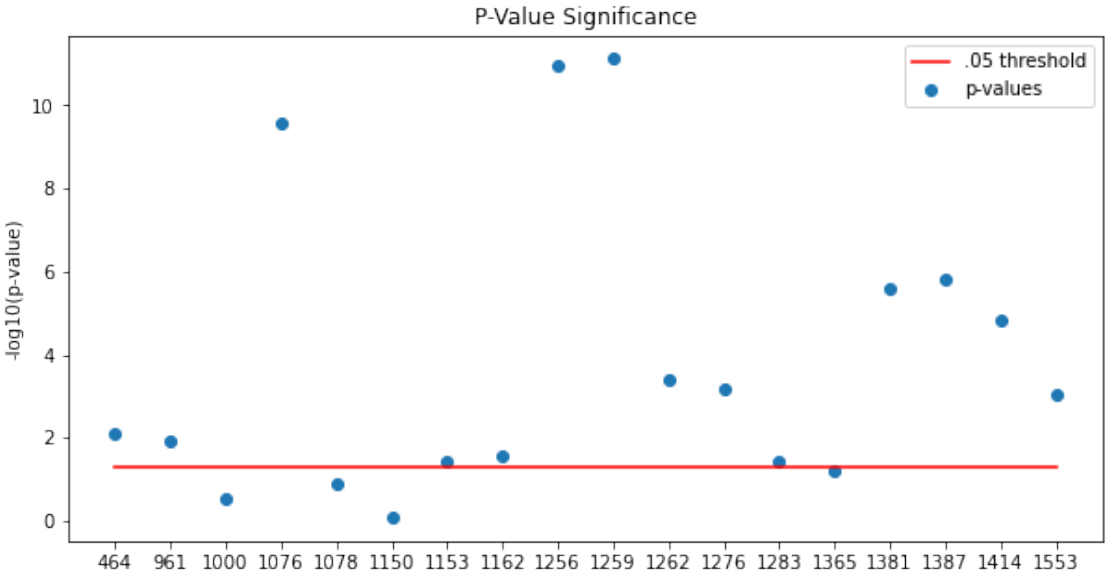
report_executed

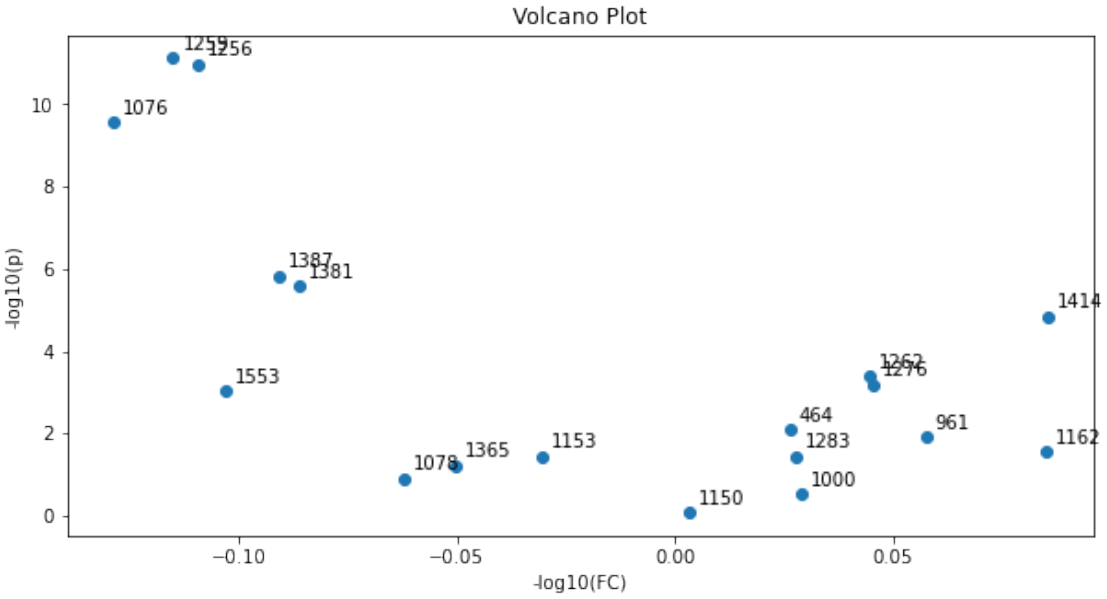
July 13, 2021

1 Statistics

T-test

[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)
t_test.plot_volcano_t(variables)
```





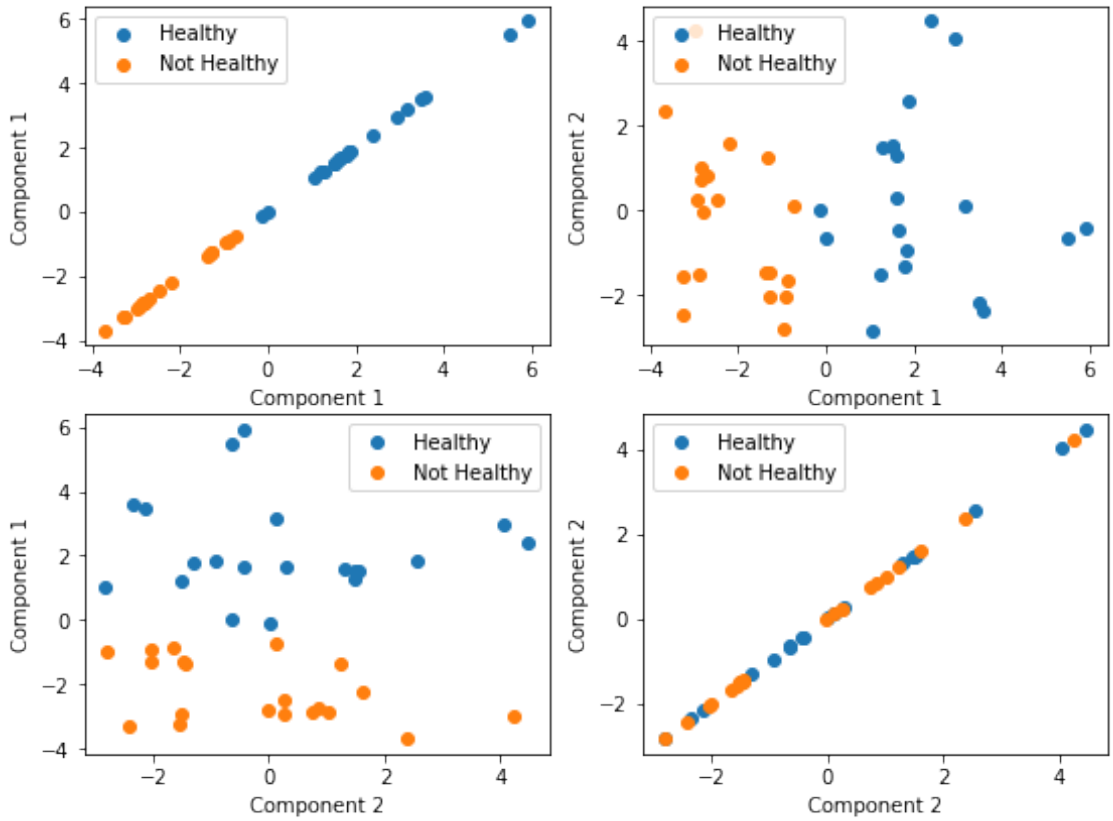
2 Dimension-Reduction

PCA, LDA

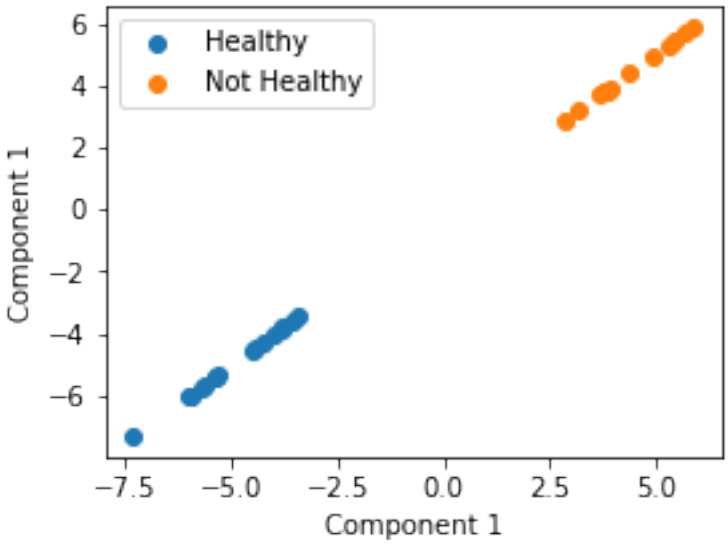
[2]:
```
data.normalizeData("autoscale")

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)
```

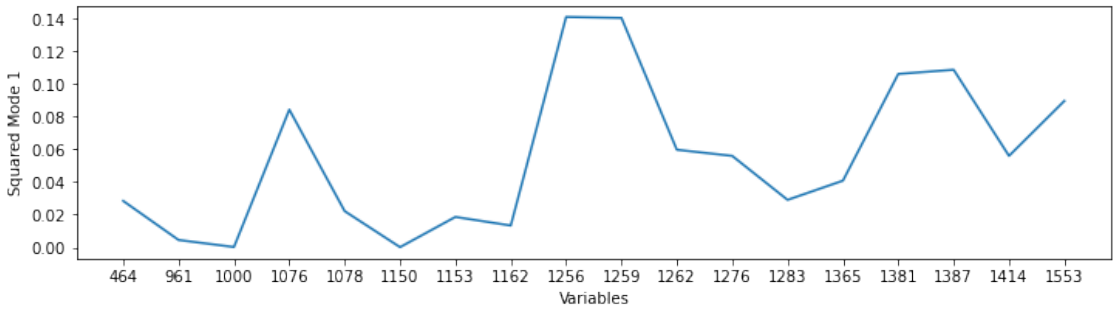
PCA Projections
Projections of data into latent space.
Data is colored by response



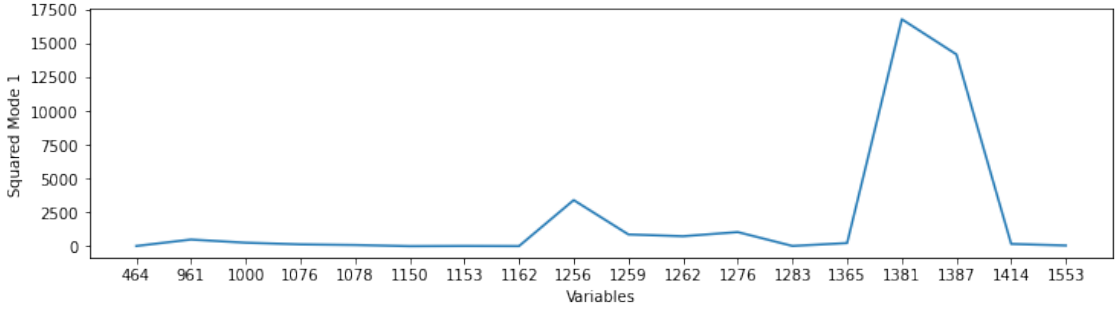
LDA Projections
Projections of data into latent space.
Data is colored by response



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

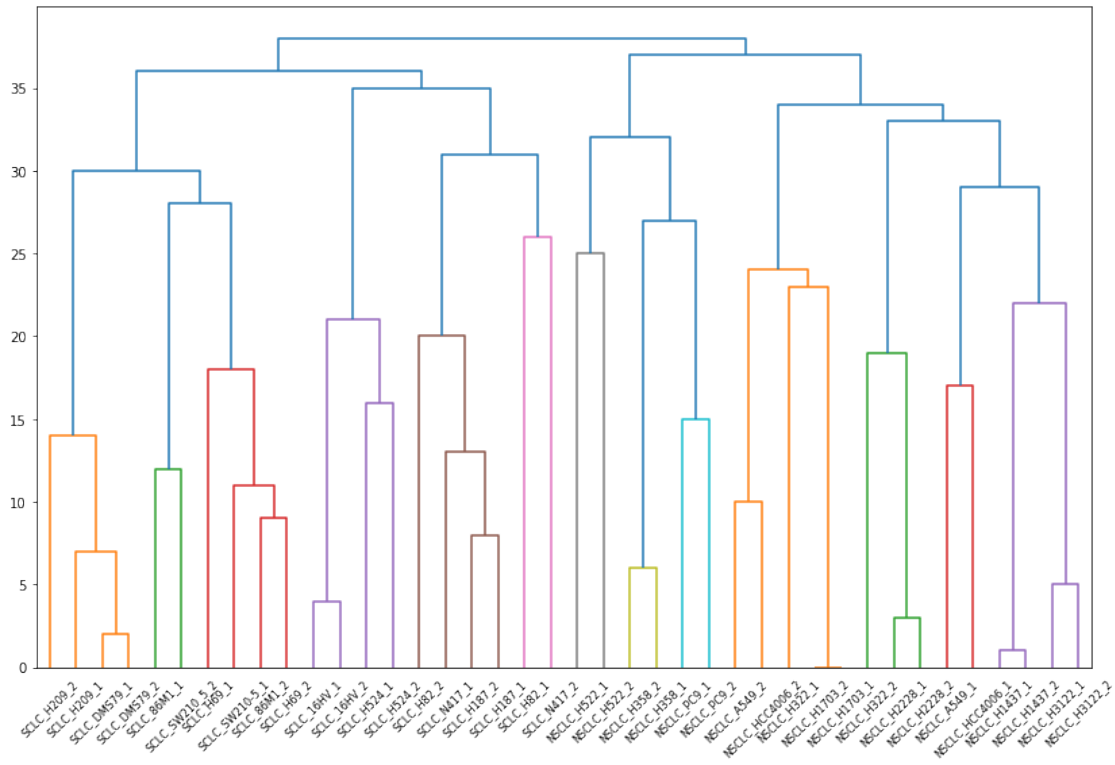
K-means, hierarchical,

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

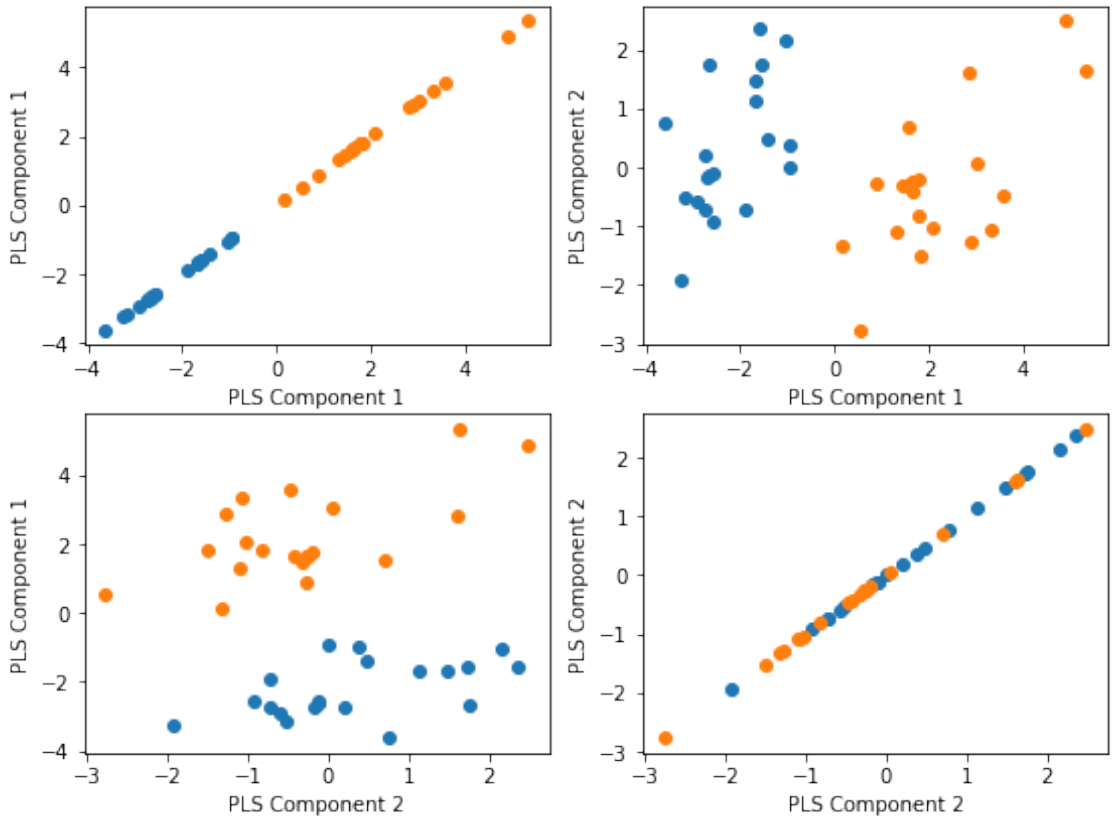


4 Classification

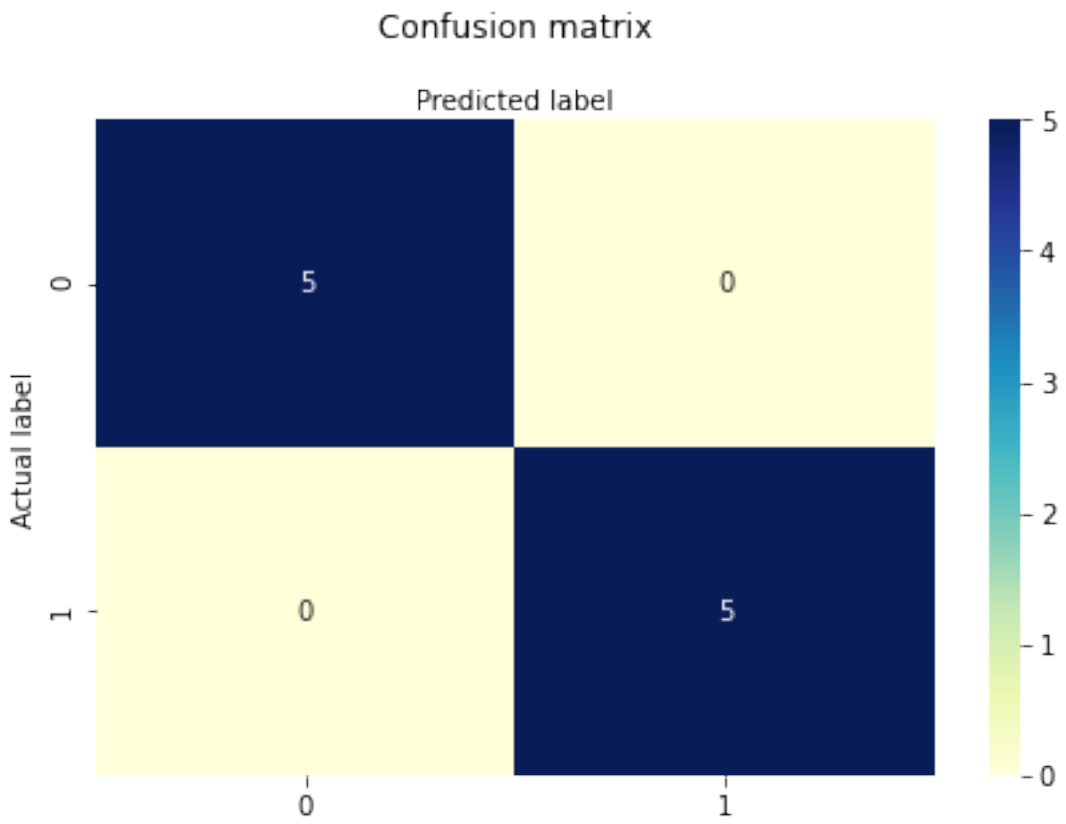
PLS-DA, SVM, random forests, logstic regression

[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)
```



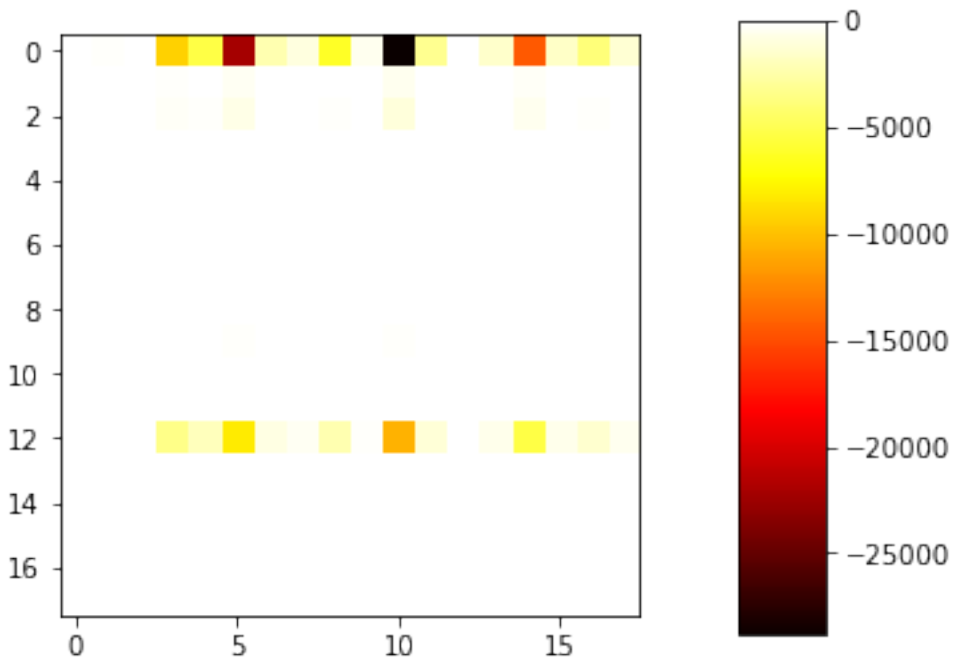

```
SVM Validated Parameters:  {'kernel': 'linear', 'shrinking': True}
Random Forest Validated Parameters:  {'criterion': 'gini', 'n_estimators': 10}
SVM: R^2=1.0 Q^2=1.0
RF: R^2=1.0 Q^2=1.0
Accuracy: 1.0
<modules.adapml_classification.Classification object at 0x7f97893fb4c0>
```



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