report_executed

August 18, 2021

1 Statistics

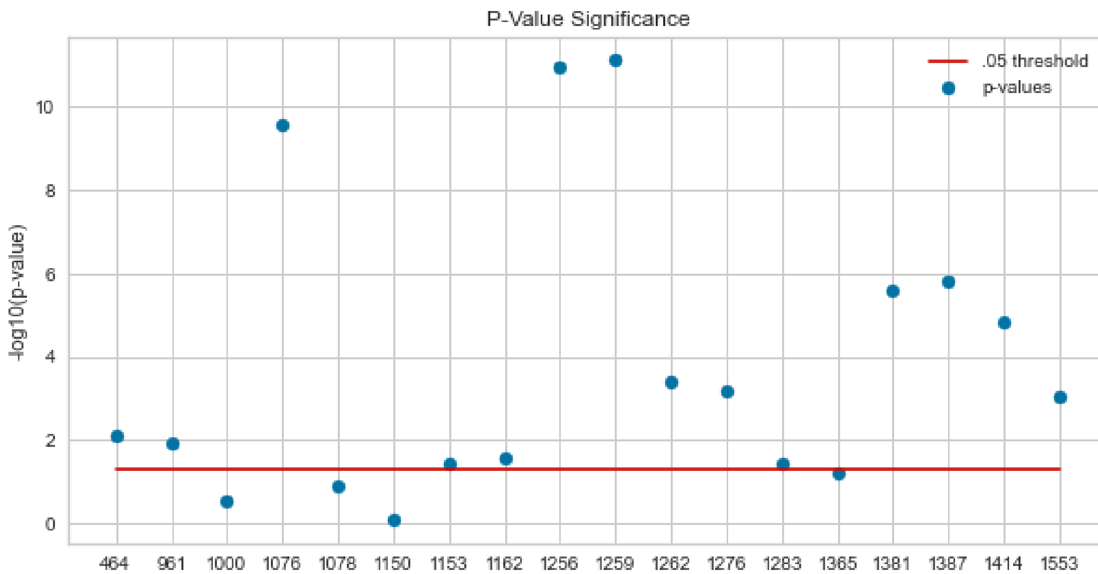
In the statistics module we analyze data for different responses and at different spectral peak locations. We use Python package scipy in this module.

1.1 T-Test

T-test checks for difference in the mean between two sample from different responses. We assume the data is independent and follows the normality assumption. Let $x_1, \ldots, x_n$ and $y_1, \ldots, y_m$ be the two samples and we test whether the means are equal. The null hypothesis states means μ_1 and μ_2 are equal and the alternative hypothesis states they are not equal. If the p-value is lower than the chosen significance level, we can reject the null hypothesis, i.e. the samples do not have the same means.

[1]:
```
import modules.adapml_data as adapml_data
import modules.adapml_classification as adapml_classification
import modules.adapml_clustering as adapml_clustering
import modules.adapml_chemometrics as adapml_chemometrics
import modules.adapml_statistics as adapml_statistics
import modules.adapml_regression as adapml_regression
import numpy as np
import modules.loadTestData as load_data
import sklearn.preprocessing as pre
from sklearn.cross_decomposition import PLSRegression as PLS
from matplotlib import pyplot as plt
from sklearn import cluster as clst
from scipy.cluster.hierarchy import dendrogram

import os

reldir = os.getcwd()
path_to_data = os.path.join(reldir, '..', 'data',␣
↪'SCLC_study_output_filtered_2.csv')

data = adapml_data.DataImport(path_to_data)

response1D = data.resp
#response1D = adapml_data.DataImport.getResponse(path_to_data)
```

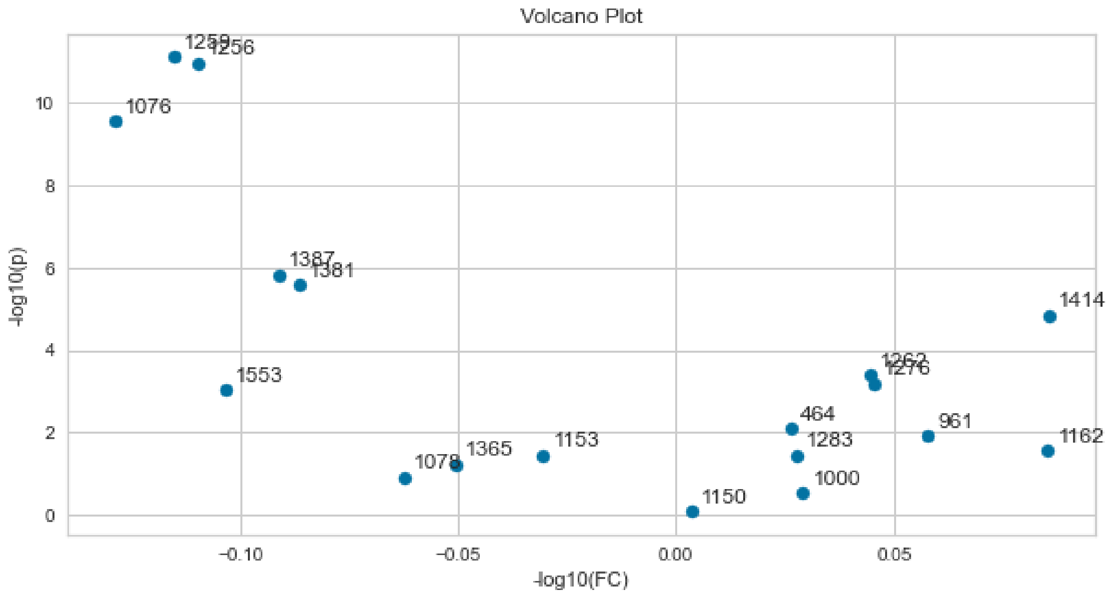
```
response2D = adapml_data.DataImport.getDummyResponse(response1D)

variables = data.getVariableNames()
samples = data.getSampleNames()

t_test = adapml_statistics.Statistics(data.data, 'anova', response1D)
t_test.plot_logp_values(variables)
```



1.2 Volcano Plot

Volcano plot is a scatter plot which demonstrates magnitude between the responses and t-test significance of the data. We can choose a significance level and fold change limit to specify the rectangle of interest.

[2]:
```
t_test.plot_volcano_t(variables)
```



2 Dimension-Reduction

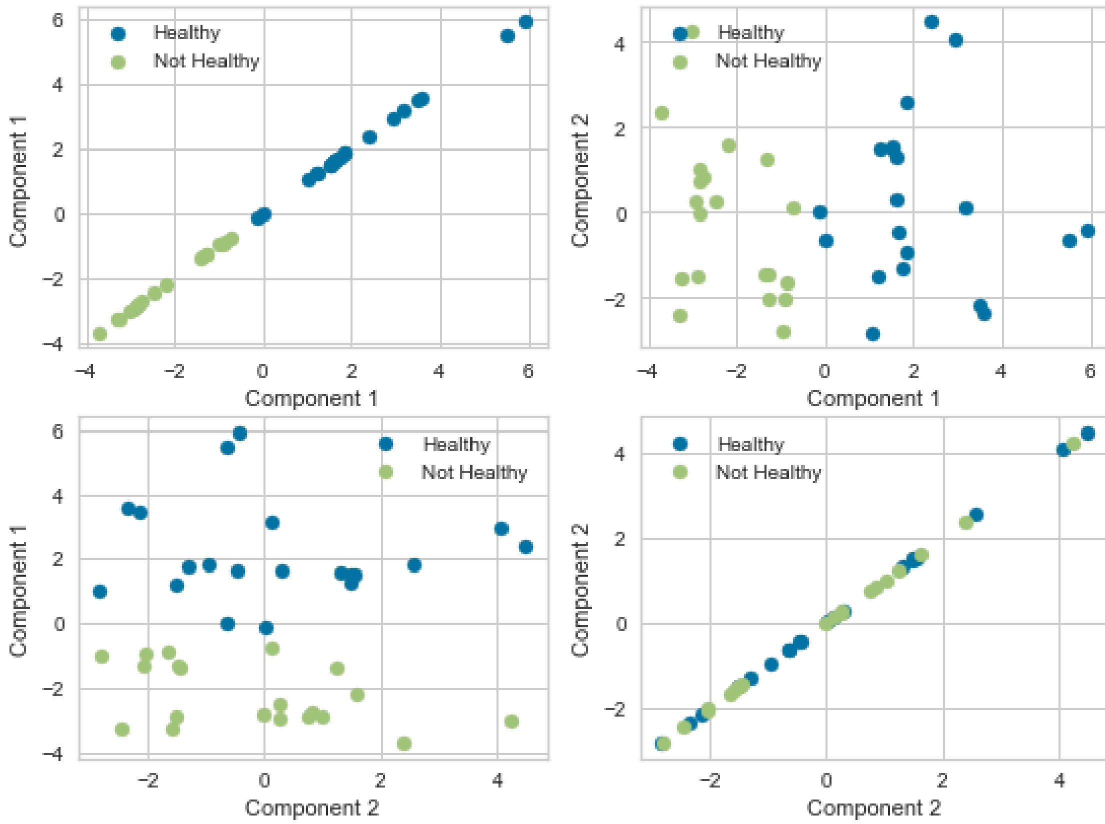
Dimension-reduction methods are used to condense high dimensional data down to dimensions which provide the most information. We have implemented the principal component analysis (PCA). It performs a change of basis and the new basis is chosen, such that the i-th principal component is orthogonal to the first i-1 principal components and the direction maximizes the variance of the projected data. We use the Python library sklearn.

2.1 Principal Component Analysis

The principal component analysis (PCA) is one of the methods for dimension-reduction. It performs a change of basis and the new basis is chosen, such that the i-th principal component is orthogonal to the first i-1 principal components and the direction maximizes the variance of the projected data. Instead of considering all the dimensions, we pick the necessary number of principal components.

[3]:
```
data.normalizeData("autoscale")

pca = adapml_chemometrics.Chemometrics(data.data, "pca", response1D)

print("PCA Projections");pca.plotProjectionScatterMultiClass(2,␣
↪labels=["Healthy", "Not Healthy"])
```

```
PCA Projections
Projections of data into latent space.
Data is colored by response
```

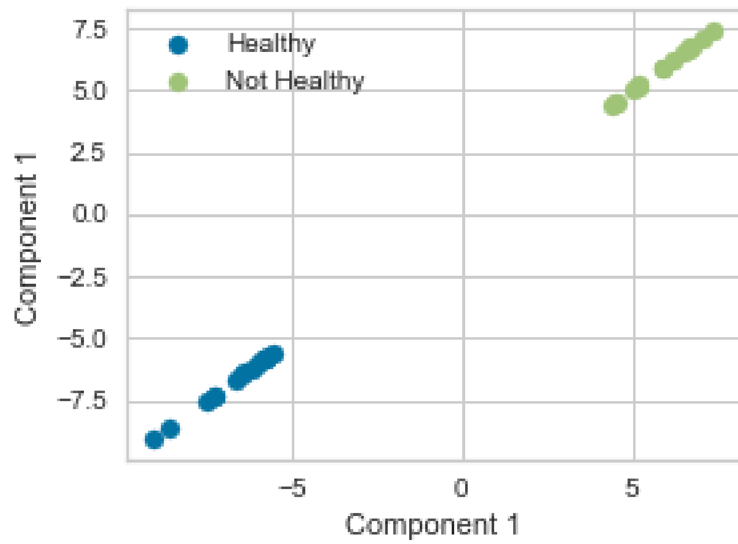


2.2 Linear Discriminant Analysis

Linear discriminant analysis is a classifier with a linear decision boundary. We assume normality and fit conditional densities $p(x \mid y = 0)$ and $p(x \mid y = 1)$ with mean and covariance parameters (μ_0, σ_0) and (μ_1, σ_1), where x, μ_0 and μ_1 are vectors. Dimensionality-reduction is done by projecting the input to the most discriminative directions.

[4]:
```
lda = adapml_chemometrics.Chemometrics(data.data, "lda", response1D) # Also␣
↪Predicts

print("LDA Projections");lda.plotProjectionScatterMultiClass(1,␣
↪labels=["Healthy", "Not Healthy"])
```

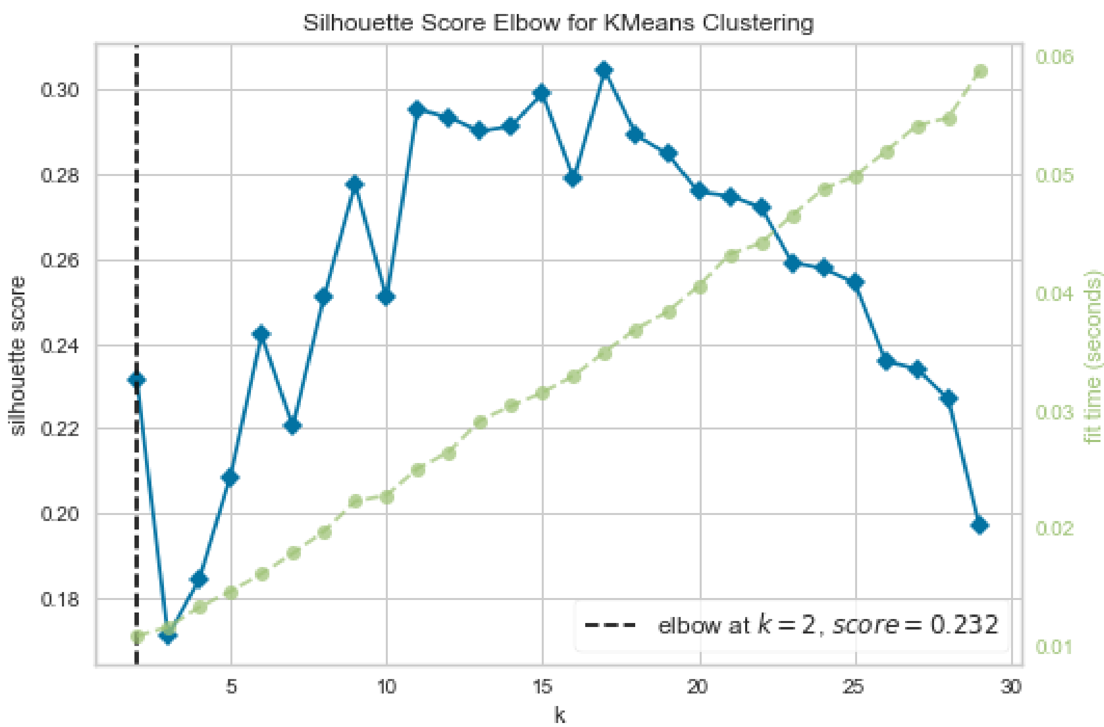
```
LDA Projections
Projections of data into latent space.
Data is colored by response
```



3 Clustering

In this module we use various different clustering methods on spectra. Clustering is done with scipy and sklearn libraries.

[5]:
```
silhouette = adapml_clustering.Clustering(data.data, 'silhouette', 3)
nr_clusters = silhouette.clustnr
```



3.1 K-Means Clustering

K-means clustering aims to partition the data into k sets and to minimize the Euclidian within-cluster sum of squares (WCSS)

$$WCSS = \sum_{i=1}^{k} \sum_{x_j \in C_i} \|x_j - \mu_i\|_2^2$$

where $x_1, \ldots, x_n$ is the data and μ_i is the centroid of C_i cluster. It is solved by either Lloyd's or Elkan's algorithm and we use sklearn module in Python.

[6]:
```
kmeans_cluster = adapml_clustering.Clustering(data.data, 'kmeans', nr_clusters)
kmeans_cluster.getClusterResults(samples)
```

	Cluster 1	Cluster 2
0	SCLC_86M1_2	NSCLC_A549_1
1	SCLC_86M1_1	NSCLC_H1703_2
2	SCLC_16HV_1	NSCLC_H1703_1
3	SCLC_16HV_2	NSCLC_A549_2
4	SCLC_DMS79_1	NSCLC_H1437_1
5	SCLC_DMS79_2	NSCLC_H2228_1
6	SCLC_H187_2	NSCLC_H2228_2
7	SCLC_H187_1	NSCLC_H1437_2
8	SCLC_H209_1	NSCLC_H3122_1
9	SCLC_H524_1	NSCLC_H322_2
10	SCLC_H209_2	NSCLC_H322_1
11	SCLC_H524_2	NSCLC_H358_2
12	SCLC_H69_1	NSCLC_H3122_2
13	SCLC_H82_1	NSCLC_H522_1
14	SCLC_H82_2	NSCLC_H522_2
15	SCLC_H69_2	NSCLC_HCC4006_1
16	SCLC_N417_2	NSCLC_H358_1
17	SCLC_N417_1	NSCLC_PC9_1
18	SCLC_SW210-5_1	NSCLC_PC9_2
19	SCLC_SW210_5_2	NSCLC_HCC4006_2

3.2 BIRCH Clustering

[7]:
```
birch_cluster = adapml_clustering.Clustering(data.data, 'birch', nr_clusters)
birch_cluster.getClusterResults(samples)
```

	Cluster 1	Cluster 2
0	NSCLC_A549_1	SCLC_86M1_2
1	NSCLC_H1703_2	SCLC_86M1_1
2	NSCLC_H1703_1	SCLC_16HV_1
3	NSCLC_A549_2	SCLC_16HV_2

4	NSCLC_H1437_1	SCLC_DMS79_1
5	NSCLC_H2228_1	SCLC_DMS79_2
6	NSCLC_H2228_2	SCLC_H187_2
7	NSCLC_H1437_2	SCLC_H187_1
8	NSCLC_H3122_1	SCLC_H209_1
9	NSCLC_H322_2	SCLC_H524_1
10	NSCLC_H322_1	SCLC_H209_2
11	NSCLC_H358_2	SCLC_H524_2
12	NSCLC_H3122_2	SCLC_H69_1
13	NSCLC_H522_1	SCLC_H82_1
14	NSCLC_H522_2	SCLC_H82_2
15	NSCLC_HCC4006_1	SCLC_H69_2
16	NSCLC_H358_1	SCLC_N417_2
17	NSCLC_PC9_1	SCLC_N417_1
18	NSCLC_PC9_2	SCLC_SW210-5_1
19	NSCLC_HCC4006_2	SCLC_SW210_5_2

3.3 DBSCAN Clustering

[8]:
```
dbscan_cluster = adapml_clustering.Clustering(data.data, 'dbscan', nr_clusters)
dbscan_cluster.getClusterResults(samples)
```

	Cluster 1	Cluster 2
0	NSCLC_A549_1	NSCLC_H1703_2
1	NSCLC_A549_2	NSCLC_H1703_1
2	NSCLC_H1437_1	NaN
3	NSCLC_H2228_1	NaN
4	NSCLC_H2228_2	NaN
5	NSCLC_H1437_2	NaN
6	NSCLC_H322_2	NaN
7	NSCLC_H322_1	NaN
8	NSCLC_H358_2	NaN
9	NSCLC_H522_1	NaN
10	NSCLC_H522_2	NaN
11	NSCLC_HCC4006_1	NaN
12	NSCLC_H358_1	NaN
13	NSCLC_PC9_1	NaN
14	NSCLC_PC9_2	NaN
15	NSCLC_HCC4006_2	NaN
16	SCLC_86M1_2	NaN
17	SCLC_86M1_1	NaN
18	SCLC_16HV_1	NaN
19	SCLC_16HV_2	NaN
20	SCLC_DMS79_1	NaN
21	SCLC_DMS79_2	NaN
22	SCLC_H187_2	NaN
23	SCLC_H187_1	NaN
24	SCLC_H209_1	NaN

```
25        SCLC_H524_1            NaN
26        SCLC_H209_2            NaN
27        SCLC_H524_2            NaN
28         SCLC_H69_1            NaN
29         SCLC_H82_1            NaN
30         SCLC_H82_2            NaN
31         SCLC_H69_2            NaN
32        SCLC_N417_2            NaN
33        SCLC_N417_1            NaN
34     SCLC_SW210-5_1            NaN
35     SCLC_SW210_5_2            NaN
```

3.4 Mean Shift Clustering

[9]:
```
meanshift_cluster = adapml_clustering.Clustering(data.data, 'meanshift',␣
 ↪nr_clusters)
meanshift_cluster.getClusterResults(samples)
```

```
            Cluster 1       Cluster 2
0       NSCLC_A549_1   NSCLC_H1703_2
1       NSCLC_A549_2   NSCLC_H1703_1
2      NSCLC_H1437_1             NaN
3      NSCLC_H2228_1             NaN
4      NSCLC_H2228_2             NaN
5      NSCLC_H1437_2             NaN
6      NSCLC_H3122_1             NaN
7       NSCLC_H322_2             NaN
8       NSCLC_H322_1             NaN
9       NSCLC_H358_2             NaN
10     NSCLC_H3122_2             NaN
11      NSCLC_H522_1             NaN
12      NSCLC_H522_2             NaN
13   NSCLC_HCC4006_1             NaN
14      NSCLC_H358_1             NaN
15       NSCLC_PC9_1             NaN
16       NSCLC_PC9_2             NaN
17   NSCLC_HCC4006_2             NaN
18       SCLC_86M1_2             NaN
19       SCLC_86M1_1             NaN
20       SCLC_16HV_1             NaN
21       SCLC_16HV_2             NaN
22      SCLC_DMS79_1             NaN
23      SCLC_DMS79_2             NaN
24       SCLC_H187_2             NaN
25       SCLC_H187_1             NaN
26       SCLC_H209_1             NaN
27       SCLC_H524_1             NaN
28       SCLC_H209_2             NaN
```

```
29       SCLC_H524_2            NaN
30        SCLC_H69_1            NaN
31        SCLC_H82_1            NaN
32        SCLC_H82_2            NaN
33        SCLC_H69_2            NaN
34       SCLC_N417_2            NaN
35       SCLC_N417_1            NaN
36    SCLC_SW210-5_1            NaN
37    SCLC_SW210_5_2            NaN
```

3.5 Gaussian Mixture Clustering

[10]:
```
gaussian_cluster = adapml_clustering.Clustering(data.data, 'gaussian',␣
 ↪nr_clusters)
gaussian_cluster.getClusterResults(samples)
```

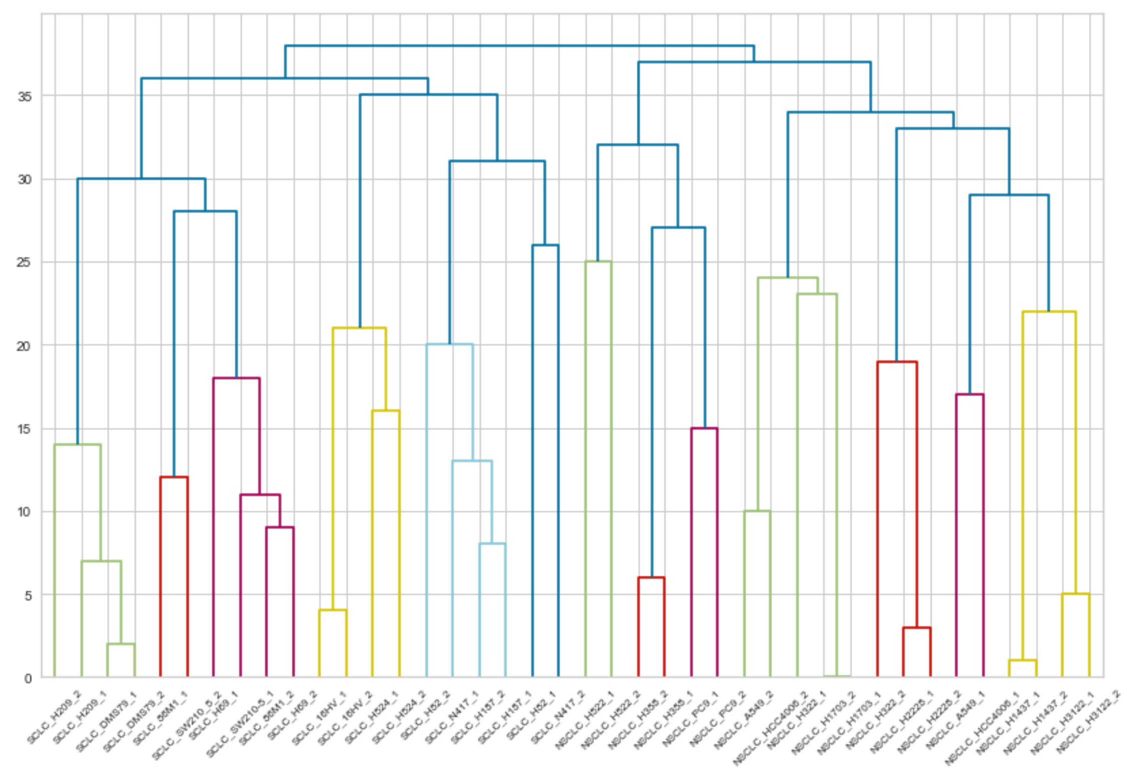
```
           Cluster 1        Cluster 2
0      NSCLC_A549_1    NSCLC_H522_1
1     NSCLC_H1703_2     SCLC_86M1_2
2     NSCLC_H1703_1     SCLC_86M1_1
3      NSCLC_A549_2     SCLC_16HV_1
4     NSCLC_H1437_1     SCLC_16HV_2
5     NSCLC_H2228_1    SCLC_DMS79_1
6     NSCLC_H2228_2    SCLC_DMS79_2
7     NSCLC_H1437_2     SCLC_H187_2
8     NSCLC_H3122_1     SCLC_H187_1
9      NSCLC_H322_2     SCLC_H209_1
10     NSCLC_H322_1     SCLC_H524_1
11     NSCLC_H358_2     SCLC_H209_2
12    NSCLC_H3122_2     SCLC_H524_2
13     NSCLC_H522_2      SCLC_H69_1
14  NSCLC_HCC4006_1      SCLC_H82_1
15     NSCLC_H358_1      SCLC_H82_2
16      NSCLC_PC9_1      SCLC_H69_2
17      NSCLC_PC9_2     SCLC_N417_2
18  NSCLC_HCC4006_2     SCLC_N417_1
19              NaN  SCLC_SW210-5_1
20              NaN  SCLC_SW210_5_2
```

3.6 Hierarchical Clustering

Hierarchical clustering builds hierarchies of clusters based on a chosen metric and a linkage scheme. We used cosine distance and average linkage scheme.

[11]:
```
hierarchical_cluster = adapml_clustering.Clustering(data.data, 'hierarchical',␣
 ↪nr_clusters)
hierarchical_cluster.getClusterResults(samples)
hierarchical_cluster.plot_dendrogram(samples)
```

	Cluster 1	Cluster 2
0	NSCLC_A549_1	SCLC_86M1_2
1	NSCLC_H1703_2	SCLC_86M1_1
2	NSCLC_H1703_1	SCLC_16HV_1
3	NSCLC_A549_2	SCLC_16HV_2
4	NSCLC_H1437_1	SCLC_DMS79_1
5	NSCLC_H2228_1	SCLC_DMS79_2
6	NSCLC_H2228_2	SCLC_H187_2
7	NSCLC_H1437_2	SCLC_H187_1
8	NSCLC_H3122_1	SCLC_H209_1
9	NSCLC_H322_2	SCLC_H524_1
10	NSCLC_H322_1	SCLC_H209_2
11	NSCLC_H358_2	SCLC_H524_2
12	NSCLC_H3122_2	SCLC_H69_1
13	NSCLC_H522_1	SCLC_H82_1
14	NSCLC_H522_2	SCLC_H82_2
15	NSCLC_HCC4006_1	SCLC_H69_2
16	NSCLC_H358_1	SCLC_N417_2
17	NSCLC_PC9_1	SCLC_N417_1
18	NSCLC_PC9_2	SCLC_SW210-5_1
19	NSCLC_HCC4006_2	SCLC_SW210_5_2

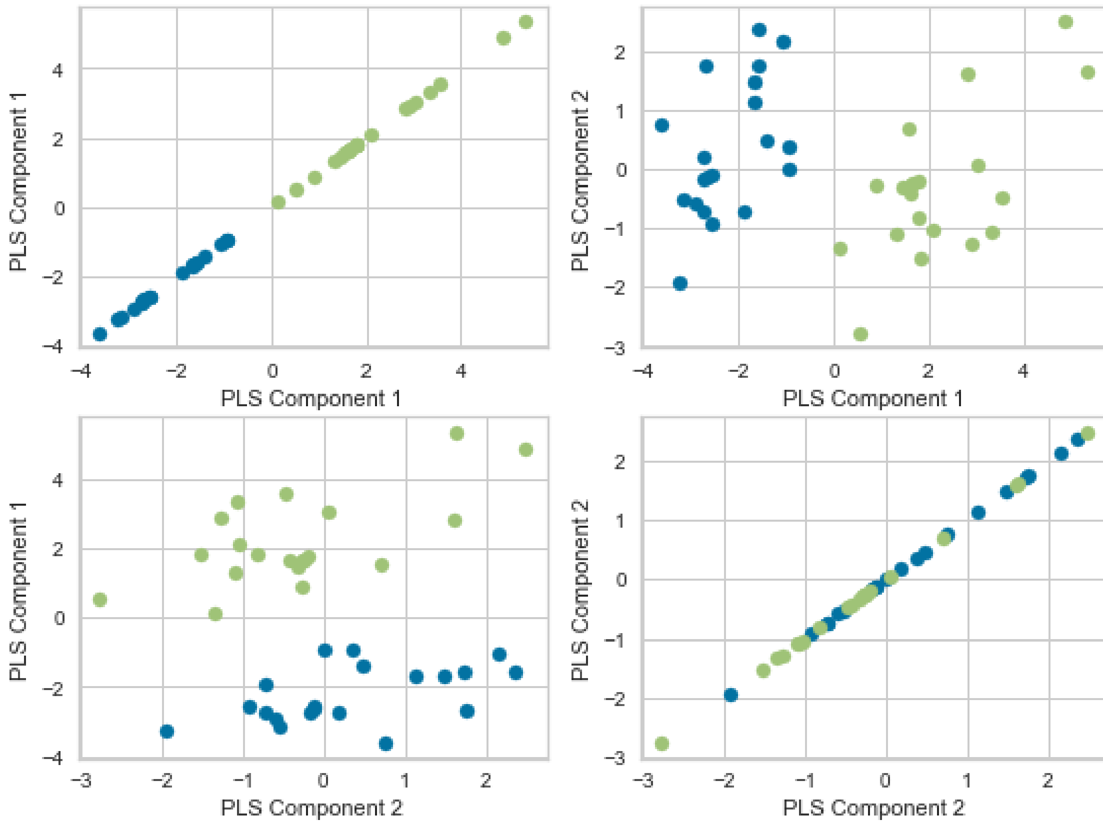


4 Classification

Classification methods aim to classify the response of samples. The given data is separated into a training set and a testing set. The model parameters are found from the training set and the testing set is used to quantify the model accuracy. The methods are from sklearn package.

4.1 Partial Least Squares-Discriminant Analysis

[12]:
```
def plotProjectionScatterMultiClass(pc, resp, num_var):
    plt.figure(figsize=(24, 18))

    for i in range(num_var):
        for j in range(num_var):
            plt.subplot(5,5,5*(i) + j + 1)
            for c in range(resp.shape[1]):
                inx = np.where(resp[:,c] == 1)[0]
                tmp = pc[inx,:]
                pc1 = tmp[:,i]
                pc2 = tmp[:,j]
                plt.scatter(pc1, pc2)
            plt.xlabel("PLS Component "+str(i+1))
            plt.ylabel("PLS Component "+str(j+1))

    plt.show()

data = load_data.loadDataPandas(path_to_data)
d = data.to_numpy()
var_index = data.columns.values.tolist()

resp = load_data.getResponseMatrix2D()

norm_trans = pre.StandardScaler().fit(d)
data_norm = norm_trans.transform(d)
#data_norm, norm_trans = pre.mean_center(d)
#In-built preprocessing method - TBD

pls = PLS().fit(data_norm, resp)
pls_trans = pls.transform(data_norm)

plotProjectionScatterMultiClass(pls_trans, resp, 2)
```



4.2 Support Vector Machines

Classification via SVM is done by fitting a linear plane to the latent space but only considering a subset of inputs in the fitting process. The quantity R^2 measures what percentage of variation was explained by the model in the training set. The quantity Q^2 shows the same measurement but for the test data set.

```
[13]: data = adapml_data.DataImport(path_to_data)
svm = adapml_classification.Classification(data.data, response1D, 'svm', .75,␣
 ↪kfolds=3)

adapml_classification.print_model_stats(svm, "SVM")
```

```
SVM Validated Parameters:  {'kernel': 'linear', 'shrinking': True}
SVM: R^2=1.0 Q^2=1.0
```

4.3 Random Forest

Random forests is an ensemble classification method. It works by constructing multiple decision trees based on the training data and then choosing the class, chosen by the most number of decision trees. The quantity R^2 measures what percentage of variation was explained by the model in the training set. The quantity Q^2 shows the same measurement but for the test data set.

[14]:
```python
data = adapml_data.DataImport(path_to_data)
rnf = adapml_classification.Classification(data.data, response1D,␣
 ↪'randomforest', .75, kfolds=3)

adapml_classification.print_model_stats(rnf, "RF")
```

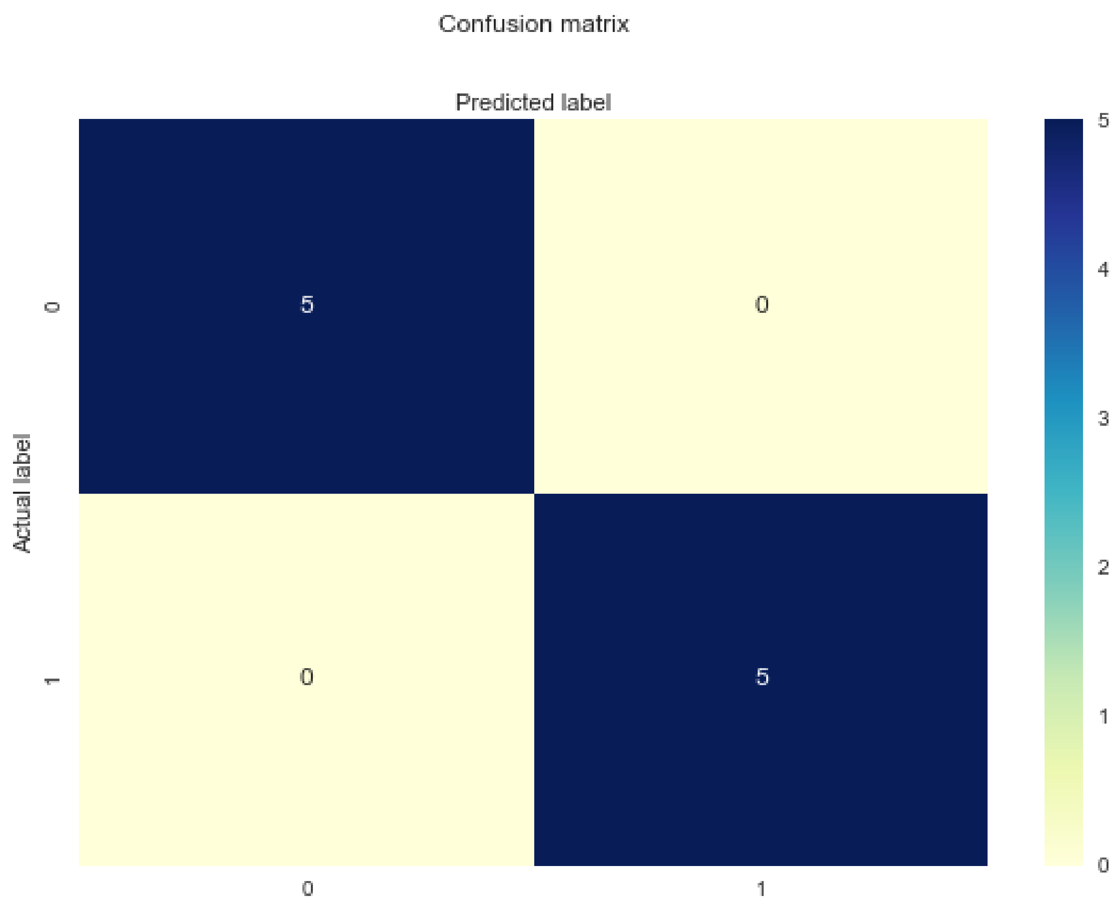
```
Random Forest Validated Parameters:  {'criterion': 'gini', 'n_estimators': 10}
RF: R^2=1.0 Q^2=1.0
```

4.4 Logistic Regression

Logistic regression uses a logistic function to model a binary dependent variable. The confusion matrix displays the accuracy of the model for the test data set. We use the packages sklearn for the logistic regression and seaborn for the confusion matrix.

[15]:
```python
data = adapml_data.DataImport(path_to_data)

logistic = adapml_classification.Classification(data.data, response1D,␣
 ↪'logistic', .25)
print(logistic)
```

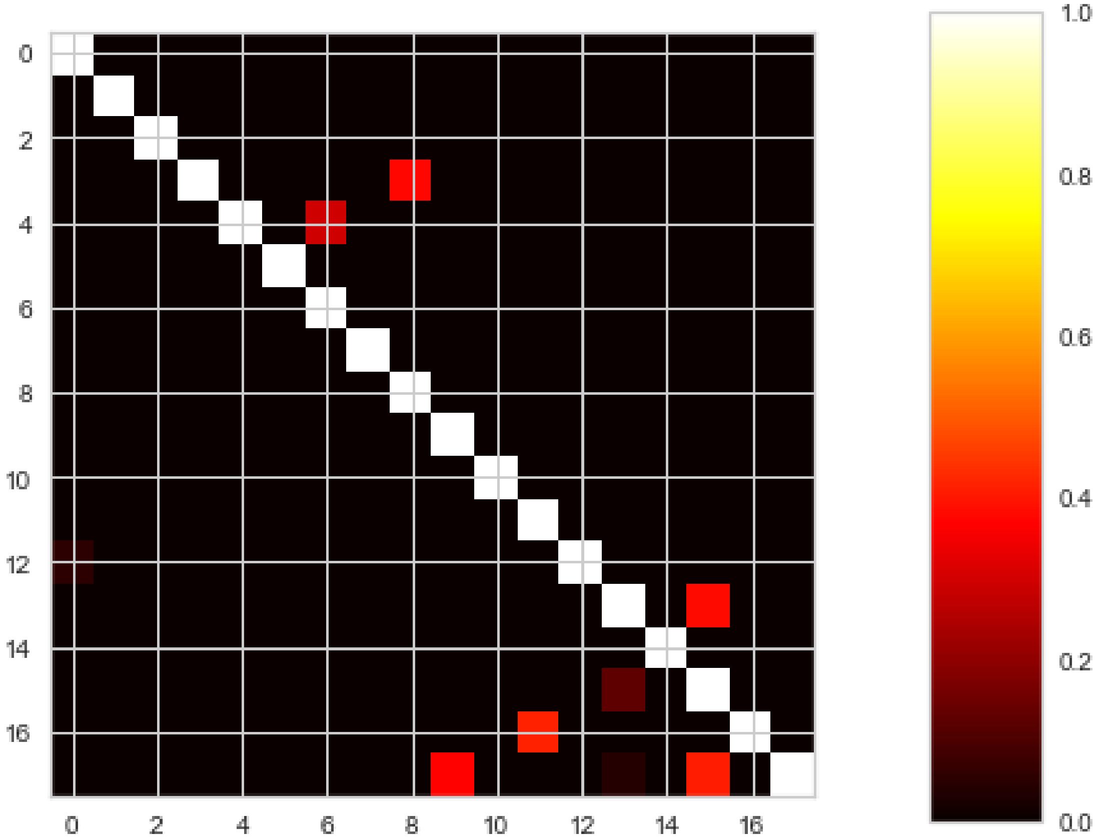
```
Accuracy: 1.0
<modules.adapml_classification.Classification object at 0x7fdc98db48b0>
```



5 Regression

5.1 Linear Regression

[16]:
```
reg = adapml_regression.Regression(data.data, "linear")
reg.linear
```


0
2
4
6
8
10
12
14
16
1.0
0.8
0.6
0.4
0.2
0.0