report_executed

July 14, 2021

1 Statistics

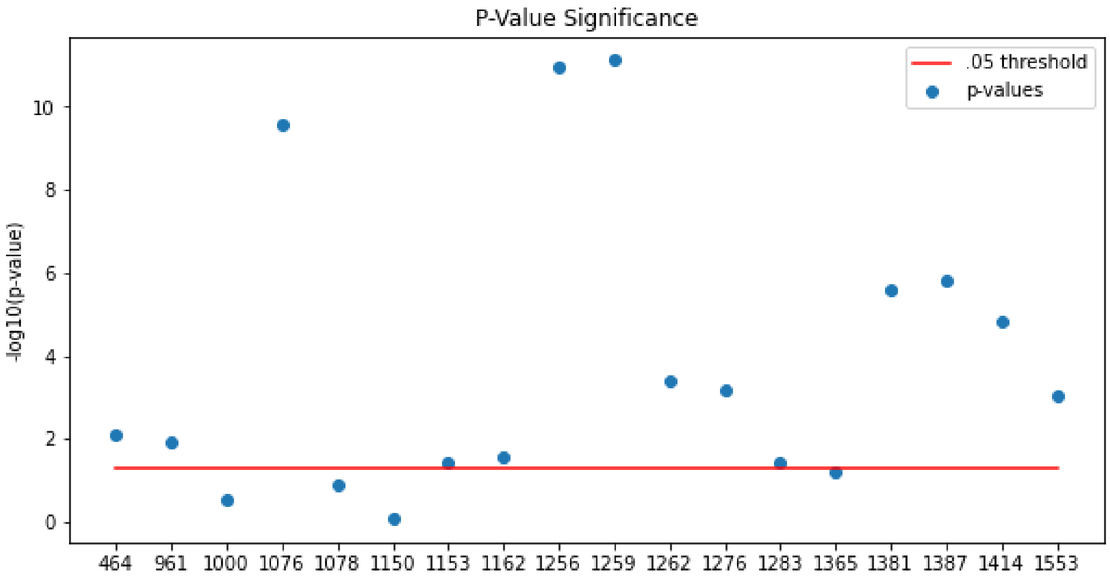
T-test

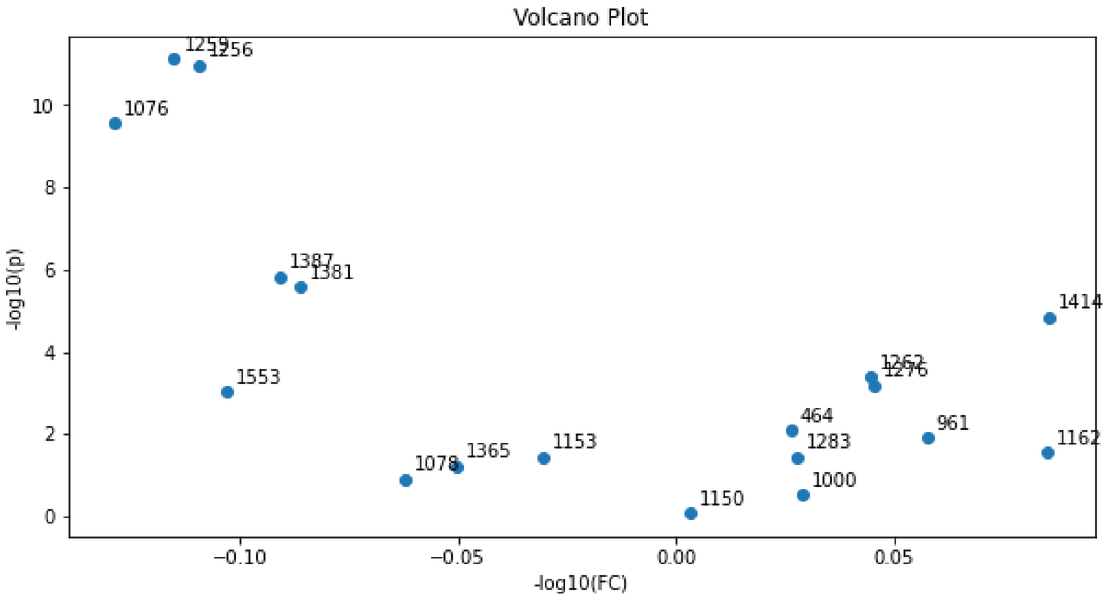
[1]:

```python
from platform import python_version

print(python_version())

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)
t_test.plot_volcano_t(variables)
```

```
3.8.8
```



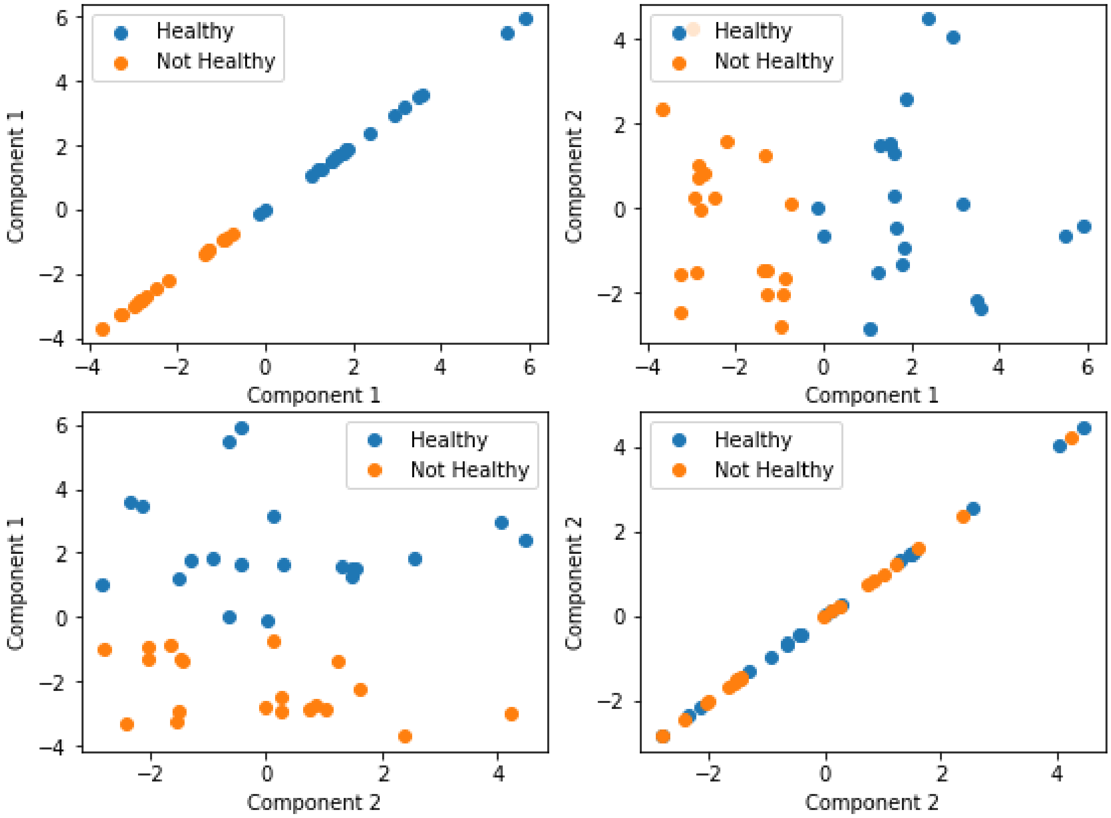


2 Dimension-Reduction

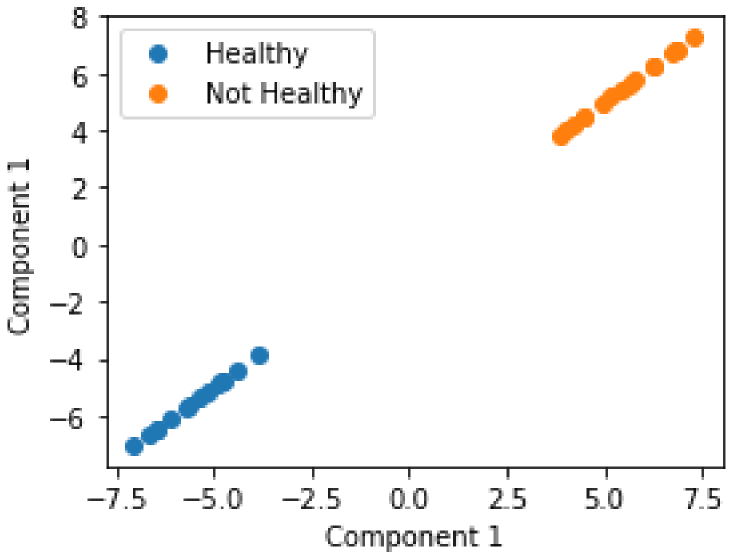
PCA, LDA

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

     pca = adapml_chemometrics.Chemometrics(data.data, "pca", response1D)
     lda = adapml_chemometrics.Chemometrics(data.data, "lda", response1D) # Also␣
      ↪Predicts

     print("PCA Projections");pca.plotProjectionScatterMultiClass(2,␣
      ↪labels=["Healthy", "Not Healthy"])
     print("LDA Projections");lda.plotProjectionScatterMultiClass(1,␣
      ↪labels=["Healthy", "Not Healthy"])

     print("PCA Vectors"); pca.plotVectorLoadings(variables, 1)
     print("LDA Vectors"); lda.plotVectorLoadings(variables, 1)
```

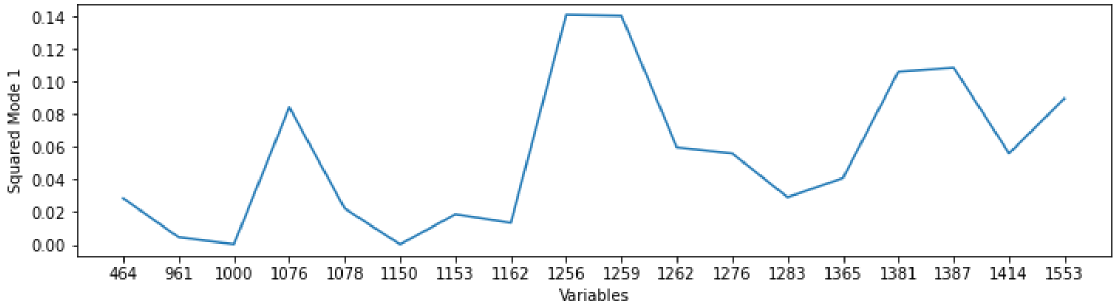
```
PCA Projections
Projections of data into latent space.
Data is colored by response
```



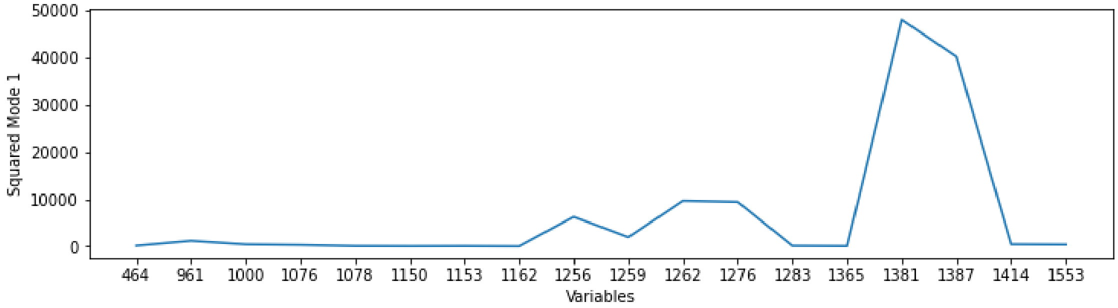
```
LDA Projections
Projections of data into latent space.
Data is colored by response
```



```
PCA Vectors
Plotting the squared loadings of the latent space transformation vectors
A Larger magnitude indicates larger importance for corresponding feature
```



```
LDA Vectors
Plotting the squared loadings of the latent space transformation vectors
A Larger magnitude indicates larger importance for corresponding feature
```



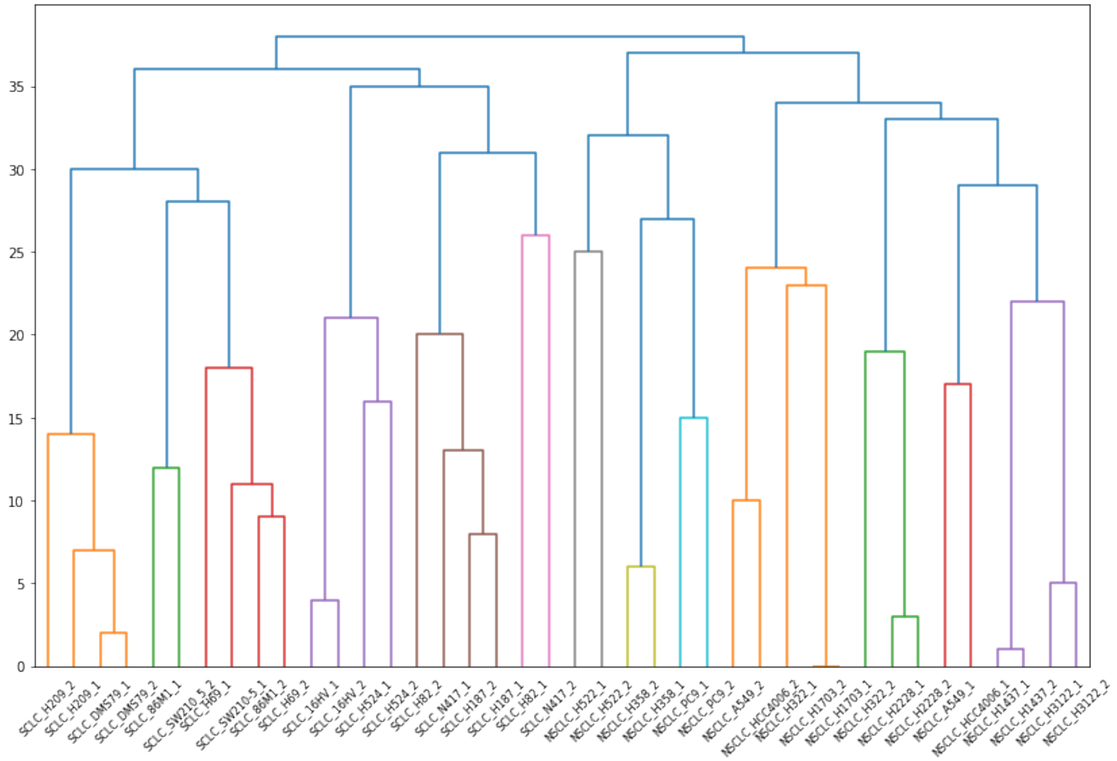
3 Clustering

K-means, hierarchical,

[3]:
```
kmeans_cluster = adapml_clustering.Clustering(data.data, 'kmeans', 3)
kmeans_cluster.getClusterResults(samples)

hierarchical_cluster = adapml_clustering.Clustering(data.data, 'hierarchical',␣
 ↪3)
hierarchical_cluster.getClusterResults(samples)
hierarchical_cluster.plot_dendrogram(samples)
```

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

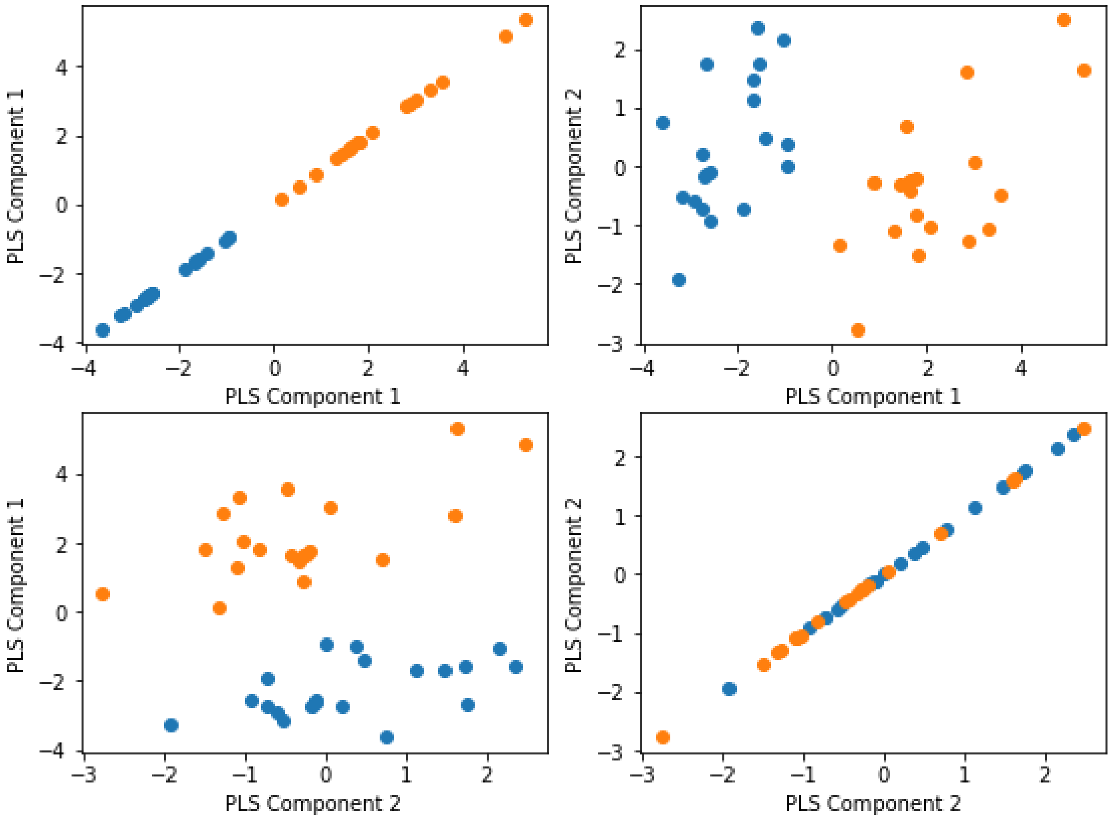
```
11     SCLC_H524_2    NSCLC_H3122_2           NaN
12      SCLC_H69_1  NSCLC_HCC4006_1           NaN
13      SCLC_H82_1  NSCLC_HCC4006_2           NaN
14      SCLC_H82_2              NaN           NaN
15      SCLC_H69_2              NaN           NaN
16     SCLC_N417_2              NaN           NaN
17     SCLC_N417_1              NaN           NaN
18  SCLC_SW210-5_1              NaN           NaN
19  SCLC_SW210_5_2              NaN           NaN
```



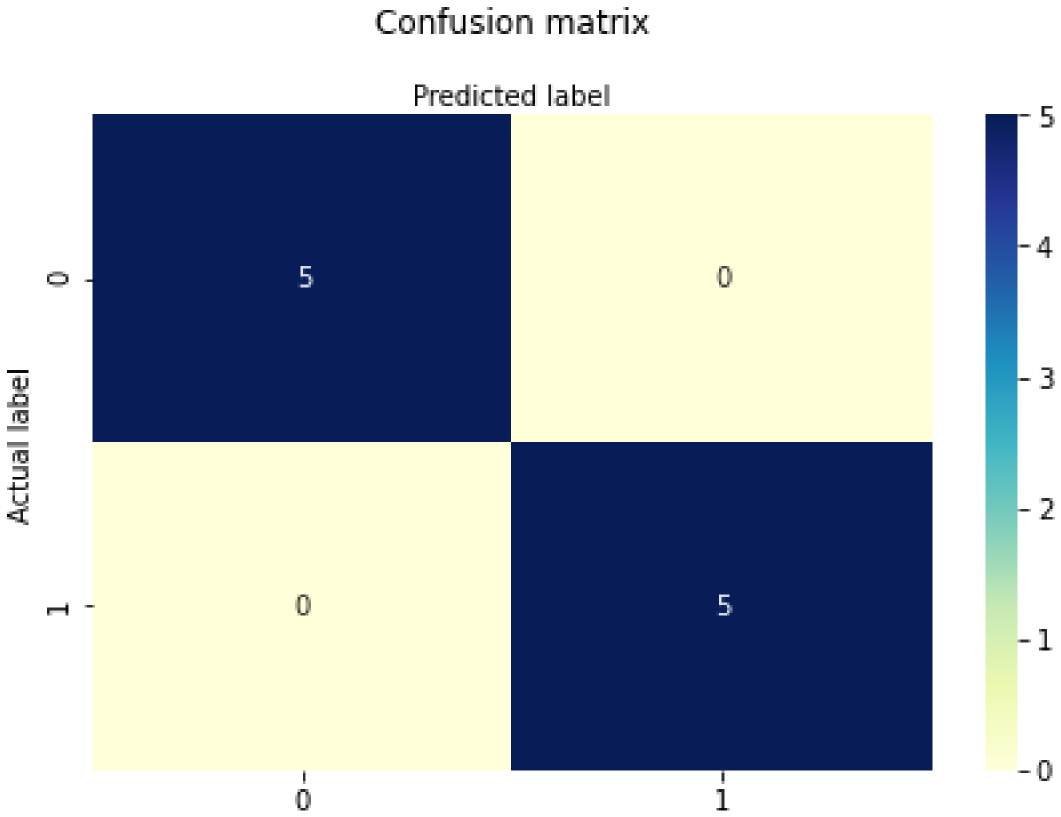
4 Classification

PLS-DA, SVM, random forests, logstic regression

[4]:
```
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)


data = adapml_data.DataImport(path_to_data)
svm = adapml_classification.Classification(data.data, response1D, 'svm', .75,␣
 ↪kfolds=3)
rnf = adapml_classification.Classification(data.data, response1D,␣
 ↪'randomforest', .75, kfolds=3)


adapml_classification.print_model_stats(svm, "SVM")
adapml_classification.print_model_stats(rnf, "RF")

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



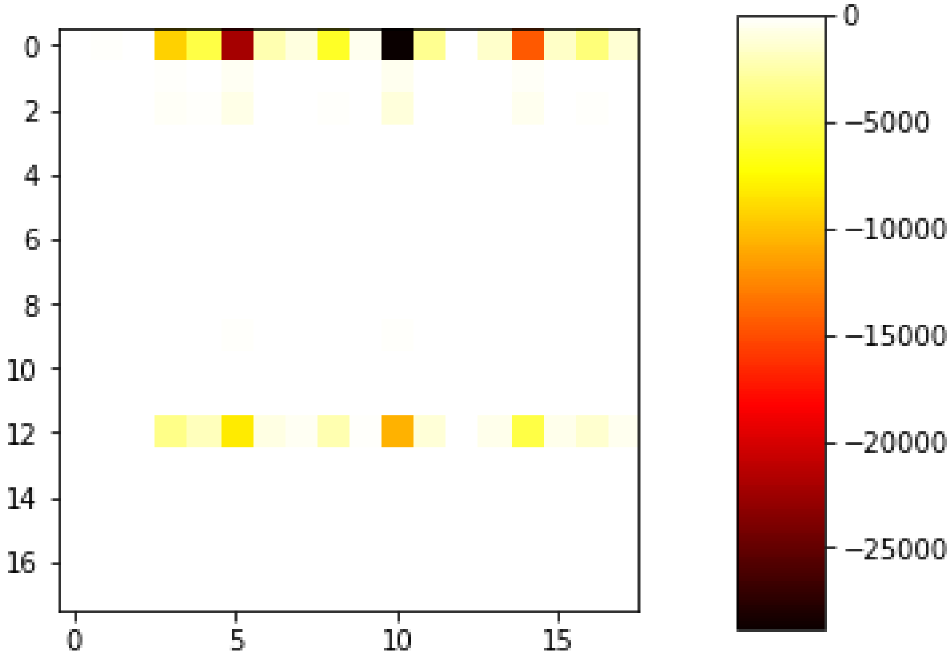
```
SVM Validated Parameters:  {'kernel': 'linear', 'shrinking': True}
Random Forest Validated Parameters:  {'criterion': 'gini', 'n_estimators': 50}
SVM: R^2=1.0 Q^2=1.0
RF: R^2=1.0 Q^2=1.0
Accuracy: 1.0
<modules.adapml_classification.Classification object at 0x7fb0a872f790>
```



5 Regression

Linear regression

[5]:
```
reg = adapml_regression.Regression(data.data, "linear")
reg.linear
```


0
2
4
6
8
10
12
14
16
0
5
10
15
0
−5000
−10000
−15000
−20000
−25000