Clustering

1 Fundamentals

- 1. Clustering: getting started
 - (a) Download the clustering datasets from the class webpage. Load the first one.
 - (b) Using sklearn library, apply KMeans algorithm on the dataframe, with 2 clusters, on the numerical columns. You can check the documentations to see how to do it, it should be something like clusters = KMeans(n_clusters=2).fit_predict(df[["weight","diameter"]]).
 - (c) Add the clusters as a column "cluster" to the dataframe
 - (d) To observe the clusters, we can plot (with seaborn library for instance, sns.scatterplot) with dot colors corresponding to clusters (hue="cluster"). Compare with using the fruit information as colors. It should correspond to your intuition.

2. Limits of k-means

- (a) Do the same with the second example. The result should not be as expected. Do you understand why?
- (b) Normalize the data, and retry.
- (c) Do the same with the next example. The result should not be as expected. Do you understand why?
- (d) Try to solve the issue using Gaussian Mixture (class BayesianGaussianMixture). Check the covariance_type parameter.
- (e) Also try the DBscan approach
- (f) Do the same (comparing ground truth, k-means, GM, DBScan) on the other examples. Every time, try to understand why each of the method succeed or fail. Try to play with the parameters to make the methods succeed.

3. Interpreting clusters

- (a) We want to describe the clusters obtained. Switch back to the synthetic car dataset we used in the first class. Use k-means with 3 clusters.
- (b) Compute the centroid (mean values for each feature), and the size for each cluster. A flexible way to proceed is to extract the clusters (fit_predict), add the resulting list as a new column (e.g., "cluster") in a copy of the feature dataframe, then compute statistics by cluster in that dataframe, for instance with _.groupby("cluster").agg(['mean', "count"])
- (c) If you had to give a manual label to those clusters, to describe the cars they contain, what would it be? (e.g.: "large and old expensive cars"...)

4. Evaluation and number of clusters

- (a) Compute the silhouette score using method silhouette_visualizer from package yellowbrick, plot the silhouette score and interpret it.
- (b) We would like to find the optimal number of clusters. Apply the silhouette score method: plot the relation between k and the silhouette score, and search for a maximum value, or a value where there is a "summit" (good luck).

2 Going Further

(a) Using this knowledge, explore the proposed Wine dataset: https://www.kaggle.com/datasets/harrywang/wine-dataset-for-clustering