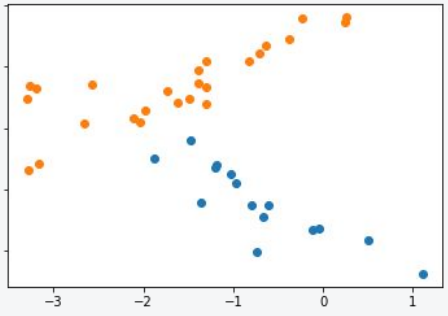
Ward, euclidean
Average, cosine



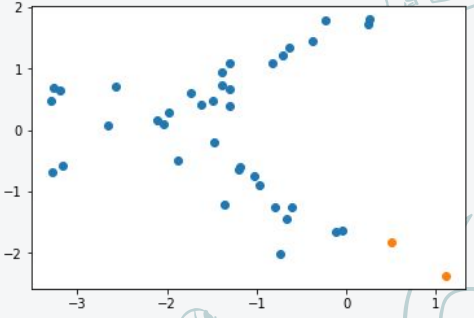
Single, euclidean
single , l1
single, l2
average, l1



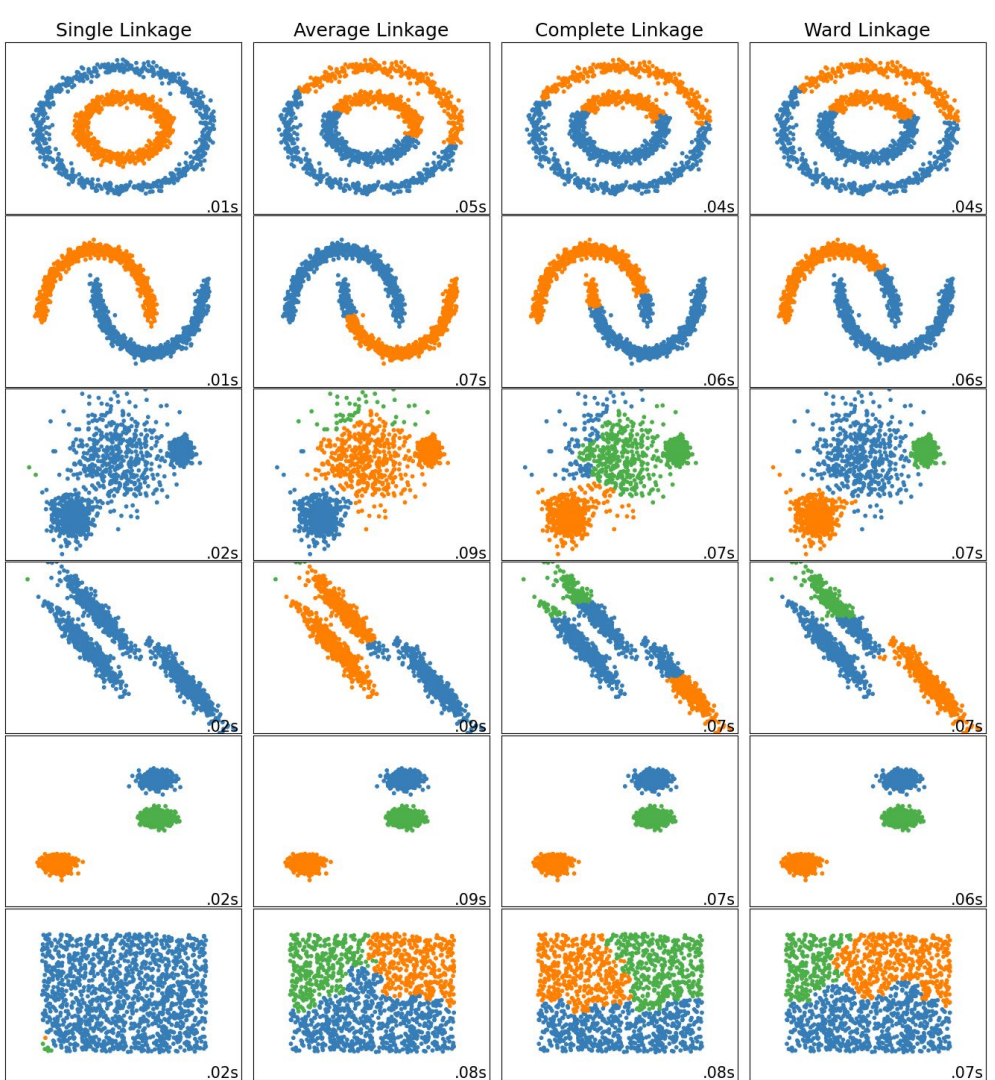
average, l2
average, euclidean



Single, cosine



Comparing Linkages across Datasets



Summary

- Each dataset needs its own distance and linkage
- Deciding on the number of clusters can be done after clustering is finished

K-means - Algorithm

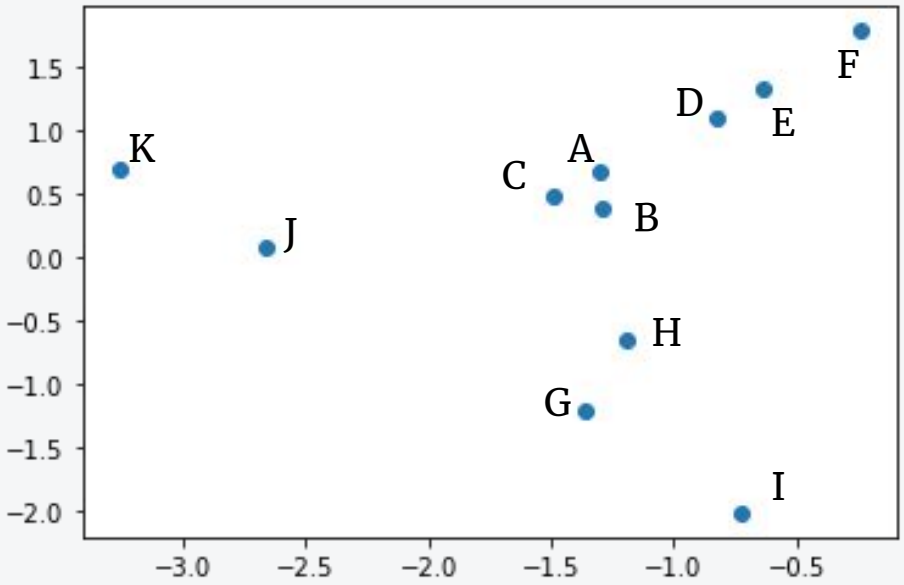
Decide on the number of clusters K

Pick K centroids at random

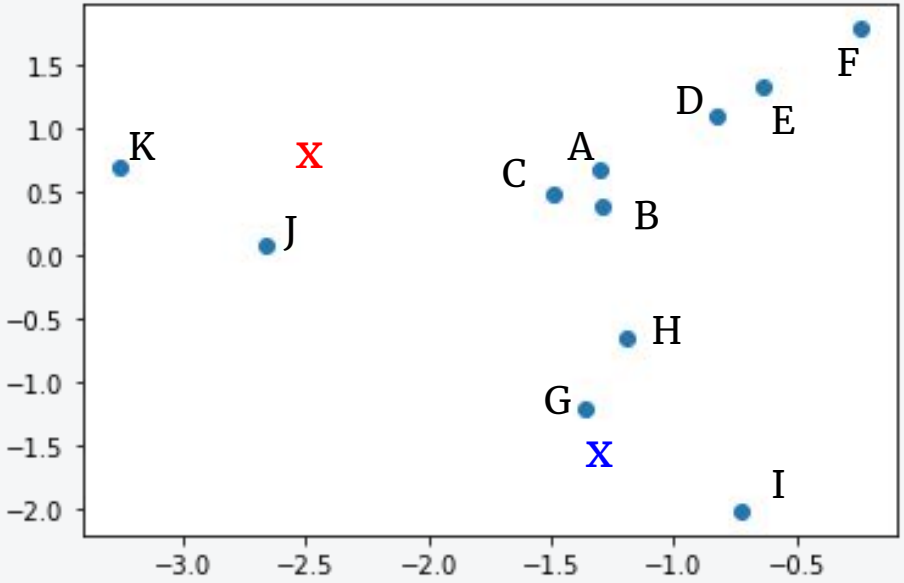
Repeat until convergence:

1) compute distance from each point to each centroid and assign points to the cluster with the closest centroid
2) Re-compute the centroid for the current cluster

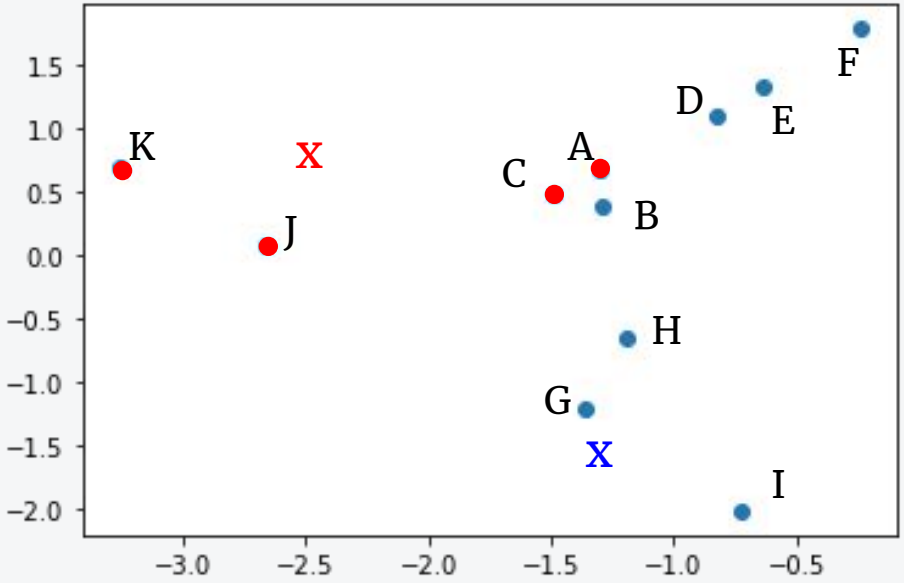
K-Means



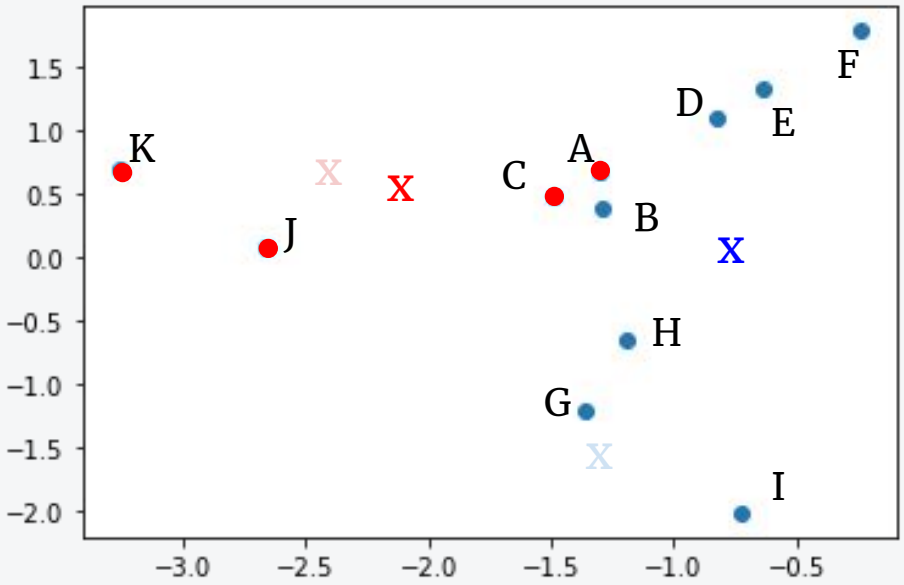
K-Means



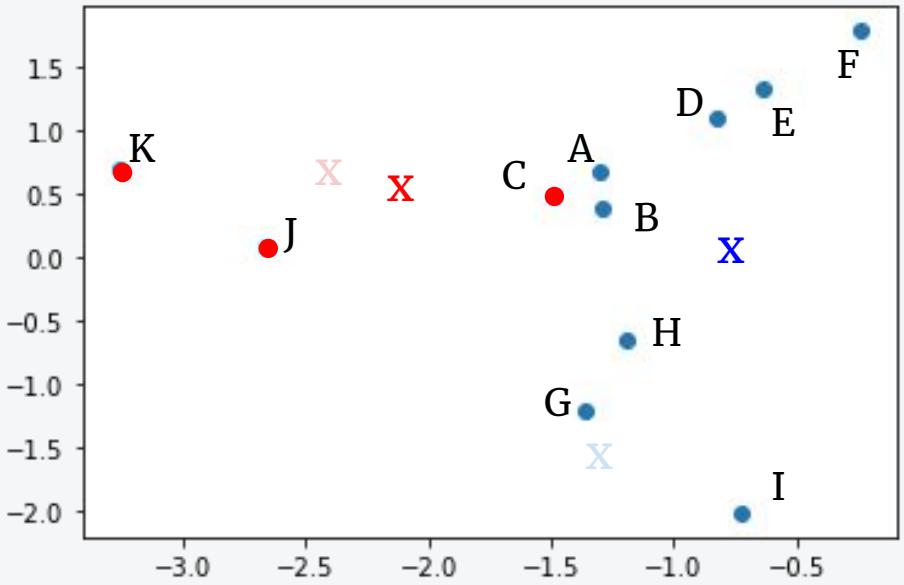
K-Means



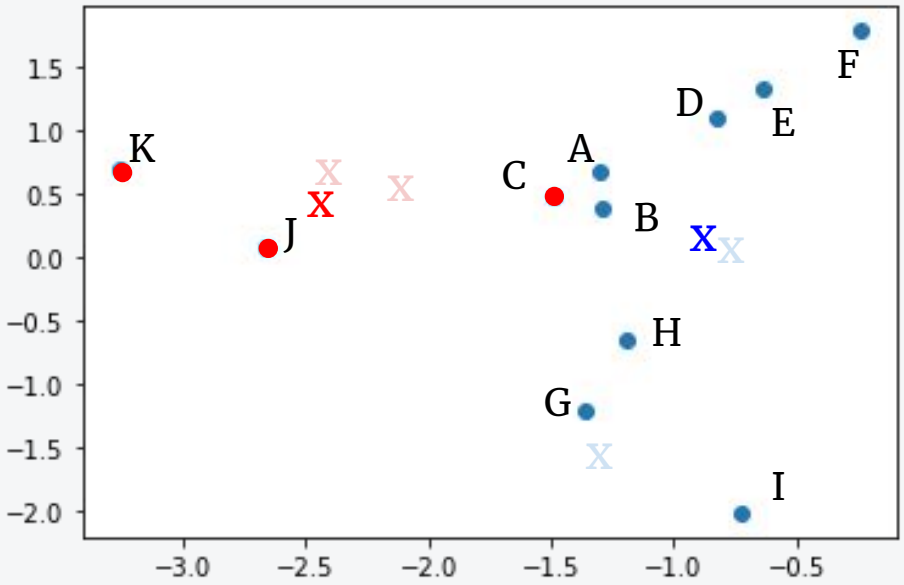
K-Means



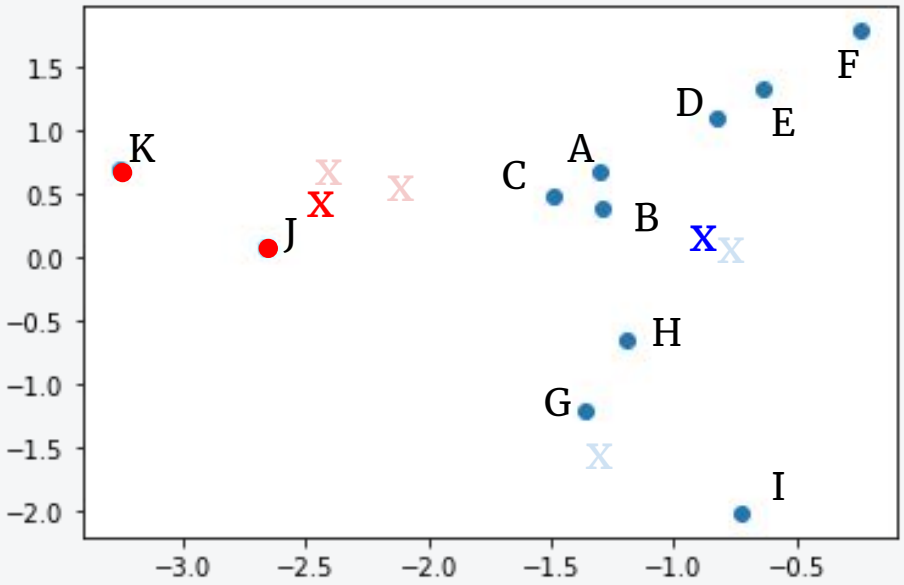
K-Means



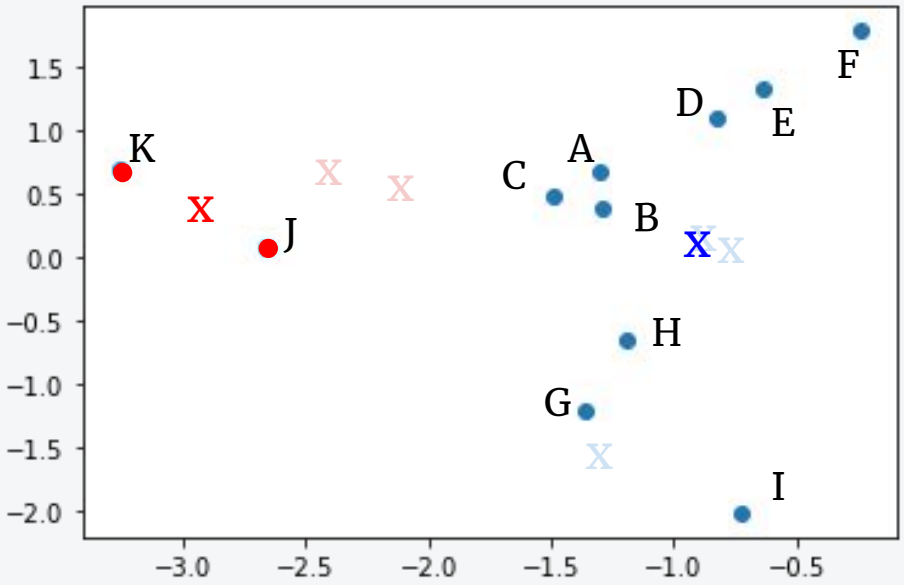
K-Means



K-Means

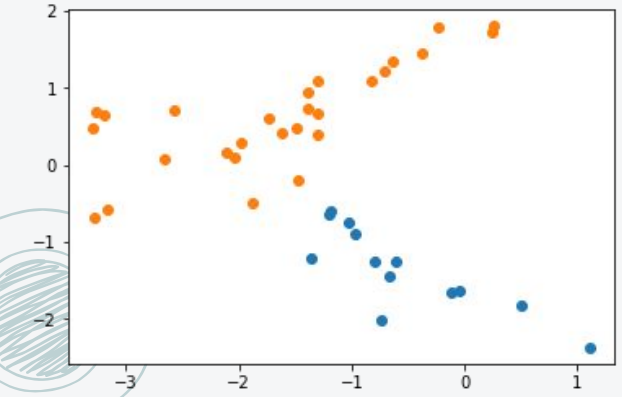


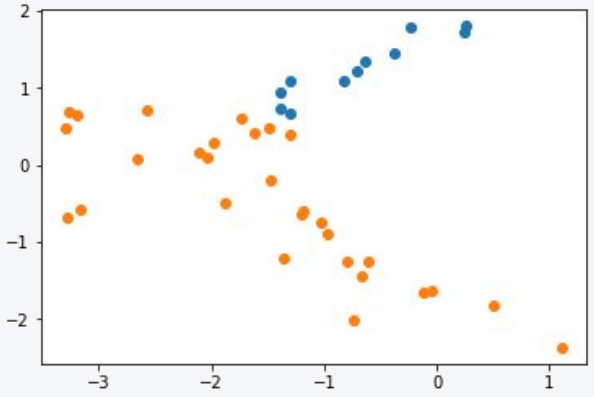
K-Means

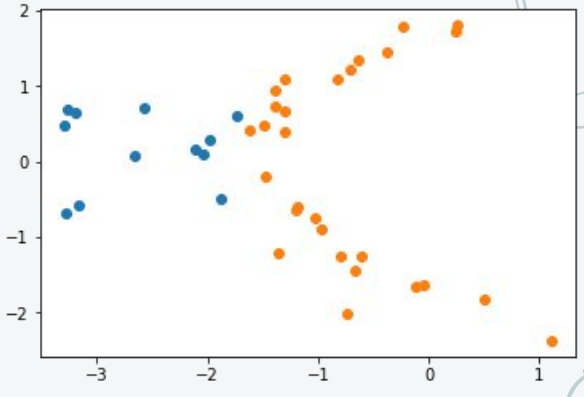


K-Means

Depends on initial conditions







How to make K-Means more robust?

How to make K-Means more robust?

- Run many times (scikit version default is 10)
- Have a better than random initialization
  - Pick data points as initializations
  - k-means++
  - Naive sharding

How to make K-Means more robust? k-means++

1. Choose one center uniformly at random among the data points.
2. For each data point x not chosen yet, compute D(x), the distance between x and the nearest center that has already been chosen.
3. Choose one new data point at random as a new center, using a weighted probability distribution where a point x is chosen with probability proportional to D(x).
4. Repeat Steps 2 and 3 until k centers have been chosen.
5. Now that the initial centers have been chosen, proceed using standard k-means clustering.

K-MEANS

Advantages:

Fast

Makes relatively few assumptions

Stable when robust initialization is used

Disadvantages:

Depends on the initialization

Can get stuck in local minimum

A bit about selecting the number of clusters

General approach

- Apply clustering for k = 1..K (e.g. K = 10)
- For each k, compute a statistic
- Plot statistic as a function of k

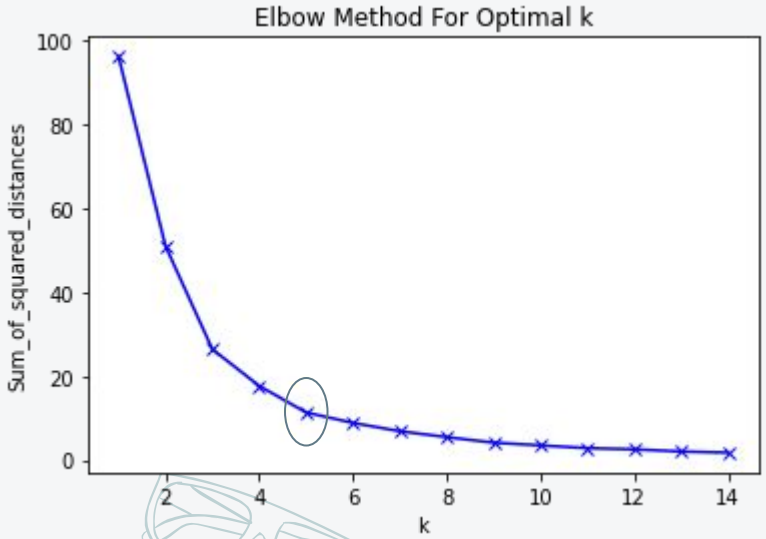
VARIOUS STATISTICS FOR SELECTING THE NUMBER OF CLUSTERS

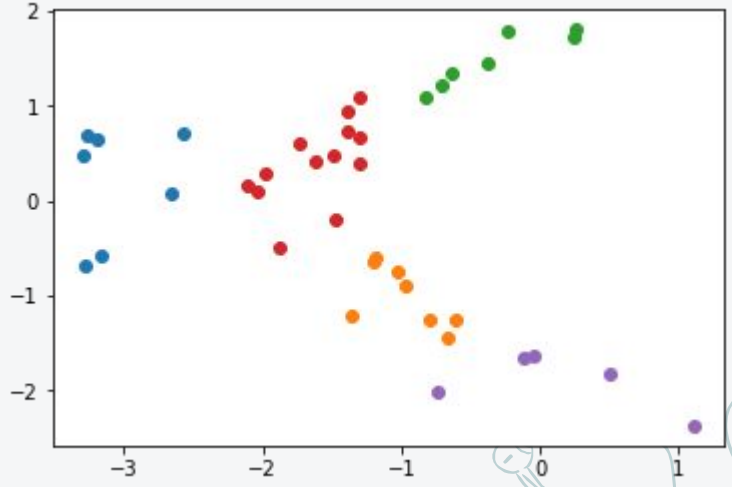
- Silhouette
- Gap
- Elbow
- Information Criterion (depend on the likelihood)
  - AIC
  - BIC
- ...

Elbow

Elbow method- heuristic

Elbow in the plot of the sum of squared distances to the nearest centre





Silhouette Score

For each data point i in cluster C_i, let

$$a(i) = \frac{1}{|C_i| - 1} \sum_{j \in C_i, i \neq j} d(i, j)$$ - average distance for point i to other points within its cluster

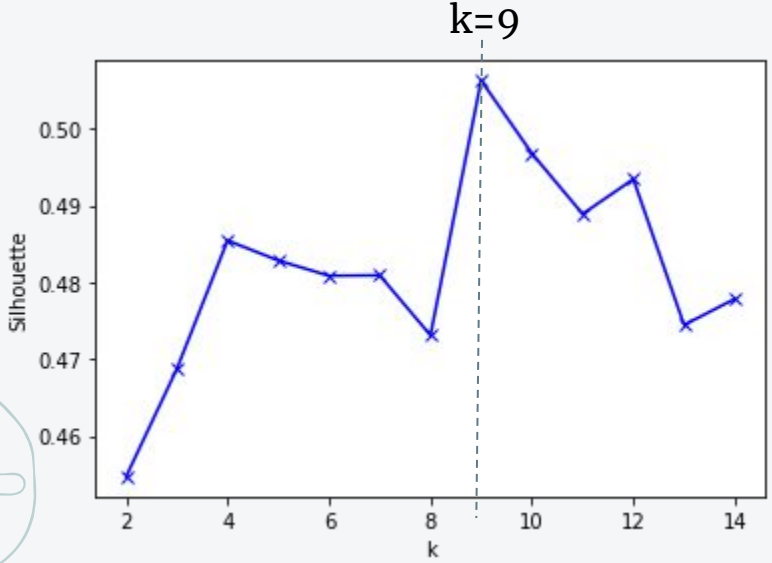
$$b(i) = \min_{k \neq i} \frac{1}{|C_k|} \sum_{j \in C_k} d(i, j)$$ - min (across clusters) of the averages of intra-cluster distances

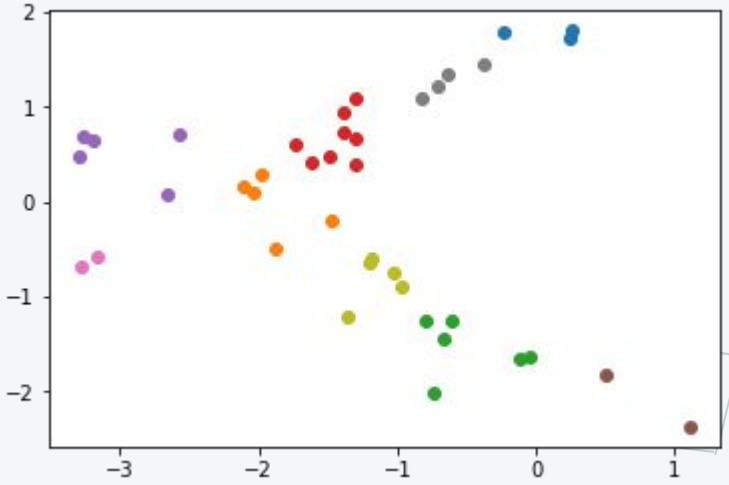
Silhouette: $$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}$$, Silhouette Coefficient: $$SC = \max_k \tilde{s}(k)$$

average over all points

Kauffman and Rousseeuw (1990)

Silhouette Score





Kauffman and Rousseeuw (1990)

GAP STATISTIC

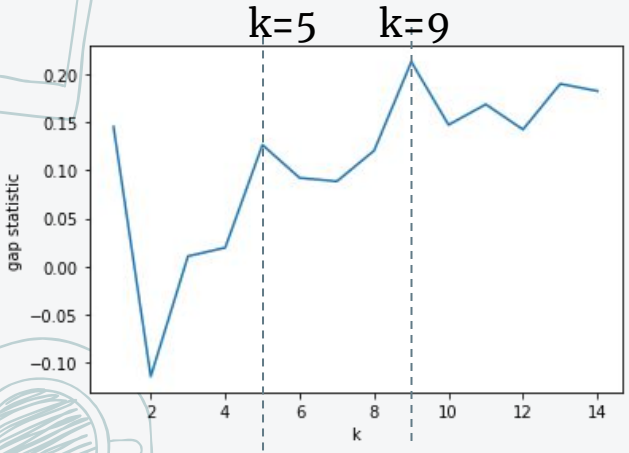
$D_r = \Sigma_{i,j \in Cr} d_{ij}$ - sum of pairwise distances in cluster i

$W_k = \Sigma_{r=1..k} 1/(2n_r) D_r$ - pooled within cluster sum of distances

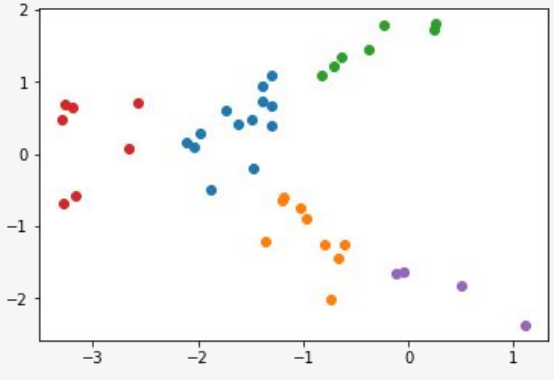
Main idea: compare $\log(W_k)$ to expectation under the null distribution $\text{Gap}_n(k) = E_n^*\{\log(W_k)\} - \log(W_k)$

Tibshirani et al (2000)

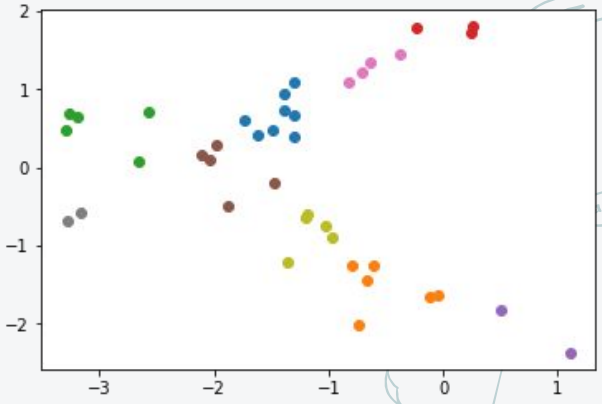
GAP STATISTIC



k=5

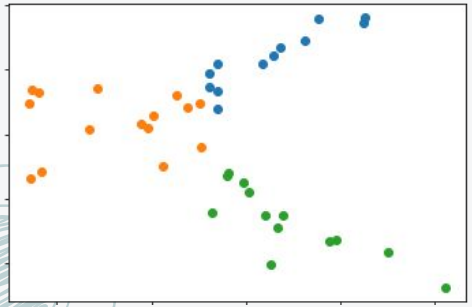


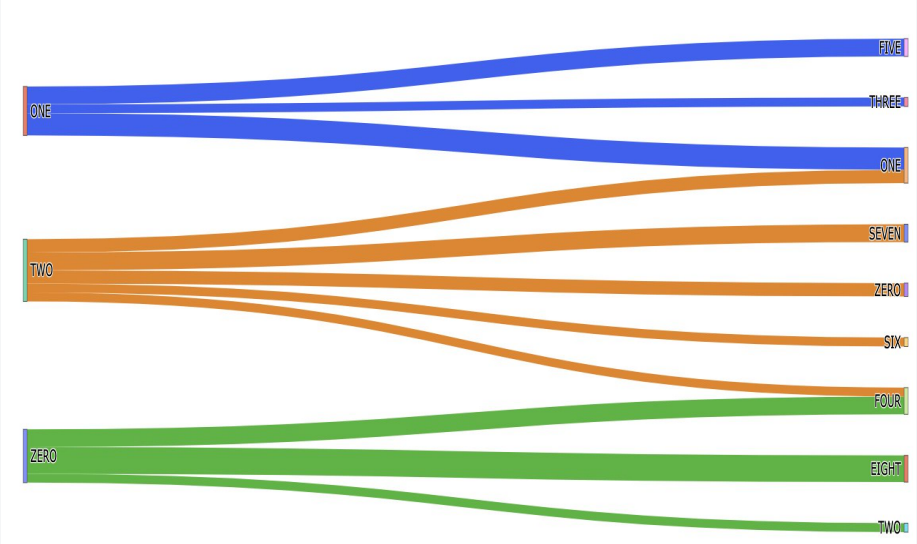
k=9



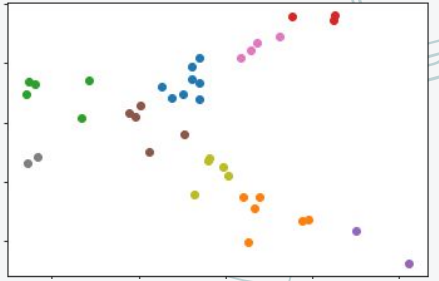
Alluvial (SANKY) plot

k=3





k=9



SUMMARY

- There are MANY clustering methods
- There is no one perfect method that works for every dataset
- There are many ways to select the number of clusters
- Examine multiple methods for each dataset
- Visualizations help to analyze clustering

Reading

5 common clustering methods:

https://towardsdatascience.com/the-5-clustering-algorithms-data-scientists-need-to-know-a36d136ef68

10 clustering methods in python:

https://machinelearningmastery.com/clustering-algorithms-with-python/

Original k-means++ presentation:
http://theory.stanford.edu/~sergei/slides/BATS-Means.pdf

Original gap statistic paper:

https://statweb.stanford.edu/~gwalther/gap

Sanky plots:
https://towardsdatascience.com/sankey-diagram-basics-with-pythons-plotly-7a13d557401a