report_executed

July 14, 2021

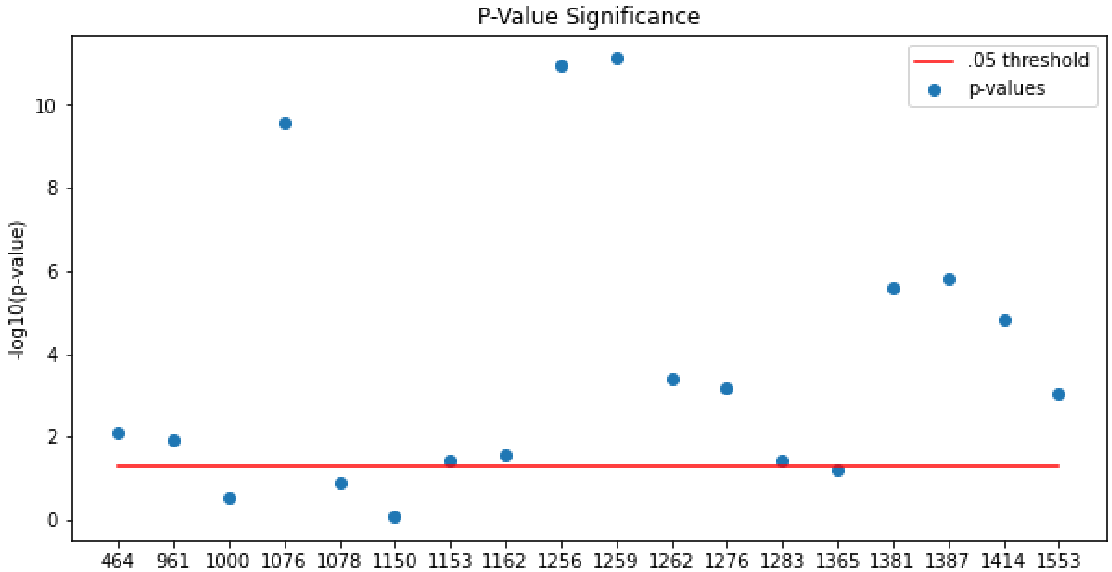
1 Statistics

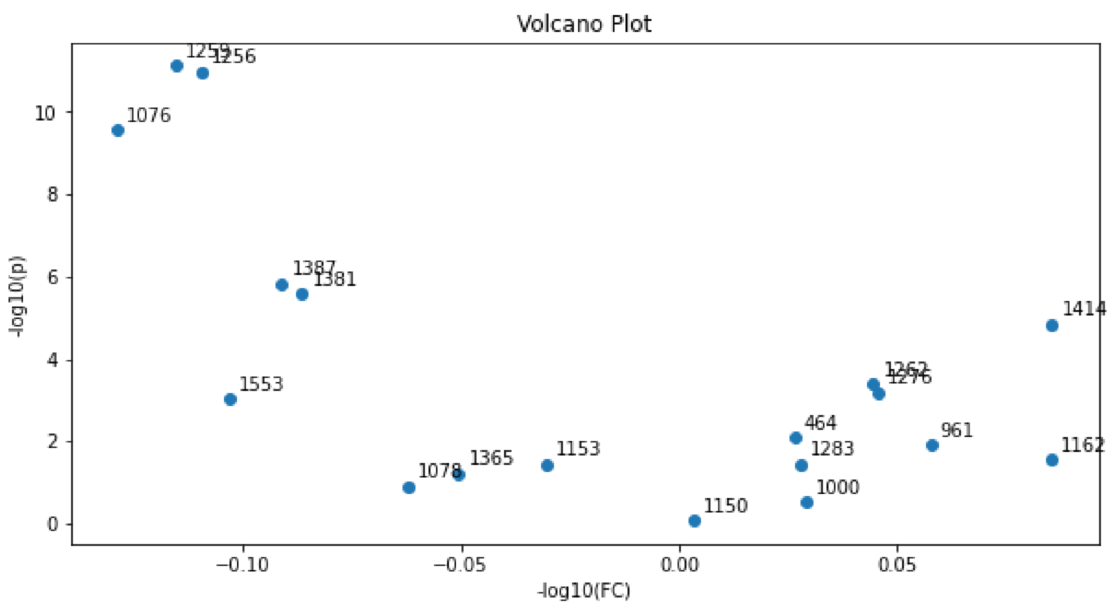
T-test

[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)
```

3.9.5





2 Dimension-Reduction

Dimension-reduction transformations are used to condense high dimensional data down to a smaller number of dimensions. We wish to leave only the dimensions which provide the most amount of information.

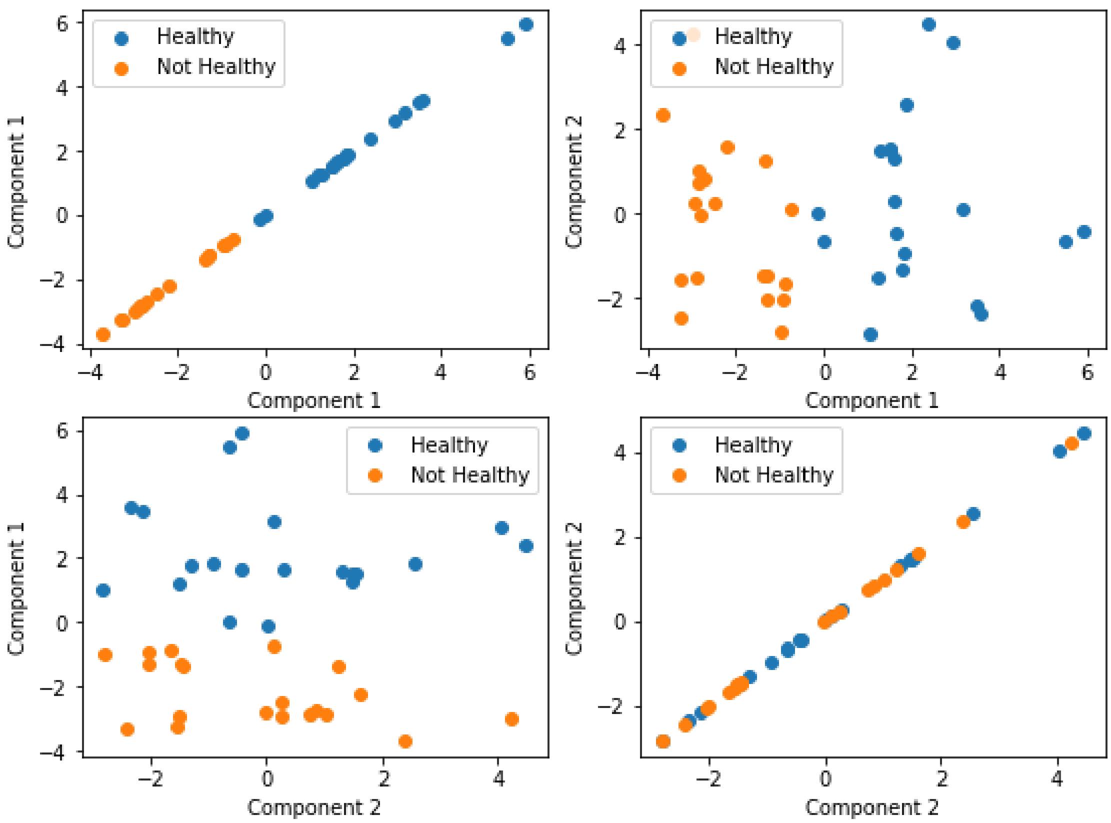
2.1 Principal Component Analysis

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. We use the Python library sklearn for both PCA.

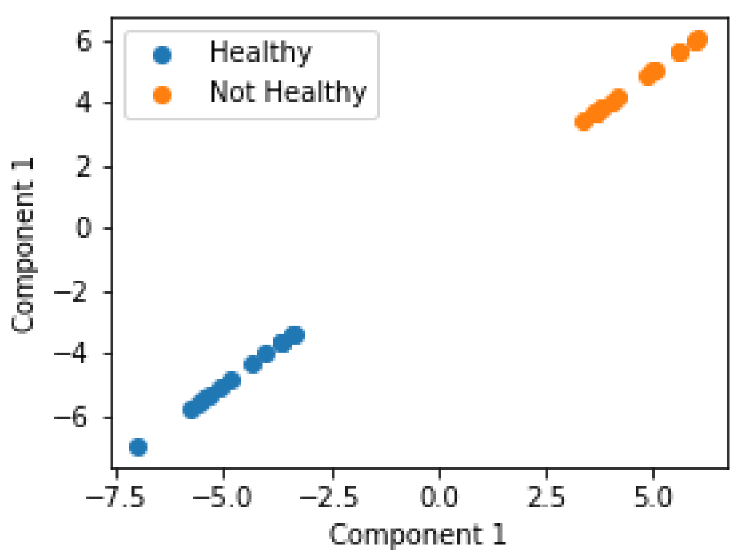
2.2 Linear Discriminant Analysis

[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)
```

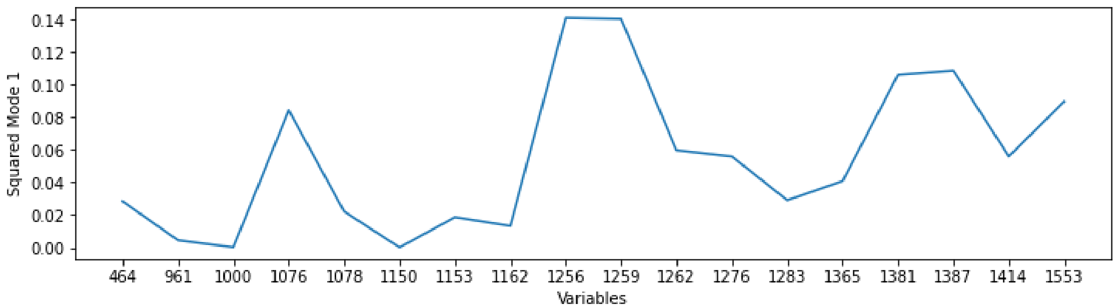
```
PCA Projections
Projections of data into latent space.
Data is colored by response
```



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



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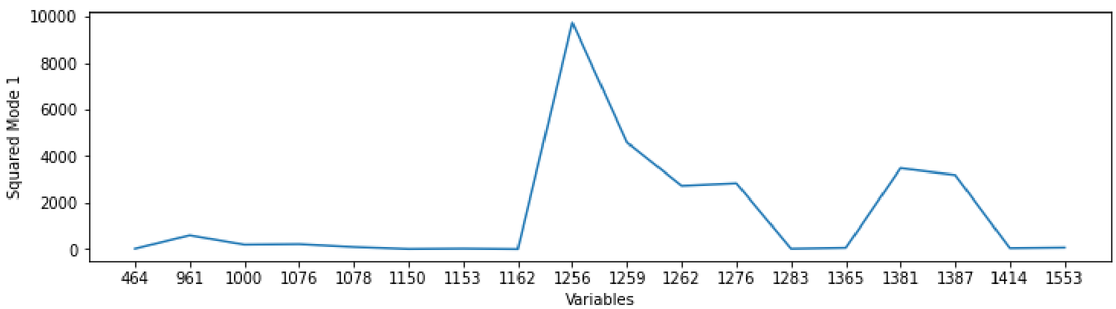


3 Clustering

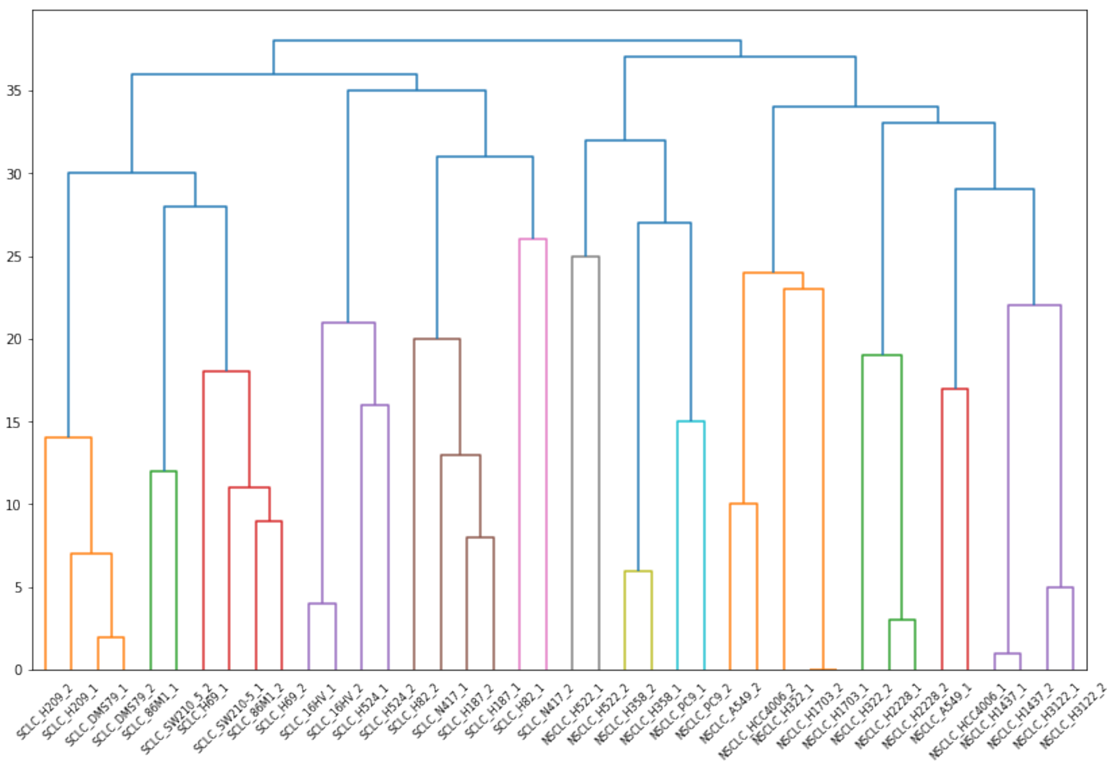
K-means, hierarchical,

[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	NSCLC_A549_1	NSCLC_H522_1	NSCLC_H1703_2

1	NSCLC_A549_2	SCLC_86M1_2	NSCLC_H1703_1
2	NSCLC_H1437_1	SCLC_86M1_1	NSCLC_H358_2
3	NSCLC_H2228_1	SCLC_16HV_1	NSCLC_H522_2
4	NSCLC_H2228_2	SCLC_16HV_2	NSCLC_H358_1
5	NSCLC_H1437_2	SCLC_DMS79_1	NSCLC_PC9_1
6	NSCLC_H3122_1	SCLC_DMS79_2	NSCLC_PC9_2
7	NSCLC_H322_2	SCLC_H187_2	NaN
8	NSCLC_H322_1	SCLC_H187_1	NaN
9	NSCLC_H3122_2	SCLC_H209_1	NaN
10	NSCLC_HCC4006_1	SCLC_H524_1	NaN
11	NSCLC_HCC4006_2	SCLC_H209_2	NaN
12	NaN	SCLC_H524_2	NaN
13	NaN	SCLC_H69_1	NaN
14	NaN	SCLC_H82_1	NaN
15	NaN	SCLC_H82_2	NaN
16	NaN	SCLC_H69_2	NaN
17	NaN	SCLC_N417_2	NaN
18	NaN	SCLC_N417_1	NaN
19	NaN	SCLC_SW210-5_1	NaN
20	NaN	SCLC_SW210_5_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

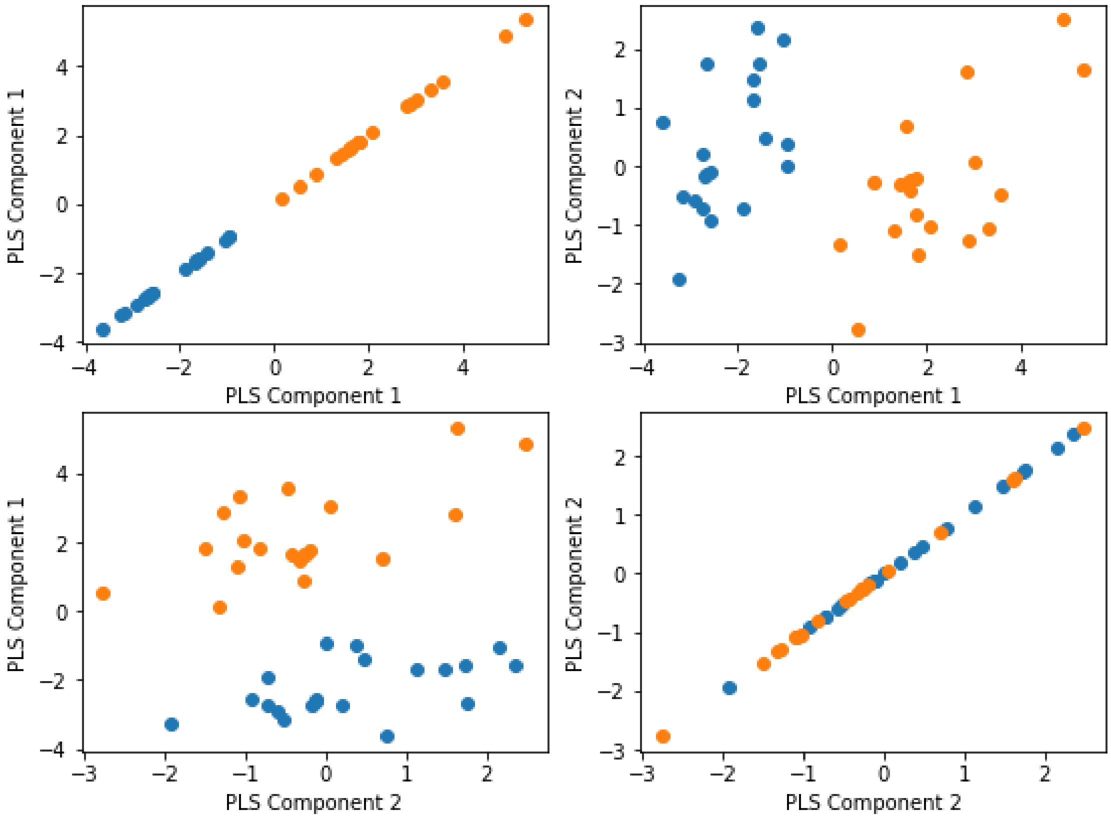


4 Classification

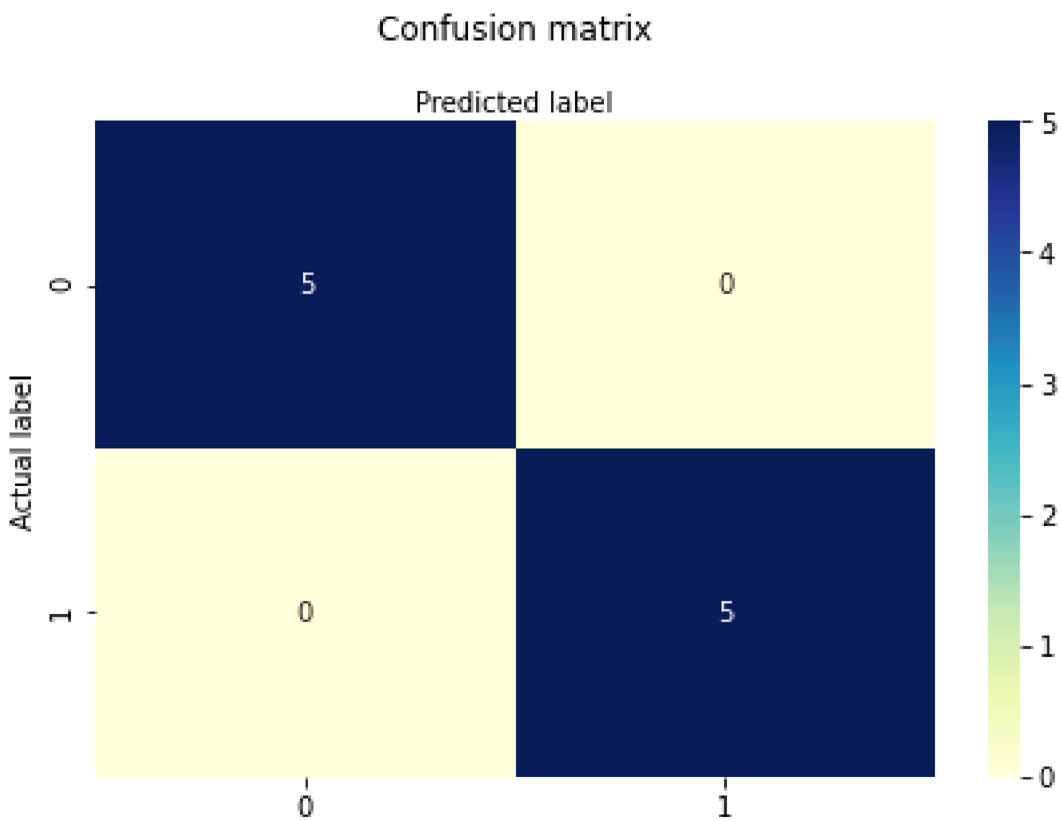
PLS-DA, SVM, random forests, logstic regression

[4]:
```python
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)
```



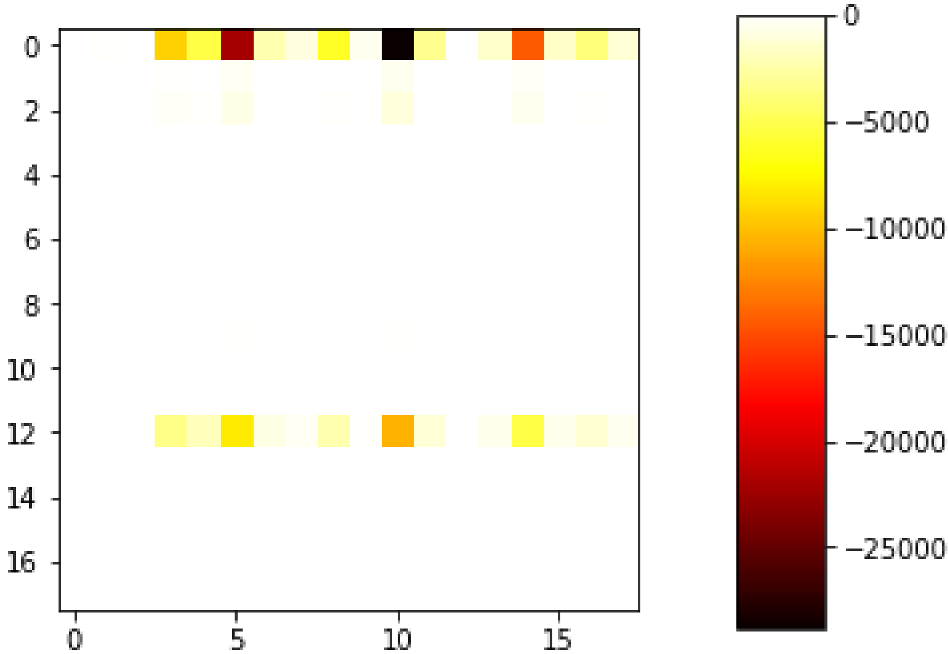

```
SVM Validated Parameters:  {'kernel': 'linear', 'shrinking': True}
Random Forest Validated Parameters:  {'criterion': 'gini', 'n_estimators': 10}
SVM: R^2=1.0 Q^2=1.0
RF: R^2=1.0 Q^2=0.55
Accuracy: 1.0
<modules.adapml_classification.Classification object at 0x122e00fd0>
```



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