

Mini-Project2

April 9, 2024

```
[293]: import math
import pickle
import gzip
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
%matplotlib inline
```

1 Mini-Project 2

1.) Topic

This project will explore PCA and KMeans clustering on the Darwin dataset, which is a dataset of handwriting data from subjects either diagnosed with Alzheimer's or not. We will use Logistic Regression on the dataset after doing PCA. In addition we will predict from the unsupervised K-means clustering based on our best permutation of labels.

2.) Data

Here is a link to the dataset from the UCI repository:
<https://archive.ics.uci.edu/dataset/732/darwin>

I couldn't find clear descriptions of the features within the repository, so I had to do some additional searching to find out a little more on the features. A detailed description of the tasks the subjects completed can be found here: [Link](#)

The subjects were tasked with 25 different handwriting tasks. The study used paper overlayed on a graphic tablet to track the pen motions and pressure applied by the subjects. Below you can see the column names for the first task. There were 25 tasks, as there are 18 features per task we end up with 450 features.

```
[314]: from sklearn.preprocessing import StandardScaler
s = StandardScaler()
X = pd.read_csv('Data/data.csv')

X.iloc[:,0:19]
```

```
[314]:      ID  air_time1  disp_index1  gmrt_in_air1  gmrt_on_paper1  \
0    id_1      5160      0.000013    120.804174      86.853334
```

1	id_2	51980	0.000016	115.318238	83.448681
2	id_3	2600	0.000010	229.933997	172.761858
3	id_4	2130	0.000010	369.403342	183.193104
4	id_5	2310	0.000007	257.997131	111.275889
..
169	id_170	2930	0.000010	241.736477	176.115957
170	id_171	2140	0.000009	274.728964	234.495802
171	id_172	3830	0.000008	151.536989	171.104693
172	id_173	1760	0.000008	289.518195	196.411138
173	id_174	2875	0.000008	235.769350	178.208024

	max_x_extension1	max_y_extension1	mean_acc_in_air1	mean_acc_on_paper1	\
0	957	6601	0.361800	0.217459	
1	1694	6998	0.272513	0.144880	
2	2333	5802	0.387020	0.181342	
3	1756	8159	0.556879	0.164502	
4	987	4732	0.266077	0.145104	
..	
169	1839	6439	0.253347	0.174663	
170	2053	8487	0.225537	0.174920	
171	1287	7352	0.165480	0.161058	
172	1674	6946	0.518937	0.202613	
173	1838	6560	0.567311	0.147818	

	mean_gmrt1	mean_jerk_in_air1	mean_jerk_on_paper1	mean_speed_in_air1	\
0	103.828754	0.051836	0.021547	1.828076	
1	99.383459	0.039827	0.016885	1.817744	
2	201.347928	0.064220	0.020126	3.378343	
3	276.298223	0.090408	0.021150	5.082499	
4	184.636510	0.037528	0.018590	3.804656	
..	
169	208.926217	0.032691	0.022786	4.074893	
170	254.612383	0.032059	0.019521	4.149653	
171	161.320841	0.022705	0.022441	2.041489	
172	242.964666	0.090686	0.023634	4.385103	
173	206.988687	0.099555	0.019198	4.898606	

	mean_speed_on_paper1	num_of_pendown1	paper_time1	pressure_mean1	\
0	1.493242	22	10730	1679.232060	
1	1.517763	11	12460	1723.171348	
2	3.308866	10	6080	1520.253289	
3	3.542645	10	5595	1913.995532	
4	2.180544	8	4080	1819.121324	
..	
169	3.390491	12	5835	1470.698372	
170	4.143594	10	4595	1880.668118	
171	3.507108	14	4060	1800.671182	

172	3.538417	8	4425	1881.701695
173	2.945370	12	4340	1860.744240

	pressure_var1	total_time1
0	288285.0449	15890
1	210516.6356	64440
2	120845.8717	8680
3	100286.6032	7725
4	160061.8198	6390
..
169	235194.3615	8765
170	155216.3567	6735
171	212575.8020	7890
172	109235.0387	6185
173	131142.3171	7215

[174 rows x 19 columns]

3.) Data Cleaning and EDA

If we use the Pandas Dataframe describe function we get some very useful data about our dataset and features. We can see the count of each column is 174, meaning there is data for all rows and columns, so we won't need to impute. There is some interesting percentile data as well for each of the features as well as mean, min and max values.

There are some features that could use scaling, for example the pressure_var25 feature could lead to some computation issues if it is multiplied many times. We will use sklearn's standard scaler to assist us in scaling and standardizing the dataset.

Below the describe table I am going to show a few histograms of the features means, so I had to do a fun list comprehension to get the indexes of columns that should be grouped together which is what makes python so great. An example of metrics that should be grouped together across tasks would be gmrt_in_air1, gmrt_in_air2 ... ,gmrt_in_air25 .

We haven't removed the label column from our data frame yet, we will do that just after this so we can shuffle the data with the labels. Before creating our list of grouped feature indexes, we should go ahead and drop the ID column because it is of no use to us.

Please read on in the next cell labeled: "3.) Data Cleaning and EDA continued"

```
[315]: X.describe()
```

```
[315]:
```

	air_time1	disp_index1	gmrt_in_air1	gmrt_on_paper1	\
count	174.000000	174.000000	174.000000	174.000000	
mean	5664.166667	0.000010	297.666685	200.504413	
std	12653.772746	0.000003	183.943181	111.629546	
min	65.000000	0.000002	28.734515	29.935835	
25%	1697.500000	0.000008	174.153023	136.524742	
50%	2890.000000	0.000009	255.791452	176.494494	
75%	4931.250000	0.000011	358.917885	234.052560	

max	109965.000000	0.000028	1168.328276	865.210522
-----	---------------	----------	-------------	------------

	max_x_extension1	max_y_extension1	mean_acc_in_air1	\
count	174.000000	174.000000	174.000000	
mean	1977.965517	7323.896552	0.416374	
std	1648.306365	2188.290512	0.381837	
min	754.000000	561.000000	0.067748	
25%	1362.500000	6124.000000	0.218209	
50%	1681.000000	6975.500000	0.275184	
75%	2082.750000	8298.500000	0.442706	
max	18602.000000	15783.000000	2.772566	

	mean_acc_on_paper1	mean_gmrt1	mean_jerk_in_air1	...	mean_gmrt25	\
count	174.000000	174.000000	174.000000	...	174.000000	
mean	0.179823	249.085549	0.067556	...	221.360646	
std	0.064693	132.698462	0.074776	...	63.762013	
min	0.096631	41.199445	0.011861	...	69.928033	
25%	0.146647	161.136182	0.029523	...	178.798382	
50%	0.163659	224.445268	0.039233	...	217.431621	
75%	0.188879	294.392298	0.071057	...	264.310776	
max	0.627350	836.784702	0.543199	...	437.373267	

	mean_jerk_in_air25	mean_jerk_on_paper25	mean_speed_in_air25	\
count	174.000000	174.000000	174.000000	
mean	0.148286	0.019934	4.472643	
std	0.062207	0.002388	1.501411	
min	0.030169	0.014987	1.323565	
25%	0.107732	0.018301	3.485934	
50%	0.140483	0.019488	4.510578	
75%	0.199168	0.021134	5.212794	
max	0.375078	0.029227	10.416715	

	mean_speed_on_paper25	num_of_pendown25	paper_time25	\
count	174.000000	174.000000	174.000000	
mean	2.871613	85.839080	43109.712644	
std	0.852809	27.485518	19092.024337	
min	0.950249	32.000000	15930.000000	
25%	2.401199	66.000000	32803.750000	
50%	2.830672	81.000000	37312.500000	
75%	3.335828	101.500000	46533.750000	
max	5.602909	209.000000	139575.000000	

	pressure_mean25	pressure_var25	total_time25
count	174.000000	174.000000	1.740000e+02
mean	1629.585962	163061.767360	1.642033e+05
std	324.142316	56845.610814	4.969397e+05
min	474.049462	26984.926660	2.998000e+04

25%	1499.112088	120099.046800	5.917500e+04
50%	1729.385010	158236.771800	7.611500e+04
75%	1865.626974	200921.078475	1.275425e+05
max	1999.775983	352981.850000	5.704200e+06

[8 rows x 450 columns]

```
[316]: X = X.drop(['ID'], axis=1)
```

```
[317]: l1 = [[y + x*18 for x in range(25)] for y in range(18)] #
l1
```

```
[317]: [[0,
18,
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449]]
```

3.) Data Cleaning and EDA continued

If you expand the cell above you can see our 18 arrays of 25 indexes that should be grouped for the histograms.

Let's use those in the next cell to pull in the means from each of those columns, I'm just going to do an arbitrary one as I don't want to show 18 histograms, but you could easily loop through the array of arrays and print out 18 histograms if so inclined. We can do this easily by just making

a new dataframe from the existing with just the columns we want. Then we can use pandas to calculate the mean of each column. This will be the data for our mean histogram for disp_index and air_time.

```
[318]: dspmn = X[X.columns[l1[1]]]
display(dspmn)

gmrtmn = X[X.columns[l1[2]]]
display(gmrtmn)
```

	disp_index1	disp_index2	disp_index3	disp_index4	disp_index5	\
0	0.000013	0.000012	0.000013	0.000027	0.000016	
1	0.000016	0.000015	0.000013	0.000045	0.000034	
2	0.000010	0.000010	0.000009	0.000023	0.000014	
3	0.000010	0.000014	0.000014	0.000026	0.000016	
4	0.000007	0.000012	0.000012	0.000027	0.000003	
..	
169	0.000010	0.000012	0.000007	0.000027	0.000015	
170	0.000009	0.000010	0.000010	0.000025	0.000015	
171	0.000008	0.000012	0.000011	0.000027	0.000015	
172	0.000008	0.000011	0.000012	0.000027	0.000015	
173	0.000008	0.000011	0.000010	0.000027	0.000015	

	disp_index6	disp_index7	disp_index8	disp_index9	disp_index10	...	\
0	0.000003	0.000004	0.000006	0.000004	0.000006	...	
1	0.000009	0.000007	0.000006	0.000007	0.000008	...	
2	0.000005	0.000005	0.000007	0.000010	0.000005	...	
3	0.000003	0.000005	0.000009	0.000007	0.000005	...	
4	0.000004	0.000005	0.000006	0.000007	0.000005	...	
..	
169	0.000006	0.000005	0.000007	0.000009	0.000004	...	
170	0.000007	0.000010	0.000007	0.000012	0.000009	...	
171	0.000004	0.000007	0.000007	0.000011	0.000007	...	
172	0.000004	0.000007	0.000007	0.000011	0.000007	...	
173	0.000004	0.000007	0.000007	0.000011	0.000007	...	

	disp_index16	disp_index17	disp_index18	disp_index19	disp_index20	\
0	0.000005	0.000025	0.000004	0.000028	0.000014	
1	0.000005	0.000030	0.000006	0.000033	0.000051	
2	0.000000	0.000029	0.000004	0.000030	0.000014	
3	0.000005	0.000026	0.000004	0.000030	0.000016	
4	0.000003	0.000019	0.000004	0.000028	0.000012	
..	
169	0.000005	0.000027	0.000005	0.000034	0.000014	
170	0.000004	0.000031	0.000005	0.000034	0.000013	
171	0.000004	0.000031	0.000005	0.000034	0.000018	
172	0.000004	0.000031	0.000005	0.000034	0.000018	
173	0.000004	0.000031	0.000005	0.000034	0.000018	

	disp_index21	disp_index22	disp_index23	disp_index24	disp_index25
0	0.000061	0.000009	0.000009	0.000019	0.000049
1	0.000036	0.000012	0.000011	0.000016	0.000070
2	0.000049	0.000010	0.000011	0.000022	0.000056
3	0.000058	0.000009	0.000010	0.000021	0.000058
4	0.000062	0.000008	0.000008	0.000021	0.000043
..
169	0.000050	0.000008	0.000009	0.000021	0.000051
170	0.000053	0.000009	0.000009	0.000020	0.000056
171	0.000053	0.000011	0.000010	0.000025	0.000059
172	0.000053	0.000011	0.000010	0.000025	0.000059
173	0.000053	0.000011	0.000010	0.000025	0.000059

[174 rows x 25 columns]

	gmrt_in_air1	gmrt_in_air2	gmrt_in_air3	gmrt_in_air4	gmrt_in_air5 \
0	120.804174	269.355789	330.487573	232.639907	125.989768
1	115.318238	272.771237	240.382372	68.602606	151.022535
2	229.933997	122.809584	82.562392	107.348186	101.628410
3	369.403342	185.278506	323.273194	219.338837	212.248278
4	257.997131	112.619685	214.958135	204.322750	134.501527
..
169	241.736477	244.639443	205.543659	91.302401	92.660767
170	274.728964	326.445362	461.017026	327.269006	106.507208
171	151.536989	303.522001	428.020268	63.105656	102.308276
172	289.518195	511.188113	385.069812	63.105656	102.308276
173	235.769350	511.188113	405.584055	63.105656	102.308276

	gmrt_in_air6	gmrt_in_air7	gmrt_in_air8	gmrt_in_air9	gmrt_in_air10 \
0	244.192448	390.168619	98.738919	1331.340031	136.057361
1	130.260917	133.477130	85.904279	67.345719	70.232324
2	156.512289	273.908579	936.464720	299.546106	201.996739
3	214.783769	162.139813	121.386016	237.756310	149.103145
4	399.201436	420.384148	198.886419	210.098311	127.444184
..
169	407.986542	319.107406	193.202877	292.564378	351.985247
170	361.434999	392.816132	193.202877	478.666791	176.547172
171	87.324640	139.288717	193.202877	178.700835	196.224808
172	87.324640	139.288717	193.202877	178.700835	196.224808
173	87.324640	139.288717	193.202877	178.700835	196.224808

	...	gmrt_in_air16	gmrt_in_air17	gmrt_in_air18	gmrt_in_air19 \
0	...	152.892221	233.520832	154.316105	161.441145
1	...	125.217229	114.279952	90.701274	103.550797
2	...	255.367051	355.428038	167.812304	160.468599
3	...	267.084079	262.309253	412.731557	134.595114
4	...	185.464449	318.563434	181.697644	119.828032


```

..      ...
169 ...      318.348482      341.258753      356.548511      95.346818
170 ...      181.009497      360.743997      356.548511      95.346818
171 ...      213.848238      360.743997      356.548511      95.346818
172 ...      213.848238      360.743997      356.548511      95.346818
173 ...      213.848238      360.743997      356.548511      95.346818

```

```

      gmrt_in_air20 gmrt_in_air21 gmrt_in_air22 gmrt_in_air23 \
0      175.234228      251.622971      141.179667      126.658709
1      185.609249      290.800361      64.153361      85.909291
2      124.719850      703.155498      147.953226      117.765304
3      235.163095      451.279786      137.080909      211.397750
4      187.584869      288.615548      129.442167      104.338067
..      ...
169      204.739473      404.320478      220.482567      249.819905
170      198.244935      305.367999      133.312847      247.462723
171      243.500435      305.367999      97.473341      249.977087
172      243.500435      305.367999      97.473341      249.977087
173      243.500435      305.367999      97.473341      249.977087

```

```

      gmrt_in_air24 gmrt_in_air25
0      218.093767      279.628181
1      79.502263      86.117902
2      110.209716      215.379542
3      101.823953      207.557650
4      91.467337      167.510556
..      ...
169      114.441189      232.999622
170      289.535604      250.394568
171      141.325005      183.261091
172      141.325005      183.261091
173      141.325005      183.261091

```

[174 rows x 25 columns]

```

[319]: dspMean = dspmn.mean(axis=0).to_numpy()
      gmrtMean = gmrtmn.mean(axis=0).to_numpy()

```

```

[320]: fig, axs = plt.subplots(1, 2, sharey=True, tight_layout=True)

```

```

axs[0].hist(dspMean)
axs[0].set_xlabel('Mean')
axs[0].set_ylabel('Freq')
axs[0].title.set_text('Disp_Index')

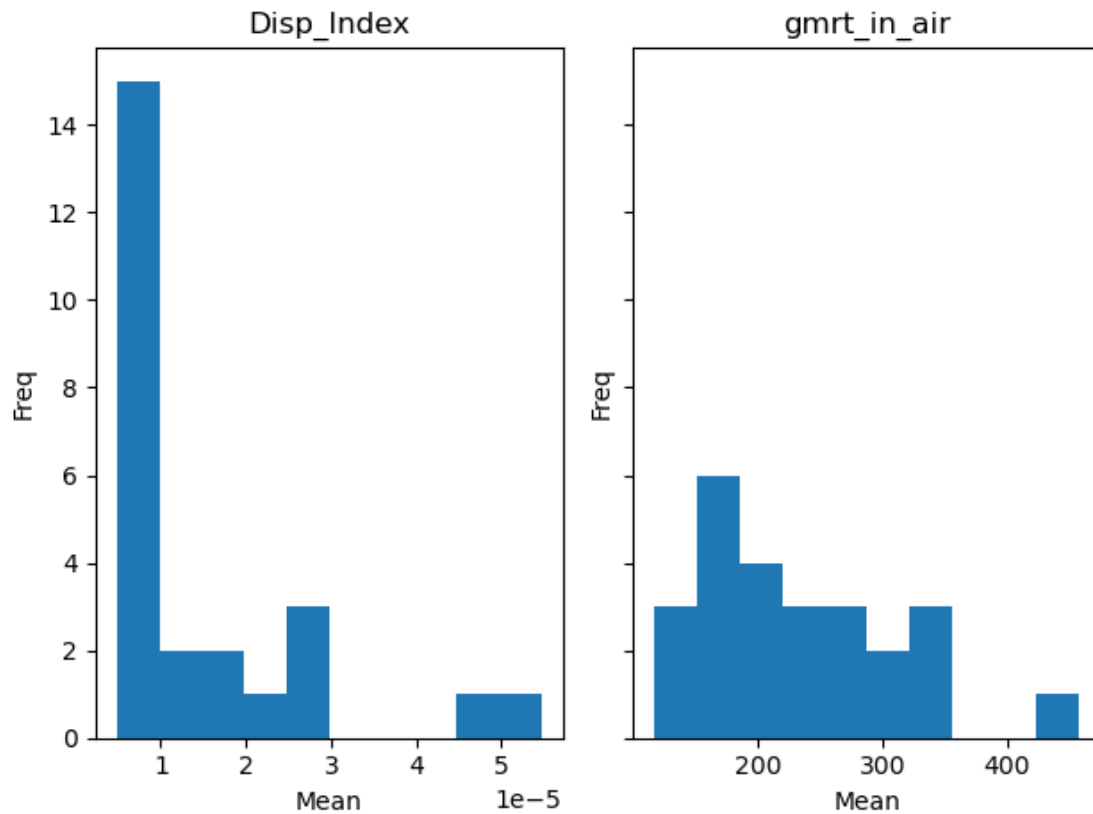
axs[1].hist(gmrtMean)

```

```

axs[1].set_xlabel('Mean')
axs[1].set_ylabel('Freq')
axs[1].title.set_text('gmrt_in_air')

```



So to conclude our EDA we will shuffle our data and then pull our label data out and apply sklearn's standard scaler. We pull the target data out after shuffling so we can keep the order when we split the data into training and test data later.

```

[321]: X[0:5]
X = X.sample(frac=1)

```

```

[322]: npt = X['class'].to_numpy()

X = X.drop(['class'], axis=1)

X = s.fit_transform(X)

X

```

```

[322]: array([[ -0.2824812 ,  0.67005885,  0.58067291, ...,  0.68059489,
                0.01161489, -0.19097171],

```

```

[-0.37362547, -0.28743257,  0.00608449, ...,  0.32867771,
 1.21002067,  0.91310364],
[ 0.57823776,  2.63873278, -0.78277519, ..., -0.14248587,
 0.04551975, -0.1365429 ],
...,
[-0.36966268, -0.68713303,  0.54116553, ...,  0.92729398,
-1.21182576, -0.2119602 ],
[ 0.24338163,  0.55074528,  0.1291487 , ...,  0.84618712,
-1.22320833,  0.35761497],
[ 0.00838791, -0.40674614, -0.90324148, ..., -0.40951536,
 0.2262976 , -0.16547271]]))

```

```
[323]: X.shape
```

```
[323]: (174, 450)
```

4.) Model Building

So the focus of this project for me is really the dimensionality reduction and clustering more so than model building; however, we will still build two models. We will use logistic regression (actually classification) after we perform PCA on the dataset. After that we will use KMeans clustering on the original dataset to see how the algorithm clusters the data into two groups. We will use the implicitly as a model for predictions, we should note that this is still an unsupervised algorithm, i.e. it knows nothing about the labels so hopefully the clusters will implicitly be our labels.

Below is my PCA implementation from Homework 6. I did have to make an adjustment to it, on the homework assignment I used the `Numpy.linalg.eig` function to compute the eigen_pairs, when I ran this initially for the DARWIN dataset I got complex numbers in the eigen_pairs. Switching the algorithm to the `numpy.linalg.eigh` resolved this issue as it is meant for Real Symmetric matrices which is what our covariance matrix that we compute should be. This made the overall algorithm much faster as well.

```

[324]: from sklearn.preprocessing import StandardScaler

class PCA1:
    def __init__(self, target_explained_variance=None):
        """
        explained_variance: float, the target level of explained variance
        """
        self.target_explained_variance = target_explained_variance
        self.feature_size = -1

    def standardize(self, X):
        """
        standardize features using standard scaler
        :param X: input data with shape m (# of observations) X n (# of
        ↪ features)
        :return: standardized features (Hint: use sklearn's StandardScaler.)

```

```

"""
    # Q1. Standardize X using sklearn's StandardScaler. Read the
    ↳ documentation's example. https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.StandardScaler.html#sklearn.preprocessing.StandardScaler
    ↳ StandardScaler
    # Hint: In the example, they used .fit() and .transform() methods
    ↳ separately. You can use another method that has both fit and transform.
    # YOUR CODE HERE
    scaler = StandardScaler()

    return scaler.fit_transform(X)

def compute_mean_vector(self, X_std):
    """
    compute mean vector
    :param X_std: transformed data
    :return mean vector of shape (# of features,)
    """
    # Q2. return mean vector of shape (# of features,). Hint: averaging
    ↳ over the rows for each column.
    # YOUR CODE HERE
    fl = X_std.shape[1]
    mv = np.empty((fl,))
    i = 0

    for col in X_std.T:
        mv[i] = np.mean(col) #Don't need to provide axis as a col(row since
        ↳ transposed) should only have one axis
        i += 1

    return mv

def compute_cov(self, X_std, mean_vec):
    """
    Covariance using mean, (don't use any numpy.cov)
    :param X_std:
    :param mean_vec:
    :return n X n matrix:: covariance matrix
    """
    # Q3. Caculate covariance matrix https://en.wikipedia.org/wiki/Covariance\_matrix
    ↳ Covariance_matrix
    # Hint:  $E[(X-\mu)^T(X-\mu)]$ . You can assume equal probability when
    ↳ calculating the expected value.
    # YOUR CODE HERE

```

```

        CVM = (1 / (X_std.shape[0] - 1))*((X_std - mean_vec).T.dot(X_std -
↪mean_vec))
        print(CVM)

        return CVM

    def compute_eigen_vector(self, cov_mat):
        """
        Eigenvector and eigen values using numpy. Uses numpy's eigenvalue_
↪function
        :param cov_mat:
        :return: (eigen_values, eigen_vector)
        """
        # Q4. Return eigenvalues and engenvectors.
        # Hint: Use appropriate function in linalg package. https://numpy.org/doc/stable/reference/routines.linalg.html
        ↪# YOUR CODE HERE
        #print(cov_mat.shape)
        eigen_vals, eigen_vecs = np.linalg.eigh(cov_mat, )

        #eigen_vals = np.array([float(x.real) for x in eigen_vals])
        #print(eigen_vecs.shape)
        return eigen_vals, eigen_vecs

    def compute_explained_variance(self, eigen_vals):
        """
        Q5. Sort eigen values and compute explained variance ratio.
        explained variance informs the amount of information (variance)
        can be attributed to each of the principal components.
        :param eigen_vals:
        :return: explained variance ratio.
        """
        ↪# YOUR CODE HERE
        lenEV = np.array(eigen_vals).shape[0]
        eigen_vals[:, : -1].sort()
        totvar = sum(eigen_vals)
        evr = np.empty((lenEV,))
        j = 0

        for v in eigen_vals:
            evr[j] = v / totvar
            j += 1

        #print(evr)
        return evr

```

```

def cumulative_sum(self, var_exp):
    """
    return cumulative sum of explained variance.
    :param var_exp: explained variance ratio
    :return: cumulative explained variance ratio
    """
    return np.cumsum(var_exp)

def compute_weight_matrix(self, eig_pairs, cum_var_exp):
    """
    compute weight matrix of top principal components conditioned on target
    explained variance.
    (Hint : use cumulative explained variance ratio and
    ↪target_explained_variance to find
    top components)

    :param eig_pairs: list of tuples containing eigenvalues and
    ↪eigenvectors,
    sorted by eigenvalues in descending order (the biggest eigenvalue and
    ↪corresponding eigenvectors first).
    :param cum_var_exp: cumulative explained variance by features
    :return: weight matrix (the shape of the weight matrix is n X k)
    """
    matrix_w = np.ones((self.feature_size, 1))
    # Q6. In this function, you will implement weight matrix calculation.
    # For each iteration, check the cumulative explained variance ratio
    ↪compared to the target explained variance (see the init variables)
    # then add the eigenvector as column of the matrix_w above.
    # matrix_w will have the dimension of (784,1) initially, but each
    ↪iteration the column will be added until
    # the cumulative explained variance reaches the target explained
    ↪variance.
    # YOUR CODE HERE
    #print(matrix_w.shape)
    #print(eig_pairs[0][1].reshape(-1,1))
    #print(eig_pairs[0][1].T.shape)
    #print(eig_pairs[0])
    #print(matrix_w)
    matrix_w = np.concatenate((matrix_w, eig_pairs[0][1].reshape(-1,1)),
    ↪axis=1)

    csi = 1
    while (cum_var_exp[csi] <= self.target_explained_variance):
        matrix_w = np.concatenate((matrix_w, eig_pairs[csi][1].
    ↪reshape(-1,1)), axis=1)
        csi += 1

```

```

        #print(matrix_w)
        return matrix_w

def transform_data(self, X_std, matrix_w):
    """
    transform data to subspace using weight matrix
    :param X_std: standardized data
    :param matrix_w: weight matrix
    :return: data in the subspace
    """
    return X_std.dot(matrix_w)

def fit(self, X):
    """
    entry point to the transform data to k dimensions
    standardize and compute weight matrix to transform data.
    The fit function returns the transformed features. k is the number of
    ↪ features which cumulative
    explained variance ratio meets the target_explained_variance.
    :param m X n dimension: train samples
    :return m X k dimension: subspace data.
    """

    self.feature_size = X.shape[1]

    # Multisteps to accomplish the fit function- 16 pts
    # step 1. Standardize X to X_std using an appropriate function you
    ↪ implemented above.
    # X_std = (complete this part)
    # YOUR CODE HERE
    X_std = self.standardize(X)

    # step 2. get mean_vec and cov_mat from the appropriate functions from
    ↪ above implementations
    # mean_vec =
    # cov_mat =
    # YOUR CODE HERE
    mean_vec = self.compute_mean_vector(X_std)
    cov_mat = self.compute_cov(X_std, mean_vec)

    # step 3. get eigenvalues and eigenvectors from the implemented
    ↪ function above.
    # eig_vals, eig_vecs =
    # YOUR CODE HERE

```

```

eig_vals, eig_vecs = self.compute_eigen_vector(cov_mat)

# step 4. Sort both eig_vals and eig_vecs by descending order in
↳eigenvalues.
# For example, the first 5 elements of the sorted eigenvalues would
↳look like array([170.57702751, 112.84212831, 45.10927112, 40.75001861, 32.
↳99731063])
# and reorder the eigenvector list accordingly.
# Make a list of tuple called eig_pairs
# eig_pairs = [(170.577, the first eigenvector), (112.84, the second
↳eigenvector), ...] (the length of this list is 784)
# Each eigenvector has a dimension of (784,)
# YOUR CODE HERE
eig_pairs = list(zip(eig_vals,eig_vecs))
eig_pairs.sort(key=lambda x: x[0], reverse=True)

# step 5. get explained variance ratio and cumulated explained variance
↳ratio using functions implemented above.
# Use the variable names below.
# var_exp =
# cum_var_exp =
# YOUR CODE HERE
var_exp = self.compute_explained_variance(eig_vals)
cum_var_exp = self.cumulative_sum(var_exp)

# This step calculates the matrix_w
matrix_w = self.
↳compute_weight_matrix(eig_pairs=eig_pairs,cum_var_exp=cum_var_exp)

print(len(matrix_w),len(matrix_w[0]))
return self.transform_data(X_std=X_std, matrix_w=matrix_w)

```

Next we run the PCA algorithm:

```

[325]: pca_handler = PCA1(target_explained_variance=0.9)
X_train_updated = pca_handler.fit(X)

```

```

[[ 1.00578035  0.36334712 -0.23407708 ... -0.04146479  0.09154482
  0.0188034 ]
 [ 0.36334712  1.00578035 -0.24779655 ... -0.11254862  0.06697624
  0.09853628]
 [-0.23407708 -0.24779655  1.00578035 ...  0.08944409 -0.12053273
 -0.08482268]
 ...
 [-0.04146479 -0.11254862  0.08944409 ...  1.00578035 -0.14329341
 -0.09395363]

```



```
[ 0.09154482  0.06697624 -0.12053273 ... -0.14329341  1.00578035
 0.12500912]
[ 0.0188034  0.09853628 -0.08482268 ... -0.09395363  0.12500912
 1.00578035]]
450 79
```

```
[326]: X_train_updated.shape
```

```
[326]: (174, 79)
```

We have reduced our dimension from 450 to 79. As we can see above our updated data set keeps the same number of rows but the columns have decreased to 54. Order of the rows has been preserved. For a small test on whether or not our PCA implementation is ok we can compare it to sklearn's PCA algorithm:

```
[327]: from sklearn.decomposition import PCA

pca = PCA(n_components=0.9)
principal_components = pca.fit_transform(X)
```

```
[328]: principal_components.shape
```

```
[328]: (174, 79)
```

As we can see we get the exact same number of dimensions!

Before fitting a logistic regression model, we need to convert the Prediction labels from “H”(Healthy) to 0 and “P”(Patient(Diagnosed with Alzheimer’s disease)) to 1

```
[329]: from sklearn.preprocessing import LabelEncoder

le = LabelEncoder()
y = le.fit_transform(npt)
```

Now we can split the data into train and test sets.

```
[330]: from sklearn.model_selection import train_test_split

X_train, X_test, Y_train, Y_test = train_test_split(X_train_updated, y,
                                                    test_size=.3)
```

Now that we have our splits, let’s run it through a quick model to see if we can get any decent predictability. Let’s use Logistic Regression as a baseline model to use after performing Unsupervised learning of some sort, in this case PCA.

5.) Model Training

Below we train a logistic regression model and use it to predict on the test set.

```
[331]: from sklearn.linear_model import LogisticRegression
```

```
LogReg = LogisticRegression(max_iter=10000)
LogReg.fit(X_train, Y_train)

ypred = LogReg.predict(X_test)
```

```
[332]: Y_test, ypred
```

```
[332]: (array([1, 0, 0, 0, 1, 0, 1, 1, 0, 1, 0, 0, 0, 1, 1, 0, 0, 1, 0, 1, 1, 1,
               0, 1, 1, 1, 0, 0, 1, 1, 1, 0, 0, 0, 1, 1, 0, 1, 1, 0, 0, 1, 0, 1,
               0, 1, 1, 1, 0, 1, 0, 0, 1])),
       array([1, 0, 0, 1, 1, 0, 0, 0, 0, 1, 0, 0, 0, 0, 1, 0, 0, 1, 0, 1, 1, 1,
               1, 1, 1, 1, 1, 0, 1, 1, 1, 0, 0, 0, 1, 1, 0, 1, 1, 0, 0, 0, 0, 1,
               0, 1, 1, 1, 0, 1, 0, 1, 1]))
```

We can see above the actual labels and the outputted prediction labels from the logistic model. Next let's use sklearn's accuracy scoring method by passing those two arrays in. As we see below we get a pretty good accuracy score of ~84.9%. Not too shabby for some handwriting data. Seems like there is definitely some indication that these handwriting tasks might be able to give a solid prediction on disease. Below that we plot the roc curve, as this is a classification problem we can use ROC to see the True positive rate(model predicted Alzheimer's and the subject did indeed have Alzheimer's) vs the false positive rate(Model Predicted Alzheimer's but subject did not have Alzheimer's).

```
[333]: from sklearn.metrics import accuracy_score
```

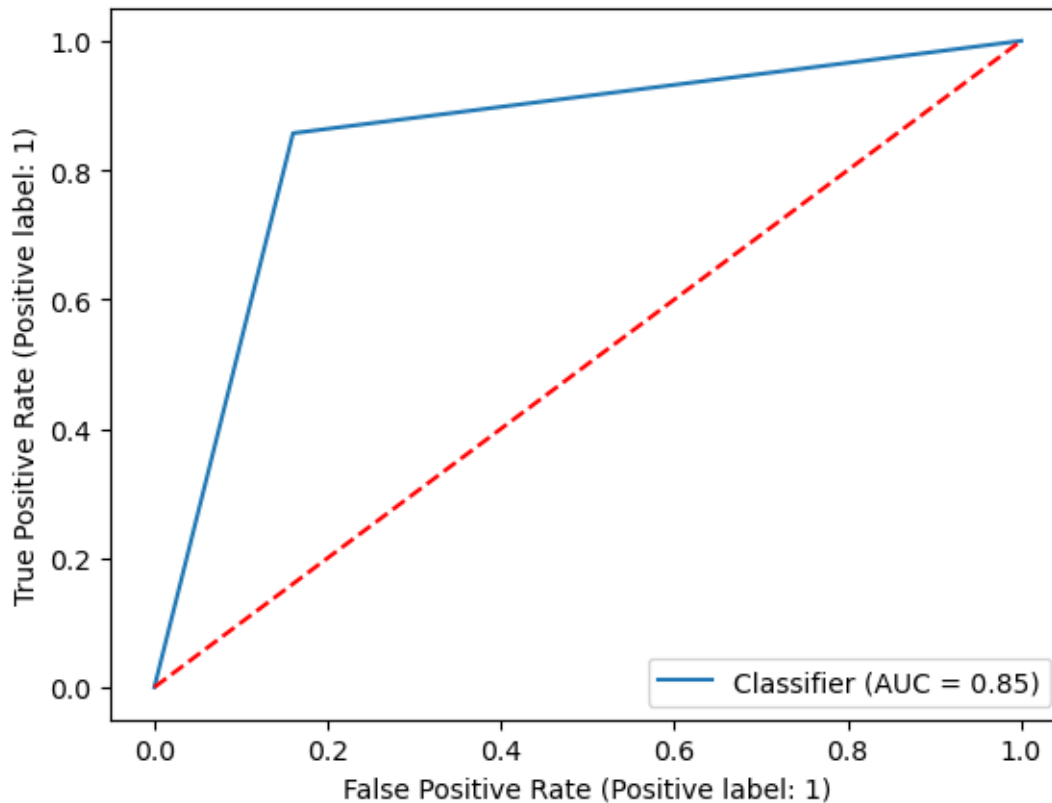
```
acc = accuracy_score(Y_test, ypred)
acc
```

```
[333]: 0.8490566037735849
```

```
[334]: from sklearn.metrics import roc_auc_score
       from sklearn.metrics import roc_curve
       from sklearn.metrics import RocCurveDisplay
```

```
fpr, tpr, thresh = roc_curve(Y_test, ypred)
rocAucScore = roc_auc_score(Y_test, ypred)

RocCurveDisplay.from_predictions(Y_test, ypred)
plt.plot(np.arange(0, 1.1, 0.1), np.arange(0, 1.1, 0.1), 'r--')
plt.show()
```



Let's do a quick GridSearch for Hyper parameter tuning so we can get our best possible model. First we will bring in the plotSearchGrid function from our Week 5 homework. Then we can display the output of our param trials on a grid.

```
[335]: import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
from matplotlib.colors import Normalize
import seaborn as sns
import copy

%matplotlib inline

class MidpointNormalize(Normalize):

    def __init__(self, vmin=None, vmax=None, midpoint=None, clip=False):
        self.midpoint = midpoint
        Normalize.__init__(self, vmin, vmax, clip)

    def __call__(self, value, clip=None):
        x, y = [self.vmin, self.midpoint, self.vmax], [0, 0.5, 1]
```

```

        return np.ma.masked_array(np.interp(value, x, y))

def plotSearchGrid(grid):

    scores = [x for x in grid.cv_results_["mean_test_score"]]
    scores = np.array(scores).reshape(len(grid.param_grid['C']), len(grid.
    ↪param_grid["penalty"]))

    plt.figure(figsize=(10, 8))
    plt.subplots_adjust(left=.2, right=0.95, bottom=0.15, top=0.95)
    plt.imshow(scores, interpolation='nearest', cmap=plt.cm.hot,
               norm=MidpointNormalize(vmin=0.2, midpoint=0.92))
    plt.xlabel('penalty')
    plt.ylabel('C')
    plt.colorbar()
    plt.xticks(np.arange(len(grid.param_grid["penalty"])), grid.
    ↪param_grid["penalty"], rotation=45)
    plt.yticks(np.arange(len(grid.param_grid["C"])), grid.param_grid["C"])
    plt.title('Validation accuracy')
    plt.show()

```

```

[336]: from sklearn.model_selection import GridSearchCV

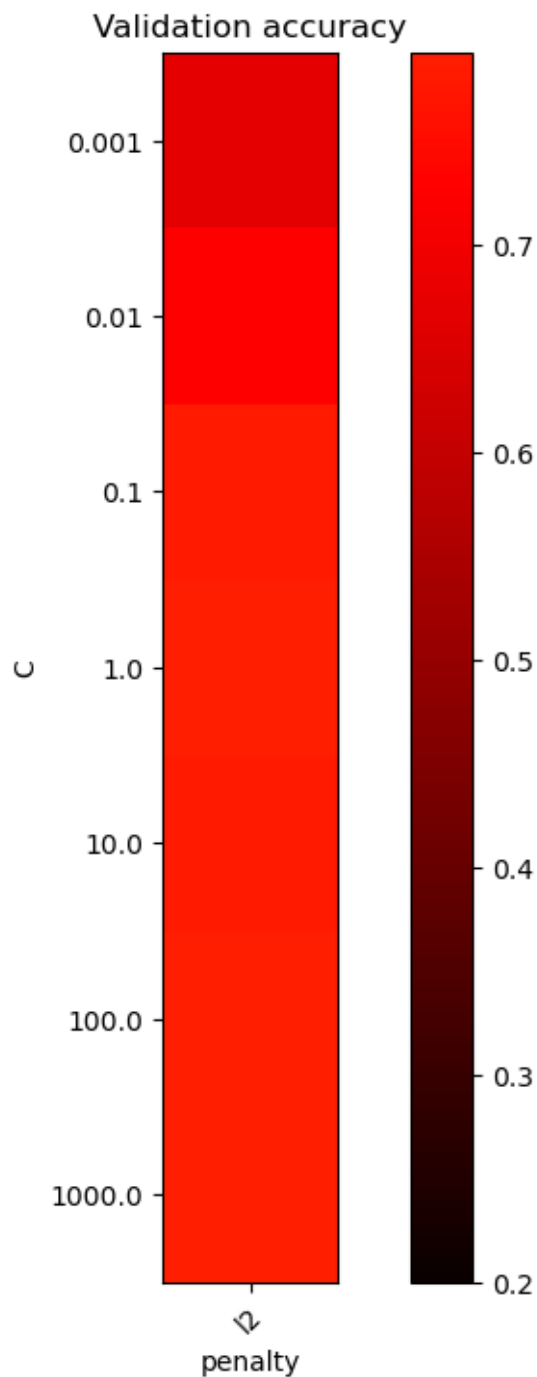
params={'C':np.logspace(-3,3,7), 'penalty':['l2']} #l2 is the only penalty_
    ↪hyper parameter that works

grid = GridSearchCV(LogisticRegression(max_iter=10000),params, cv=3)
grid.fit(X_train, Y_train)

plotSearchGrid(grid)

display(grid.best_params_, grid.best_score_)

```



```
{'C': 1.0, 'penalty': 'l2'}
```

```
0.7928861788617887
```

From the grid search it looks like the default hyperparameter settings are the best for our use. Only the l2 penalty would work for me so that's all I could test for that hyperparameter.

Now let's see what K means can tell us. We should fit a K means model with 2 clusters to see if it can possibly group the samples in either 0(Healthy) or 1(Patient)

```
[174]: from sklearn.cluster import KMeans
from sklearn.metrics import confusion_matrix

kmeans = KMeans(n_clusters=2, n_init="auto").fit(X)

print(kmeans.labels_)
print(y)
```

```
[1 1 0 1 0 1 1 1 0 1 1 1 1 1 1 1 1 0 1 1 0 1 1 1 1 1 1 0 0 1 0 1 1 1 1 1
 1 1 1 1 1 0 1 0 1 1 1 1 1 1 1 1 1 0 1 1 1 1 1 1 0 1 0 0 1 0 0 1 1 0 0 1
 1 1 1 1 0 1 0 1 1 0 0 1 1 0 1 1 1 1 0 1 1 0 1 1 1 1 1 1 1 0 1 1 1 1 1 0 1
 1 1 1 1 1 0 1 0 0 0 1 1 1 1 1 1 1 0 1 1 1 1 1 1 1 0 1 1 0 0 1 1 0 1 1 1 1
 1 1 1 0 0 1 0 1 0 0 0 1 0 1 1 0 0 1 0 1 1 1 1 1 1 1 0]
[0 0 1 0 1 0 0 0 1 0 0 0 0 0 0 0 1 1 1 0 1 1 0 1 0 1 0 0 1 1 0 1 1 0 1 0 0
 1 0 0 0 0 1 1 1 1 1 0 1 0 1 1 1 0 0 0 0 0 0 1 1 1 1 0 1 1 0 1 1 1 0 0 1 1
 0 0 1 0 1 0 1 1 0 1 1 1 0 1 0 1 0 0 1 0 1 1 1 1 0 0 0 0 1 0 0 1 1 0 1 1 0
 0 0 0 0 0 1 0 1 1 1 0 1 0 0 0 1 1 1 1 0 0 0 1 0 1 0 0 1 1 1 0 1 0 1 1 1
 0 0 1 1 1 0 1 0 1 1 1 1 1 1 0 1 1 1 1 0 0 0 0 0 0 1]
```

At this point K Means knows nothing about the labels. The nice thing about only having two clusters is that there are only two possible permutation interpretations of the labels, i.e. ((0,1) means (Patient, Healthy) or (0,1) means (Healthy, Patient)). We could just try either permutation and pick the best accuracy, but we built up a nice label permutor in week 7 so let's modify that to run it, sure it's overkill for only two permutations, but you could run it for more.

```
[197]: import itertools
import functools
import operator

def label_permute_compare(ytdf, yp, n=2):
    """
    ytdf: labels dataframe object
    yp: clustering label prediction output
    Returns permuted label order and accuracy.
    Example output: (3, 4, 1, 2, 0), 0.74
    """
    # YOUR CODE HERE
    curBestAcc = 0.0
    curBestPerm = (0,0)
    #ytdf = ytdf.to_numpy()
    #actLabel = dict(map(lambda i,j : (i,j) , ['P', 'H'], [0,1]))
    #ytdf2 = list(map(lambda x: actLabel[x[0]], ytdf))
    for itp in itertools.permutations([0,1]):
        #Need to update the prediction output with different permutations
        yp2 = list(map(lambda x,y: 1 if itp[x]==y else 0, yp, ytdf))
```

```

yp2Numerator = functools.reduce(operator.add, yp2)
yp2Acc = yp2Numerator/174 #Updated denominator here to be number of
↪ samples

    if(yp2Acc > curBestAcc):
        curBestPerm = itp
        curBestAcc = yp2Acc
    return curBestPerm, curBestAcc

```

```
[204]: bestperm,bestacc = label_permute_compare(y,kmeans.labels_)
```

```
bestperm,bestacc
```

```
[204]: ((1, 0), 0.735632183908046)
```

6 Results Analysis

So we can see above that K-Means gives us accuracy around 73.5%. Let's look at a confusion matrix to see what kind of predictions the model may be good at (i.e. maybe it's better at predicting Healthy vs predicting Alzheimer's)

```
[275]: from sklearn.metrics import confusion_matrix, f1_score
from sklearn import metrics

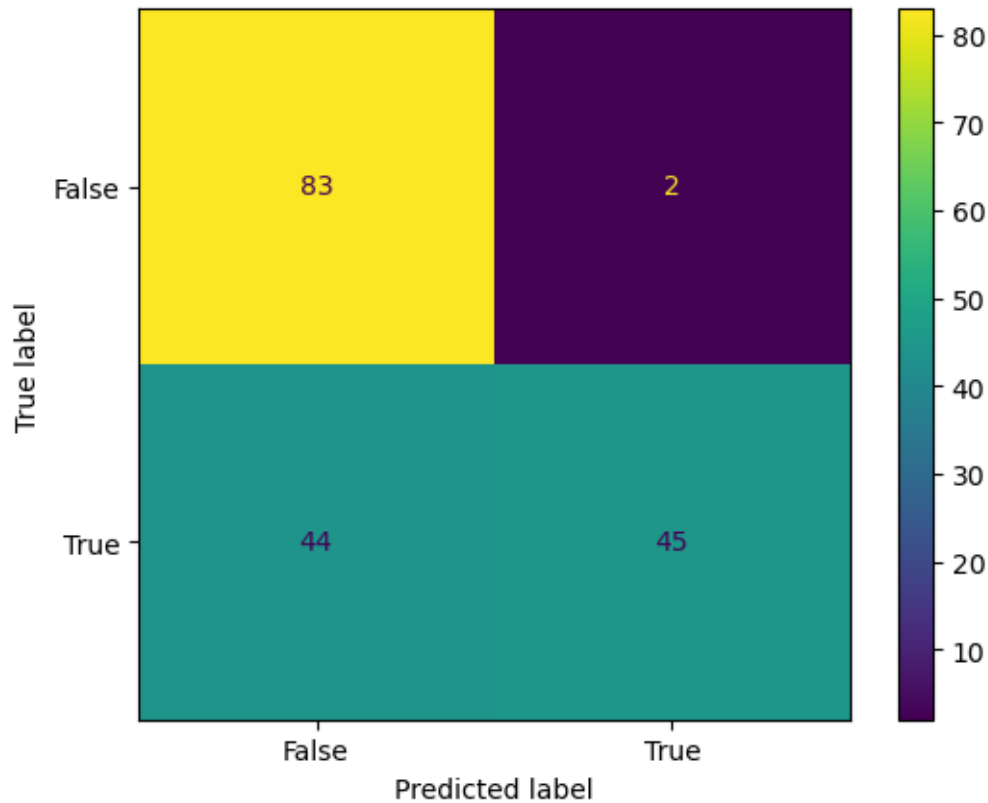
cmkm = confusion_matrix(y,list(map(lambda x: bestperm[x], kmeans.labels_)))

cm_display = metrics.ConfusionMatrixDisplay(confusion_matrix = cmkm,
↪ display_labels = [False, True])
plt.figure(figsize = (8,5))
cm_display.plot()
plt.show()

display(f1_score(y, list(map(lambda x: bestperm[x], kmeans.labels_))))

```

<Figure size 800x500 with 0 Axes>



0.6617647058823529

Let's analyze this confusion matrix a little bit to see how this KMeans clustering does as a predictor. The first thing I notice is that we obtained very few false positives, there were only 2, this gives us a false positive rate of $2/85$ or .0235 or 2.35%. This means when the model predicts true it is very likely that the subject has Alzheimer's.

The next thing of note is there seems to be a lot of false negatives, there were 44 false negatives making the false negative rate $44/89$ or .494 or 49.4%. This means if the model predicts a negative(healthy) then it's only right about half the time.

The specificity of this model is $83/85$ or .9765 or 97.65%. This means that when the actual diagnosis is negative the model predicts it with 97.65% probability.

The recall of this model is $45/89$ or .5056 or 50.56%. This means that if the actual diagnosis is positive the model only predicts correctly about half of the time.

Our F1 score of .661 isn't great, but it does show that the model does have some validity.

If we compare the accuracy of our two models, the first model with PCA and Logistic Classifier is clearly better than the KMeans. There is a chance that K Means has a False-Positive rate, but it's extremely unlikely that you would want to use this model over the PCA and Logistic model.

7 Conclusion

This has been a very interesting project to see if there are any unsupervised methods that can lead to insights into potential Alzheimer's diagnoses through handwriting. It seems that PCA with a simple logistic regression can provide a decently accurate prediction on whether or not a patient has Alzheimer's through their handwriting. It should be noted that it is decently accurate on THIS dataset. It has some problems, the main issue is it's a relatively small dataset, so the sample size might not be sufficient to offer truly accurate predictions. Another shortcoming is we don't actually know how we could differentiate Alzheimer's from some other disease like Parkinson's that might cause differences in handwriting, it is within the realm of possibility that this model prediction could lead to a misdiagnosis of Alzheimer's when maybe someone just had a stroke that affected their motor skills. An improved dataset could potentially have more classification classes for different diseases, that would be very interesting to see if you could differentiate different diseases based solely on handwriting. It should also be noted that there are likely better models than logistic regression that could be used; however, our focus in this project was on the unsupervised learning models and that did help us in regards to dimensionality reduction. In addition clustering was at least able to give us a better than guessing prediction knowing nothing about the labels, which is pretty neat, clearly there is likely some correlation in motor skill dysfunction with these neurological diseases and these unsupervised methods seem to bear that out. Further improvements could be made with a better model like Gradient Boosting or maybe using SVM or Random Forest. I'd also be interested in seeing how this could do in a deep learning model and may explore that for the next project. Thanks for taking the time to read my project!

Dataset citation:

Fontanella, Francesco. (2022). DARWIN. UCI Machine Learning Repository. <https://doi.org/10.24432/2022-01-Fontanella>

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