Part II: Practical applications 2.1 K-means clustering In Python you can use the function KMeans() from the module sklearn.cluster to perform K-means clustering. To begin you will perform Kmeans with simulated data. Follow the steps: (a) The simulated data will consist in 50 observations described by two normal-distributed variables. In order to define classes in the data the first 25 observations have a mean shift relative to the next 25 observations. In [21]: import numpy as np X = np.random.randn(50,2)X[0:25, 0] = X[0:25, 0] + 3X[0:25, 1] = X[0:25, 1] - 4You can plot the observations and notice that there are two well separated clusters: In [22]: import matplotlib.pyplot as plt plt.plot(X[:, 0], X[:,1], "o") plt.xlabel("X1") plt.ylabel("X2") Text(0, 0.5, 'X2') Out[22]: 2 1 0 -1-2 -3-4-5 -6 -1(b) Performs K-means clustering with K=2. Use the following command: In [23]: from sklearn.cluster import KMeans kmeans = KMeans(n clusters = 2, random state = 100).fit(X) Then, the cluster assignments can be obtained by running print(kmeans.labels_). The final clusters centroids can be known using the command print(kmeans.clustercenters). In addition, you can plot the observations using a different color per cluster by running the following code: In [24]: for i in range(0, X.shape[0]): if kmeans.labels [i]==0: plt.plot(X[i:, 0], X[i:, 1], "o", color = "red") plt.plot(X[i:,0], X[i:,1], "o", color = "blue") centroid1=kmeans.cluster centers [0] centroid2=kmeans.cluster centers [1] plt.plot(centroid1[0], centroid1[1], "*", color = "black", markersize = 15) plt.plot(centroid2[0], centroid2[1], "*", color = "black", markersize = 15) plt.xlabel("X1") plt.ylabel("X2") Text(0, 0.5, 'X2') Out[24]: 2 1 0 -1 \aleph -4 -5 -6 X1 (c)Now, you are going to perform K-means with real data. The fileHCVdata.csv contains laboratory values of blood donors and Hepatitis C patients and demographic values like age. There are 12 variables, features 4-12 concern laboratory data (ALB, ALT, AST, BIL,CHE, CHOL, CREA, GGT and PROT). Import the data set and get familiar with the data. Answer the following questions : 1. How many observations are there? There are 567 observations. 2. How many variables are there? There are 13 variables. 3. What type of variables (numeric, categorical)? For each categorical variable (if any)give the number of levels and categories. You will denote the resulting dataframe objectdfHVC. Let's read the data from the csv file and see the variables' data types. In [25]: import pandas as pd dfHVC = pd.read csv('HCVdata.csv', sep=';') dfHVC.columns.tolist() ['Unnamed: 0', Out[25]: 'Category', 'Sex', 'Age', 'ALB', 'ALT', 'AST', 'BIL', 'CHE', 'CHOL', 'CREA', 'GGT', 'PROT'] In [26]: dfHVC.head(20) CHE CHOL CREA GGT PROT Out[26]: Unnamed: 0 Category Sex Age ALB ALT AST BIL 0 1 0=Blood Donor 38.5 7.7 22.1 7.5 6.93 3.23 106.0 12.1 69.0 0=Blood Donor 38.5 18.0 24.7 3.9 11.17 4.80 74.0 15.6 76.5 2 3 0=Blood Donor 46.9 36.2 52.6 6.1 8.84 5.20 86.0 33.2 79.3 4 0=Blood Donor 3 32 43.2 30.6 22.6 18.9 7.33 4.74 80.0 33.8 75.7 32 39.2 4 5 0=Blood Donor 32.6 24.8 9.6 9.15 4.32 76.0 29.9 68.7 m 0=Blood Donor 46.3 17.5 17.8 7.01 4.79 70.0 16.9 74.5 6 8 0=Blood Donor 42.2 35.8 31.1 16.1 5.82 4.60 109.0 21.5 67.1 0=Blood Donor 7 32 50.9 23.2 21.2 8.69 83.0 13.7 71.3 4.10 8 0=Blood Donor m 32 42.4 20.3 20.0 35.2 5.46 4.45 81.0 15.9 69.9 0=Blood Donor 32 44.3 21.7 22.4 4.15 78.0 24.1 75.4 3.57 10 12 0=Blood Donor 46.4 10.3 20.0 5.7 7.36 4.30 79.0 18.7 68.6 m 33 36.3 23.6 22.0 7.0 78.0 19.4 13 0=Blood Donor 8.56 5.38 68.7 24.0 12 14 0=Blood Donor 39.0 15.9 3.38 65.0 7.0 70.4 6.46 13 0=Blood Donor 33 38.7 22.5 23.0 4.63 4.97 63.0 15.2 71.9 14 0=Blood Donor 41.8 33.1 38.0 8.83 4.43 71.0 24.0 72.7 6.6 40.9 17.2 22.9 10.0 6.98 90.0 14.7 72.4 0=Blood Donor 16 0=Blood Donor 45.2 32.4 31.2 10.1 9.78 5.51 102.0 48.5 76.5 m 17 0=Blood Donor 36.6 38.9 40.3 24.9 9.62 5.50 112.0 27.6 69.3 m 18 0=Blood Donor m 42.0 32.6 34.9 7.01 4.05 105.0 19.1 68.1 32.1 21.6 103.0 30.2 74.0 0=Blood Donor 13.1 In [27]: dfHVC.tail(20) CHE CHOL CREA **GGT PROT** Unnamed: 0 Out[27]: Category Sex Age ALB **ALT AST** BIL 547 3=Cirrhosis 33.0 66.6 91.0 4.02 4.08 75.9 28.5 62.3 m 4.5 548 3=Cirrhosis 27.0 17.0 319.8 37.0 1.42 3.54 66.9 93.7 65.3 m 56 549 597 3=Cirrhosis 56 23.0 123.0 43.0 1.80 2.40 62.7 35.9 62.8 m 550 598 3=Cirrhosis m 56 30.0 0.9 80.3 119.0 1.88 1.43 79.3 17.6 54.2 551 3=Cirrhosis 31.0 181.8 58.0 3.29 3.92 66.4 273.7 78.1 58 m 552 36.0 110.1 37.0 2.29 3.68 118.2 56.9 74.8 3=Cirrhosis m 553 3=Cirrhosis 59 27.0 65.2 209.0 2.47 3.61 71.7 28.5 60.6 m 3=Cirrhosis 602 31.0 95.4 117.0 1.57 3.51 60.5 53.6 68.5 554 59 m 555 603 3=Cirrhosis 61 39.0 27.3 143.2 15.0 5.38 4.88 72.3 400.3 73.4 m 556 74 23.0 2.1 90.4 22.0 2.50 3.29 51.0 46.8 3=Cirrhosis 57.1 m 557 606 3=Cirrhosis 42 33.0 3.7 55.7 200.0 1.72 5.16 89.1 146.3 69.9 f 607 49 33.0 1.2 36.3 7.0 6.92 3.82 485.9 112.0 58.5 558 3=Cirrhosis 559 608 3=Cirrhosis 39.0 1.3 30.4 21.0 6.33 3.78 158.2 142.5 82.7 f 560 3=Cirrhosis 58 34.0 15.0 150.0 8.0 6.26 3.98 56.0 49.7 80.6 19.6 561 610 3=Cirrhosis 59 39.0 285.8 40.0 5.77 4.51 136.1 101.1 70.5 32.0 5.9 110.3 50.0 5.57 6.30 55.7 650.9 68.5 562 3=Cirrhosis 563 3=Cirrhosis 24.0 2.9 44.4 20.0 1.54 3.02 63.0 35.9 71.3 64 564 29.0 99.0 48.0 82.0 3=Cirrhosis 3.5 1.66 3.63 66.7 64.2 565 3=Cirrhosis 46 33.0 39.0 62.0 20.0 3.56 4.20 52.0 50.0 71.0 615 3=Cirrhosis 36.0 100.0 0.08 12.0 9.07 5.30 67.0 34.0 68.0 In [28]: dfHVC.dtypes Unnamed: 0 int64 Out[28]: Category object object Age int64 ALB float64 ALT float64 AST float64 BIL float64 CHE float64 CHOL float64 CREA float64 GGT float64 PROT float64 dtype: object In [29]: dfHVC['Sex'] = dfHVC['Sex'].astype('category'); dfHVC['Category'] = dfHVC['Category'].astype('category'); dfHVC.dtypes Unnamed: 0 int64 Out[29]: Category category Sex category Age int64 ALB float64 ALT float64 AST float64 BIL float64 CHE float64 CHOL float64 CREA float64 float64 GGT PROT float64 dtype: object The Category variable can be simplifies, so that there can be only numbers. For '0=Blood Donors' the value would be '0', for '1=Hepatitis' the value would be '1', and for '2=Fibrosis' would be '2', then for the '3=Cirrhosis' the value would be '3'. In [30]: dfHVC["Category"].replace({"0=Blood Donor": "0", "1=Hepatitis": "1", "2=Fibrosis": "2", "3=Cirrhosis":"3"}, inplace=True) dfHVC.tail(30) Out[30]: Unnamed: 0 Category Sex **ALT AST** CHE CHOL **CREA GGT PROT** Age ALB 537 583 2 51 37.0 164.0 70.0 9.0 3.99 4.20 67.0 43.0 72.0 7.75 538 584 2 39.0 42.0 34.0 10.0 5.00 80.0 84.0 78.0 56 539 586 3 38 44.0 94.0 60.0 12.0 4.37 3.20 61.0 99.0 77.0 m 540 587 3 39 34.0 4.8 35.6 9.0 3.65 4.82 519.0 133.4 57.5 m 541 588 3 41 31.0 4.8 60.2 200.0 1.80 5.34 106.4 151.0 71.8 m 542 589 3 42 36.0 14.9 263.1 40.0 3.61 3.93 49.6 68.6 61.0 m 590 543 3 45 29.0 7.1 101.9 31.0 1.73 3.71 76.7 65.6 70.0 m 544 592 3 46 35.0 2.3 19.2 11.0 7.10 4.10 1079.1 105.6 69.1 m 545 593 3 47 42.0 159.0 102.0 11.0 6.29 5.50 58.0 201.0 79.0 m 29.6 546 594 3 51 39.0 185.0 19.0 2.00 3.60 58.3 399.5 79.4 m 547 595 3 51 33.0 4.5 66.6 91.0 4.02 4.08 75.9 28.5 62.3 m 56 27.0 548 596 3 17.0 319.8 37.0 3.54 66.9 93.7 65.3 1.42 m 549 597 3 56 23.0 5.1 123.0 43.0 1.80 2.40 62.7 35.9 62.8 m 550 598 3 56 30.0 0.9 80.3 119.0 1.88 1.43 79.3 17.6 54.2 m 551 599 3 58 31.0 7.0 181.8 58.0 3.29 3.92 66.4 273.7 78.1 m 552 600 3 59 36.0 110.1 37.0 2.29 3.68 118.2 74.8 5.2 56.9 m 553 601 3 59 27.0 4.0 65.2 209.0 2.47 3.61 71.7 28.5 60.6 m 554 602 3 59 31.0 5.4 95.4 117.0 1.57 3.51 60.5 53.6 68.5 m 555 603 3 61 39.0 27.3 143.2 15.0 5.38 4.88 72.3 400.3 73.4 m 556 605 3 74 23.0 90.4 22.0 2.50 3.29 51.0 46.8 2.1 57.1 m 557 606 3 f 42 33.0 3.7 55.7 200.0 1.72 5.16 89.1 146.3 69.9 558 607 49 33.0 36.3 7.0 6.92 3.82 485.9 112.0 58.5 f 1.2 559 608 3 f 52 39.0 1.3 30.4 21.0 6.33 3.78 158.2 142.5 82.7 560 609 58 34.0 15.0 150.0 8.0 6.26 3.98 56.0 49.7 80.6 561 610 3 f 59 39.0 19.6 285.8 40.0 5.77 4.51 136.1 101.1 70.5 562 611 62 32.0 5.9 110.3 50.0 5.57 6.30 55.7 650.9 68.5 64 563 612 24.0 2.9 44.4 20.0 1.54 3.02 63.0 35.9 71.3 564 613 64 29.0 3.5 99.0 48.0 1.66 3.63 66.7 64.2 82.0 565 614 f 46 33.0 39.0 62.0 20.0 3.56 4.20 52.0 50.0 71.0 566 615 59 36.0 100.0 80.0 12.0 9.07 5.30 67.0 34.0 68.0 In [31]: dfHVC = dfHVC.drop(columns=['Unnamed: 0']) dfHVC.head(20) CHE CHOL CREA GGT PROT Out[31]: Category Sex Age ALB ALT AST BIL 0 32 38.5 7.7 22.1 7.5 6.93 3.23 106.0 12.1 69.0 m 1 0 32 38.5 18.0 24.7 3.9 11.17 4.80 74.0 15.6 76.5 m 2 0 32 46.9 36.2 52.6 6.1 8.84 5.20 86.0 33.2 79.3 m 3 32 43.2 30.6 22.6 18.9 7.33 4.74 0.08 33.8 75.7 m 4 0 32 39.2 32.6 24.8 9.6 9.15 4.32 76.0 29.9 68.7 m 5 0 32 46.3 17.5 17.8 8.5 7.01 4.79 70.0 16.9 74.5 m 6 0 32 42.2 35.8 31.1 16.1 5.82 4.60 109.0 21.5 67.1 m 7 0 32 50.9 23.2 21.2 6.9 8.69 4.10 83.0 13.7 71.3 m 32 42.4 20.3 20.0 35.2 8 0 5.46 4.45 81.0 15.9 69.9 m 0 32 44.3 21.7 22.4 17.2 4.15 3.57 78.0 24.1 75.4 m 10 0 33 46.4 10.3 20.0 5.7 7.36 4.30 79.0 18.7 68.6 m 33 36.3 11 23.6 22.0 7.0 8.56 5.38 78.0 19.4 68.7 m 12 0 33 39.0 15.9 24.0 6.8 6.46 3.38 65.0 7.0 70.4 m 13 0 33 38.7 22.5 23.0 4.1 4.63 4.97 63.0 15.2 71.9 m 14 0 33 41.8 33.1 38.0 6.6 8.83 4.43 71.0 24.0 72.7 m 15 33 40.9 17.2 22.9 10.0 6.98 5.22 90.0 14.7 72.4 m 16 0 33 45.2 32.4 31.2 10.1 9.78 5.51 102.0 48.5 76.5 m 33 36.6 17 0 38.9 40.3 24.9 9.62 5.50 112.0 27.6 69.3 m 18 0 33 42.0 32.6 34.9 11.2 7.01 4.05 105.0 19.1 68.1 m 19 33 44.3 32.1 21.6 13.1 7.44 5.59 103.0 30.2 74.0 Let for the 'Sex' variable 0 is female, and 1 is male. In [32]: dfHVC["Sex"].replace({"m": "1", "f": "0"}, inplace=True) dfHVC.tail(40) Out[32]: Category Sex Age ALB **ALT AST** BIL CHE CHOL **CREA GGT PROT** 54 41.0 91.0 104.9 527 2 41.5 187.9 21.0 8.59 5.85 79.1 1 57 47.0 10.2 55.9 70.9 69.6 80.9 528 12.0 6.60 4.64 529 2 59 44.0 9.45 65.0 95.3 69.7 1 8.9 74.5 6.0 4.45 53.0 64 38.0 70.0 530 7.1 41.3 13.0 7.10 4.52 66.8 2 9.92 531 71 37.0 130.0 90.0 15.0 79.0 77.0 76.0 1 4.70 2 532 0 36 46.0 67.1 161.9 13.0 9.24 4.81 65.3 60.0 73.9 2 533 0 38 40.0 68.9 8.55 60.5 40.1 76.5 14.9 11.0 4.31 2 0 57 43.0 8.3 35.8 18.0 8.61 6.19 71.4 27.9 82.0 534 68 43.0 535 2 0 5.0 42.1 12.0 7.29 4.89 80.9 11.9 76.1 0 49 39.0 46.0 39.0 9.0 10.21 3.10 89.0 53.0 79.0 536 51 37.0 537 2 0 164.0 70.0 9.0 3.99 4.20 67.0 43.0 72.0 2 0 56 39.0 42.0 10.0 7.75 5.00 80.0 84.0 78.0 538 34.0 4.37 539 3 38 44.0 94.0 60.0 12.0 3.20 61.0 99.0 77.0 1 3 540 39 34.0 35.6 3.65 4.82 519.0 133.4 57.5 4.8 9.0 3 541 41 31.0 200.0 1.80 151.0 1 4.8 60.2 5.34 106.4 71.8 542 42 36.0 14.9 263.1 40.0 3.61 3.93 49.6 61.0 68.6 3 543 45 29.0 31.0 76.7 65.6 70.0 1 7.1 101.9 1.73 3.71 3 46 35.0 7.10 1079.1 105.6 69.1 544 2.3 19.2 11.0 4.10 3 545 1 47 42.0 159.0 102.0 11.0 6.29 5.50 58.0 201.0 79.0 51 39.0 29.6 185.0 19.0 2.00 58.3 399.5 546 3.60 79.4 547 3 51 33.0 66.6 91.0 4.02 4.08 75.9 28.5 1 4.5 62.3 3 319.8 37.0 3.54 66.9 93.7 548 56 27.0 17.0 1.42 65.3 3 549 1.80 35.9 1 56 23.0 5.1 123.0 43.0 2.40 62.7 62.8 550 56 30.0 0.9 80.3 119.0 1.88 1.43 79.3 17.6 54.2 3 551 7.0 181.8 3.29 3.92 273.7 78.1 1 58 31.0 58.0 66.4 3 59 36.0 5.2 110.1 2.29 3.68 118.2 56.9 552 37.0 74.8 3 60.6 553 209.0 28.5 1 59 27.0 4.0 65.2 2.47 3.61 71.7 554 59 31.0 60.5 53.6 5.4 95.4 117.0 1.57 3.51 68.5 3 555 1 61 39.0 27.3 143.2 15.0 5.38 4.88 72.3 400.3 73.4 3 556 23.0 90.4 22.0 2.50 3.29 51.0 46.8 74 2.1 57.1 557 3 42 33.0 200.0 146.3 69.9 0 3.7 55.7 1.72 5.16 89.1 558 3 6.92 0 49 33.0 1.2 36.3 7.0 3.82 485.9 112.0 58.5 3 559 0 52 39.0 6.33 158.2 142.5 82.7 1.3 30.4 21.0 3.78 3 560 0 58 34.0 15.0 150.0 8.0 6.26 3.98 56.0 49.7 80.6 3 561 59 39.0 285.8 40.0 101.1 70.5 0 19.6 5.77 4.51 136.1 562 3 50.0 5.57 650.9 0 62 32.0 5.9 110.3 6.30 55.7 68.5 3 563 0 24.0 2.9 3.02 35.9 64 44.4 20.0 1.54 63.0 71.3 3 564 0 29.0 99.0 48.0 64.2 82.0 64 3.5 1.66 3.63 66.7 3 565 0 46 33.0 39.0 62.0 20.0 3.56 4.20 52.0 50.0 71.0 100.0 566 0 59 36.0 80.0 12.0 9.07 5.30 67.0 34.0 68.0 (d) Since all the clustering approaches used in this lab are based upon distancesor dissimilarity measures, it is strongly recommended to scale the variables previously. The following code allows to scale all the variables in a dataframe called dfHVC: In [33]: from sklearn.preprocessing import StandardScaler scaler = StandardScaler() dfHVC_scaled = scaler.fit_transform(dfHVC) Create a dataframe containing all the numeric variables after being scaled, you will name theresulting output dfHVC_scaled. In [34]: dfHVC_scaled = pd.DataFrame(dfHVC_scaled) type(dfHVC_scaled) pandas.core.frame.DataFrame In [57]: dfHVC_Kmeans4=KMeans(n_clusters = 2, n_init = 50, random_state = 1000).fit(dfHVC_scaled) dfHVC_Kmeans4.cluster_centers_ array([[-0.24487944, -0.01427549, -0.03516566, 0.08789789, -0.04734399, -0.20142963, -0.13943136, 0.11561622, 0.08670992, -0.06274669, -0.15746062, 0.00580842], [3.06099296, 0.17844356, 0.43957073, -1.09872364, 0.59179983, 2.51787043, 1.74289203, -1.44520281, -1.08387394, 0.78433365, 1.96825773, -0.07260523]]) In [60]: pd.crosstab(index=dfHVC.Sex, columns=dfHVC_Kmeans4.labels_, rownames=['Real groups'], colnames=['K-means cluster] Out[60]: K-means clusters Real groups **0** 212 13 **1** 313 29 2.2 In [67]: from scipy.cluster.hierarchy import linkage hc_complete = linkage(X, "complete") Let's plot the associated dendogram using the previous results: In [68]: from scipy.cluster.hierarchy import dendrogram import matplotlib.pyplot as plt plt.figure(figsize=(25, 10)) dendrogram(hc_complete) plt.show() We remark the 2 clusters are clearly identified, which is normal because we performed hierarchical clustering with simulated data. To determine the cluster labels for each observation associated with a given cut of the dendrogram, you can use the cut_tree() function from the scipy.cluster.hierarchy module. For example, to obtain two clusters you can execute the code In [69]: from scipy.cluster.hierarchy import cut tree print(cut_tree(hc_complete, n_clusters=2).T) 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1]] (a) Perform hierarchical clustering using the HCVdata using complete, average and single linkage. To begin you will cut the dendrogram at 4 clusters. Similarly to the previous section, calculate the matching matrix and comment the results. Complete In [70]: from scipy.cluster.hierarchy import linkage from scipy.cluster.hierarchy import dendrogram import matplotlib.pyplot as plt hc complete = linkage(dfHVC, "complete") plt.figure(figsize=(25, 10)) dendrogram (hc complete) plt.show() 1200 1000 800 600 400 200 In [71]: print(cut_tree(hc_complete, n_clusters=4).T) 2 0 0 0 3 0 1 0 0 0 0 1 0 0 0 1 0 0 2 0 0 0 1 0 0 0]] **Average** In [72]: hc average = linkage(dfHVC, "average") plt.figure(figsize=(25, 10)) dendrogram (hc average) plt.show() 800 600 200 In [73]: print(cut_tree(hc_average, n_clusters=4).T) 2 0 0 0 3 0 1 0 0 0 0 1 0 0 0 1 0 0 2 0 0 0 1 0 0 0]] Single In [74]: hc_single = linkage(dfHVC, "single") plt.figure(figsize=(25, 10)) dendrogram(hc single) plt.show() In [75]: print(cut_tree(hc_single, n_clusters=4).T) $\ \, 0\ \,$ 1 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 3 0 0 0]]