Member of the project : Alexis Ribat Advanced Machine Learning Project We will analyse the Concret Slump Test data. Data file and variables name are available on the slump.data and slump\_test.names files. Link of the Dataset: https://lipn.univ-paris13.fr/~grozavu/PredA/dataProject/6%20-%20slump/ The Dataset contains: Input variables (7) (component kg in one M^3 concrete): Cement Slag Fly ash Water SP Coarse Aggr. Fine Aggr. Output variables (3): SLUMP (cm) FLOW (cm) 28-day Compressive Strength (Mpa) What is Compressive Strength of Concrete? Compressive strength of concrete is the Strength of hardened concrete measured by the compression test. The compression strength of concrete is a measure of the concrete's ability to resist loads which tend to compress it. It is measured by crushing cylindrical concrete specimens in compression testing machine. Compressive strength results are primarily used to determine that the concrete mixture as delivered on site meets the requirements of the specified strength. A test result is the average of at least two standard-cured strength specimens made from the same concrete batch and tested at the same age. In most cases strength requirements for concrete are at 28 days. As we face the problem of pollution and optimization of our ressources, we might want to find the Concrete with the best capacity required, and with the lest costs of construction. In order to do that, we will see the impact of other ingredients and their role in the Compressive Strength of Concrete. In [62]: from platform import python\_version print(python\_version()) 3.8.3 In [1]: import pandas as pd import numpy as np import matplotlib.pyplot as plt import seaborn as sns from sklearn.model\_selection import train\_test\_split from sklearn import tree from sklearn.model\_selection import cross\_val\_score from sklearn.tree import export\_graphviz from sklearn.metrics import r2\_score from sklearn.metrics import SCORERS import statistics In [2]: f = open('slump\_test.data',"r") data = []for x in f: data.append(x) df = pd.DataFrame(data) df = df[0].str.split(',', expand=True) df.iloc[:, -1] = df.iloc[:, -1].apply(lambda x: x.rstrip()) df.columns = df.iloc[0] df = df.rename(columns = {'SLUMP(cm)': 'Slump', 'FLOW(cm)': 'Flow', 'Compressive Strength (28-day) (Mpa) ': 'CS'}) df = df.iloc[1:, 1:]df = df.apply(pd.to\_numeric) #convert to numeric format df = df.drop\_duplicates(keep='first') #delete potential duplicates with open('slump\_test.names', 'r') as myfile: description = myfile.read().replace('\n', '').replace('\r', '') df.head(10) In [3]: Out[3]: Cement CS Slag Fly ash Water SP Coarse Aggr. Fine Aggr. Slump Flow 1 273.0 82.0 105.0 210.0 9.0 904.0 680.0 23.0 62.0 34.99 2 163.0 149.0 191.0 180.0 12.0 843.0 746.0 0.0 20.0 41.14 3 162.0 148.0 191.0 179.0 16.0 840.0 743.0 20.0 41.81 1.0 4 162.0 148.0 190.0 179.0 19.0 838.0 741.0 3.0 21.5 42.08 154.0 112.0 144.0 220.0 10.0 923.0 20.0 5 658.0 64.0 26.82 6 147.0 89.0 115.0 202.0 9.0 860.0 829.0 23.0 55.0 25.21 944.0 0.0 7 152.0 139.0 178.0 168.0 18.0 695.0 20.0 38.86 8 145.0 0.0 227.0 240.0 6.0 750.0 853.0 14.5 58.5 36.59 9 152.0 785.0 0.0 237.0 204.0 6.0 892.0 15.5 51.0 32.71 10 304.0 0.0 140.0 214.0 6.0 895.0 722.0 19.0 51.0 38.46 Comme on a des valeurs continue, on effectue un Histogramme sur la colonne 'Compressive\_Strength' df.hist('CS') In [4]: Out[4]: array([[<matplotlib.axes.\_subplots.AxesSubplot object at 0x00000219A58C8E80>]], dtype=object) CS 20 15 10 5 In [5]: features to analyse = df.columns[:7] current\_palette = sns.color\_palette("Blues") fig, axes = plt.subplots(round(len(features\_to\_analyse)/4), 4, figsize = (20, 15)) for i, ax in enumerate(fig.axes): if i < len(features to analyse):</pre> sns.boxplot(x=features to analyse[i], data = df, ax = ax, orient = 'v') fig.delaxes(ax = axes[1,3])240 250 175 350 230 150 200 220 300 125 210 150 ge 100 Oement 250 700 Water 75 100 200 50 180 50 25 170 150 160 1050 1000 850 16 950 14 800 900 12 Сh 750 850 10 800 700 750 700 Conclusion. There is no a lot of ouliers in the data set, we can only observe 2 points of outliers in SP (superplasticizer). Almost all features (except for Coarse aggr.) are dispersed. Since we will us tree-base model, we will no need to normalize or scale data because tree-base models are not sensitive to this. In [6]: Out[6]: SP Coarse Aggr. Fine Aggr. Slump Flow CS Cement Slag Fly ash Water 273.0 82.0 105.0 210.0 9.0 904.0 680.0 23.0 62.0 34.99 2 163.0 149.0 191.0 180.0 12.0 843.0 746.0 0.0 20.0 41.14 840.0 743.0 162.0 148.0 191.0 179.0 16.0 20.0 41.81 190.0 838.0 741.0 658.0 154.0 112.0 144.0 220.0 10.0 923.0 20.0 64.0 26.82 99 248.3 101.0 239.1 168.9 7.7 954.2 640.6 0.0 20.0 49.97 100 248.0 101.0 239.9 169.1 7.7 949.9 644.1 2.0 20.0 50.23 101 258.8 88.0 239.6 175.3 7.6 938.9 646.0 0.0 20.0 50.50 297.1 40.9 239.9 194.0 908.9 651.8 102 7.5 27.5 67.0 49.17 103 348.7 223.1 208.5 786.2 758.1 29.0 78.0 48.77 103 rows × 10 columns We want to get a total count of missing values. df.isnull().sum().sum() Out[7]: 0 There is no missing value In [8]: df.dtypes Out[8]: 0 Cement float64 Slag float64 Fly ash float64 Water float64 float64 Coarse Aggr. float64 Fine Aggr. float64 float64 Slump Flow float64 CS float64 dtype: object Checking if there are some outliers df.describe() In [9]: Out[9]: SP Coarse Aggr. CS Cement Fly ash Slump Flow Slag Water Fine Aggr. **count** 103.000000 103.000000 103.000000 103.000000 103.000000 103.000000 103.000000 103.000000 103.00000 103.000000 mean 229.894175 18.048544 49.61068 36.039417 77.973786 149.014563 197.167961 8.539806 883.978641 739.604854 7.838232 std 78.877230 60.461363 85.418080 20.208158 2.807530 88.391393 63.342117 8.750844 17.56861 17.190000 min 137.000000 0.000000 0.000000 160.000000 4.400000 708.000000 640.600000 0.000000 20.00000 152.000000 0.050000 115.500000 180.000000 6.000000 819.500000 684.500000 14.500000 38.50000 30.900000 248.000000 100.000000 164.000000 196.000000 8.000000 879.000000 742.700000 21.500000 54.00000 35.520000 50% 303.900000 125.000000 235.950000 209.500000 10.000000 952.800000 788.000000 24.000000 63.75000 41.205000 max 374.000000 193.000000 260.000000 240.000000 78.00000 58.530000 19.000000 1049.900000 902.000000 29.000000 In [10]: df.info() <class 'pandas.core.frame.DataFrame'> Int64Index: 103 entries, 1 to 103 Data columns (total 10 columns): Column Non-Null Count Dtype 0 103 non-null Cement float64 Slag 103 non-null 103 non-null Fly ash float64 Water 103 non-null float64 103 non-null float64 Coarse Aggr. 103 non-null float64 Fine Aggr. 103 non-null float64 6 7 103 non-null float64 Slump 8 103 non-null float64 Flow 9 CS 103 non-null float64 dtypes: float64(10) memory usage: 8.9 KB Interquartile range In [11]: Q1 = df.quantile(0.25)Q3 = df.quantile(0.75)IQR = Q3 - Q1print(IQR) 0 151.900 Cement 124.950 Fly ash 120.450 29.500 Water 4.000 Coarse Aggr. 133.300 Fine Aggr. 103.500 Slump 9.500 Flow 25.250 10.305 dtype: float64 The above output prints the IQR scores, which can be used to detect outliers. The code below generates an output with the 'True' and 'False' values. Points where the values are 'True' represent the presence of the outlier. In [12]: print((df < (Q1 - 1.5 \* IQR)) & (df > (Q3 + 1.5 \* IQR)))Cement Slag Fly ash Water SP Coarse Aggr. Fine Aggr. Slump \ False False
False False False False
False False False False
False False False False
False False False False
False False False False
False False False False False 4 False . . . False False False False 99 100 False False False False False False False False 101 False False False False 102 False False False False False False 103 False False False False False False False Flow CS False False 1 False False 2 3 False False 4 False False False False ... False False 100 False False 101 False False 102 False False 103 False False [103 rows x 10 columns] This technique uses the IQR scores calculated earlier to remove outliers. The rule of thumb is that anything not in the range of (Q1 - 1.5 IQR) and (Q3 + 1.5 IQR) is an outlier, and can be removed. The first line of code below removes outliers based on the IQR range and stores the result in the data frame 'df\_out'.  $df = df[\sim((df < (Q1 - 1.5 * IQR)) | (df > (Q3 + 1.5 * IQR))).any(axis=1)]$ In [13]: Out[13]: (91, 10) After removing outliers, we now have a table of 91 rows and 10 columns. It removed 12 rows. Our new clean Dataset df out looks like that now In [14]: Out[14]: Cement Slag Fly ash Water SP Coarse Aggr. Fine Aggr. Slump Flow CS 273.0 82.0 105.0 210.0 9.0 904.0 680.0 23.0 62.0 34.99 3 148.0 840.0 743.0 162.0 191.0 179.0 16.0 1.0 20.0 41.81 5 154.0 112.0 144.0 220.0 10.0 923.0 658.0 20.0 64.0 26.82 829.0 55.0 25.21 6 147.0 89.0 115.0 202.0 9.0 860.0 23.0 8 145.0 0.0 227.0 240.0 6.0 750.0 853.0 14.5 36.59 58.5 ••• 97 215.6 112.9 239.0 198.7 7.4 884.0 649.1 27.5 64.0 39.13 25.0 722.9 98 295.3 0.0 239.9 236.2 8.3 780.3 77.0 44.08 100 248.0 101.0 239.9 169.1 7.7 949.9 644.1 2.0 20.0 50.23 40.9 194.0 7.5 908.9 651.8 102 297.1 239.9 27.5 67.0 49.17 348.7 223.1 208.5 786.2 758.1 29.0 78.0 48.77 91 rows × 10 columns Now that we have a clean dataset to work with, we will evaluate the correlations between the data **Correlation Matrix** In [15]: df.corr() Out[15]: Water Slag Fly ash SP Coarse Aggr. Fine Aggr. CS Cement Slump Flow 0 1.000000 0.075126 Cement -0.162138 -0.521057 0.203663 -0.006840 -0.311702 0.024127 0.138550 0.484557 Slag -0.162138 1.000000 -0.408213 0.097353 0.249394 -0.296474 -0.119900 -0.121791 -0.211580 -0.406423 Fly ash -0.521057 -0.408213 1.000000 -0.190889 -0.184992 0.165525 -0.222959 -0.012493 0.047922 0.399072 Water 0.203663 0.097353 -0.190889 1.000000 -0.100577 -0.619445 0.039414 0.243352 0.520136 -0.135579 SP -0.006840 0.249394 -0.184992 -0.100577 1.000000 -0.121950 0.073446 -0.095434 -0.058584 -0.043374 Coarse Aggr. -0.311702 -0.296474 0.165525 -0.619445 -0.121950 1.000000 -0.479102 -0.142116 -0.322205 -0.211781 Fine Aggr. 0.024127 -0.119900 -0.222959 0.039414 0.073446 -0.479102 1.000000 0.114184 0.113157 -0.111977 Slump 0.075126 -0.121791 -0.012493 0.243352 -0.095434 -0.142116 0.114184 1.000000 0.852936 -0.026058 Flow 0.138550 -0.211580 0.047922 0.520136 -0.058584 -0.322205 0.113157 0.852936 1.000000 0.069205 0.484557 -0.406423 0.399072 -0.135579 -0.043374 -0.211781 -0.111977 -0.026058 0.069205 1.000000 In [16]: corr = df.corr() plt.figure(figsize=(15,12)) sns.heatmap(corr, xticklabels=corr.columns.values, yticklabels=corr.columns.values, linewidth=2,annot = True) plt.title("Correlation matrix") plt.show() Correlation matrix -1.0 -0.52 -0.0068 -0.31 0.024 0.14 -0.160.2 0.075 Cement - 0.8 -0.41 0.097 0.25 -0.3 -0.12 -0.12 -0.21 -0.41 -0.161 -0.52 -0.41 -0.18 0.17 -0.22 -0.012 0.048 - 0.6 1 -0.19 ash 늗 0.097 -0.19 -0.1 -0.62 0.039 0.24 -0.14 1 Water - 0.4 -0.0068 0.25 -0.1 -0.12 0.073 -0.095 -0.059 -0.18 1 -0.043 გ 0.2 0 -0.12 -0.31 -0.3 0.17 -0.62 1 -0.48 -0.14 -0.32 -0.21 Fine Aggr. Coarse Aggr - 0.0 0.024 -0.12 -0.22 0.039 0.073 -0.48 1 0.11 0.11 -0.11 - -0.2 -0.12 -0.012 0.24 -0.095 -0.14 0.11 0.85 -0.026 1 0.14 -0.21 0.048 -0.059 -0.32 0.85 1 0.069 Flow -0.4 -0.41 -0.14 -0.043 -0.21 -0.11 -0.026 0.069 1 S Slump Slag SΡ Flow Cement Fly ash Water Coarse Aggr. Fine Aggr. ĊS We can see high correlation between: . Cement & Fly\_Ash . Water & Coarse Aggregation . Flow & Slump For the Compressive Strength, we can see that the best correlations are Cement and Fly\_ash. Now, we will cut the data in order to segment and sort data values into bins, since we have a continuous variableas target and we want to convert it into categorical data to analyze it. This technique is very usefull to convert a Regression Problems into a Classification one. correlation mat = corr.corr() corr\_pairs = correlation\_mat.unstack() This will show the correlation that are > 0.5 and <-0.5 sorted pairs = corr pairs.sort values(kind="quicksort") strong pairs = sorted pairs[abs(sorted pairs) > 0.5] print(strong pairs) -0.790030 Coarse Aggr. Water -0.790030 Coarse Aggr. Water -0.625808 Slag CS CS Slag -0.625808 Fine Aggr. Coarse Aggr. -0.625003 Coarse Aggr. Fine Aggr. -0.625003 Slag -0.594630 Fly ash Slag Fly ash -0.594630 Cement Fly ash -0.523353 Fly ash -0.523353 Cement SP Slag 0.504440 0.504440 Slag SP 0.525532 Slump Water 0.525532 Water Slump Flow Water 0.707778 0.707778 Water Flow 0.949211 Flow Slump 0.949211 Flow Slump Cement Cement 1.000000 1.000000 Slump Slump Fine Aggr. Fine Aggr. 1.000000 1.000000 Coarse Aggr. Coarse Aggr. SP 1.000000 Water 1.000000 Water Fly ash Fly ash 1.000000 Slag Slag 1.000000 Flow Flow 1.000000 1.000000 dtype: float64 In [19]: plt.scatter(df['Fine Aggr.'], df['CS']) Out[19]: <matplotlib.collections.PathCollection at 0x219a63880d0> 50 45 40 35 30 25 20 700 750 800 850 650 900 In [20]: sns.pairplot(df) Out[20]: <seaborn.axisgrid.PairGrid at 0x219a65f28e0> 1050 1000 950 In [21]: | X = df[['Cement', 'Fly ash']].values y = df['CS'].values **KMeans before PCA** In [22]: import matplotlib.pyplot as plt from kneed import KneeLocator from sklearn.datasets import make blobs from sklearn.cluster import KMeans from sklearn.metrics import silhouette score from sklearn.preprocessing import StandardScaler In [23]: model = KMeans(n clusters = 3) model.fit(X) In [24]: model.predict(X) Out[24]: array([2, 1, 1, 1, 1, 1, 2, 1, 1, 1, 0, 0, 1, 1, 2, 2, 0, 0, 2, 0, 1, 2, 2, 2, 2, 2, 2, 2, 1, 2, 2, 0, 1, 1, 1, 1, 1, 0, 0, 0, 2, 2, 2, 2, 0, 0, 2, 2, 0, 0, 0, 1, 1, 2, 2, 0, 0, 2, 1, 1, 1, 2, 0, 0, 0, 1, 2, 2]) In [25]: plt.scatter(X[:,0], X[:,1], c=model.predict(X)) Out[25]: <matplotlib.collections.PathCollection at 0x219ac747f10> 250 200 150 100 50 0 200 250 In [26]: model.cluster centers #Affiche les centoïdes Out[26]: array([[ 2.93947368e+02, -2.84217094e-14], [ 1.54731707e+02, 2.06778049e+02], [ 3.01254839e+02, 1.50409677e+02]]) In [27]: | plt.scatter(X[:,0], X[:,1], c=model.predict(X)) plt.scatter(model.cluster\_centers\_[:,0],model.cluster\_centers\_[:,1], c='r') Out[27]: <matplotlib.collections.PathCollection at 0x219ac7a1d60> 200 150 100 50 0 250 150 200 300 In [28]: model.score(X) Out[28]: -231626.0702637791 In [29]: inertia = [] In [30]:  $K_range = range(1,50)$ for k in K range: model=KMeans(n clusters=k).fit(X) inertia.append(model.inertia ) C:\Users\alrib\anaconda3\lib\site-packages\sklearn\cluster\\_kmeans.py:881: UserWarning: KMeans is kno wn to have a memory leak on Windows with MKL, when there are less chunks than available threads. You can avoid it by setting the environment variable OMP\_NUM\_THREADS=1. warnings.warn( In [31]: plt.plot(K range, inertia) plt.xlabel('Number of clusters') plt.ylabel('Numer of model') Out[31]: Text(0, 0.5, 'Numer of model') le6 1.2 1.0 0.8 0.6 0.6 0.4 0.2 0.0 10 20 30 Number of clusters Optimal number of cluster is 5 or 6 In [32]: model = KMeans(n clusters = 6) In [33]: model.fit(X) model.predict(X) Out[33]: array([2, 5, 5, 5, 0, 0, 2, 5, 5, 1, 1, 5, 0, 2, 2, 1, 1, 2, 4, 5, 2, 2, 2, 2, 2, 3, 3, 2, 0, 2, 2, 4, 0, 0, 0, 5, 5, 1, 1, 1, 2, 2, 2, 2, 1, 1, 2, 2, 4, 1, 1, 5, 5, 2, 2, 1, 1, 2, 0, 0, 0, 2, 1, 1, 1, 3, 3, 3]) In [34]: plt.scatter(X[:,0], X[:,1], c=model.predict(X)) Out[34]: <matplotlib.collections.PathCollection at 0x219ad9250d0> 250 200 150 100 50 150 200 250 300 350 In [35]: model.cluster\_centers\_ #Affiche les centoïdes Out[35]: array([[ 1.53920000e+02, 2.34760000e+02], [ 3.19687500e+02, -2.84217094e-14], [ 2.95160000e+02, 1.34200000e+02], [ 3.15414286e+02, 2.21085714e+02], [ 1.56666667e+02, 0.00000000e+00], [ 1.49866667e+02, 1.57933333e+02]]) In [36]: plt.scatter(X[:,0], X[:,1], c=model.predict(X)) plt.scatter(model.cluster\_centers\_[:,0],model.cluster\_centers\_[:,1], c='r') Out[36]: <matplotlib.collections.PathCollection at 0x219ad971a90> 150 100 50 0 150 In [37]: model.score(X) Out[37]: -65935.78797619048 -65937 is still a bad score but it is better than the old score of -231626 In [38]: model.fit(X) model.predict(X) plt.scatter(X[:,0], X[:,1], c=model.predict(X)) model.cluster\_centers\_ #Affiche les centoïdes plt.scatter(X[:,0], X[:,1], c=model.predict(X)) plt.scatter(model.cluster\_centers\_[:,0],model.cluster\_centers\_[:,1], c='r') model.score(X) Out[38]: -67475.9969767544 200 150 100 50 150 200 250 300 350 **PCA** from sklearn.decomposition import PCA In [39]: Xpca = df[['Cement','Slag', 'Fly ash','Water','SP','Coarse Aggr.','Fine Aggr.']].values In [40]: In [41]: Xpca.shape Out[41]: (91, 7) In [42]: model = PCA(n components=7) In [43]: Xpca reduced = model.fit transform(Xpca) In [44]: | np.cumsum(model.explained\_variance\_ratio\_) Out[44]: array([0.43991165, 0.68943404, 0.86352295, 0.98144686, 0.99935413, 0.99990526, 1. ])

	We want to reduce the dataset AND having the most amount of information. Let say that 98% of the information is enough. It means we will keep 4 variables.   plt.plot(np.cumsum(model.explained_variance_ratio_))  [ <matplotlib.lines.line2d 0x219ada23610="" at="">]  10  09  08</matplotlib.lines.line2d>
	0.7 0.6 0.5 0.5 0.7 0.6 0.7 0.7 0.6 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7
<pre>In [48]: Out[48]: In [49]:</pre>	<pre>segmentation_std = scaler.fit_transform(df)  pca = PCA(n_components = 4) pca.fit(segmentation_std)  PCA(n_components=4)  plt.figure(figsize = (10,8)) plt.plot(range(1,8),</pre>
	[ <matplotlib.lines.line2d 0x219ada7ae20="" at="">]  10 -</matplotlib.lines.line2d>
	0.7 - 0.6 - 0.5 -
In [51]:	<pre>scores_pca = pca.transform(segmentation_std)</pre> <pre>KMeans after PCA</pre> inertia = [] <pre>K_range = range(1,21)</pre>
	<pre>for k in K_range:     kmeans_pca = KMeans(n_clusters=k , init = "k-means++", random_state = 42)     kmeans_pca.fit(scores_pca)     inertia.append(kmeans_pca.inertia_)  C:\Users\alrib\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:881: UserWarning: KMeans is kno wn to have a memory leak on Windows with MKL, when there are less chunks than available threads. You can avoid it by setting the environment variable OMP_NUM_THREADS=1.     warnings.warn(  plt.plot(K_range, inertia) plt.xlabel('Number of clusters') plt.ylabel('Numer of model')</pre>
Out[53]:	Text(0, 0.5, 'Numer of model')  600  100  100  100  100  100  100  10
In [541:	200 100 2.5 5.0 7.5 10.0 12.5 15.0 17.5 20.0  Optimal number of cluster is 5 or 6  Now, let implement it into our KMeans algo  kmeans_pca = KMeans(n_clusters = 6, init = "k-means++", random_state = 42)
<pre>In [55]: Out[55]: In [56]: In [57]:</pre>	<pre>kmeans_pca = kmeans(n_crusters = 0, fift = k=means++ , fandom_state = 42)  kmeans_pca.fit(scores_pca)  KMeans(n_clusters=6, random_state=42)  labels = kmeans_pca.predict(scores_pca)  PCA_components = pd.DataFrame(segmentation_std) kmeans_pca.fit(PCA_components.iloc[:,:4])  KMeans(n_clusters=6, random_state=42)</pre>
In [58]:	<pre>labels = kmeans_pca.predict(PCA_components.iloc[:,:4]) plt.scatter(PCA_components[0], PCA_components[1], c=labels) plt.show()</pre> 20 15 10 0.5 0.0
	-0.51.0 -0.5 0.0 0.5 10 1.5