report_executed

August 16, 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.

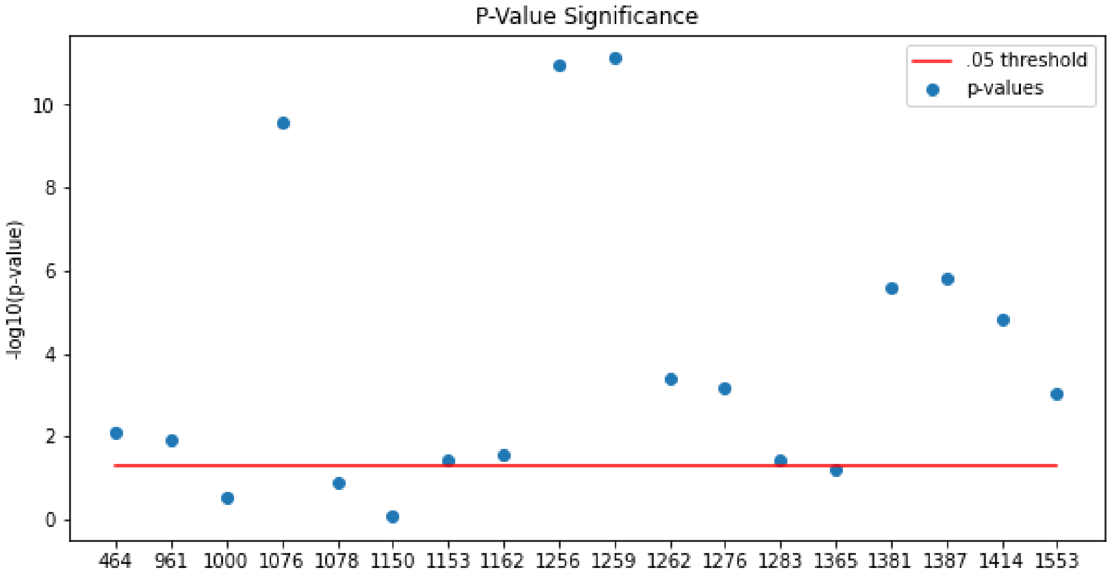
1.1 T-Test

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)
```

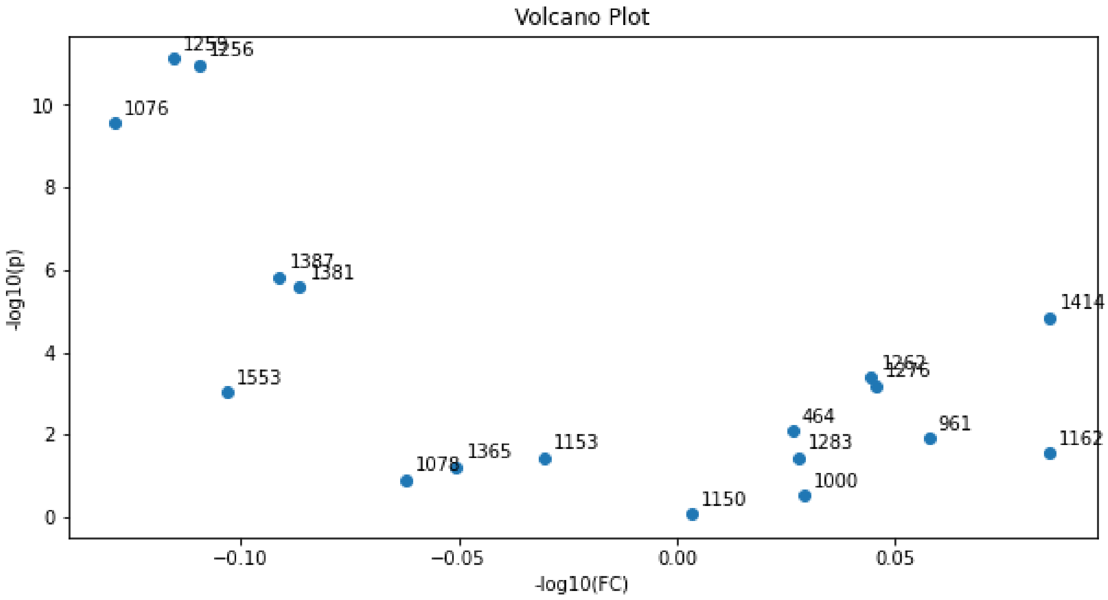


1.2 Volcano Plot

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.

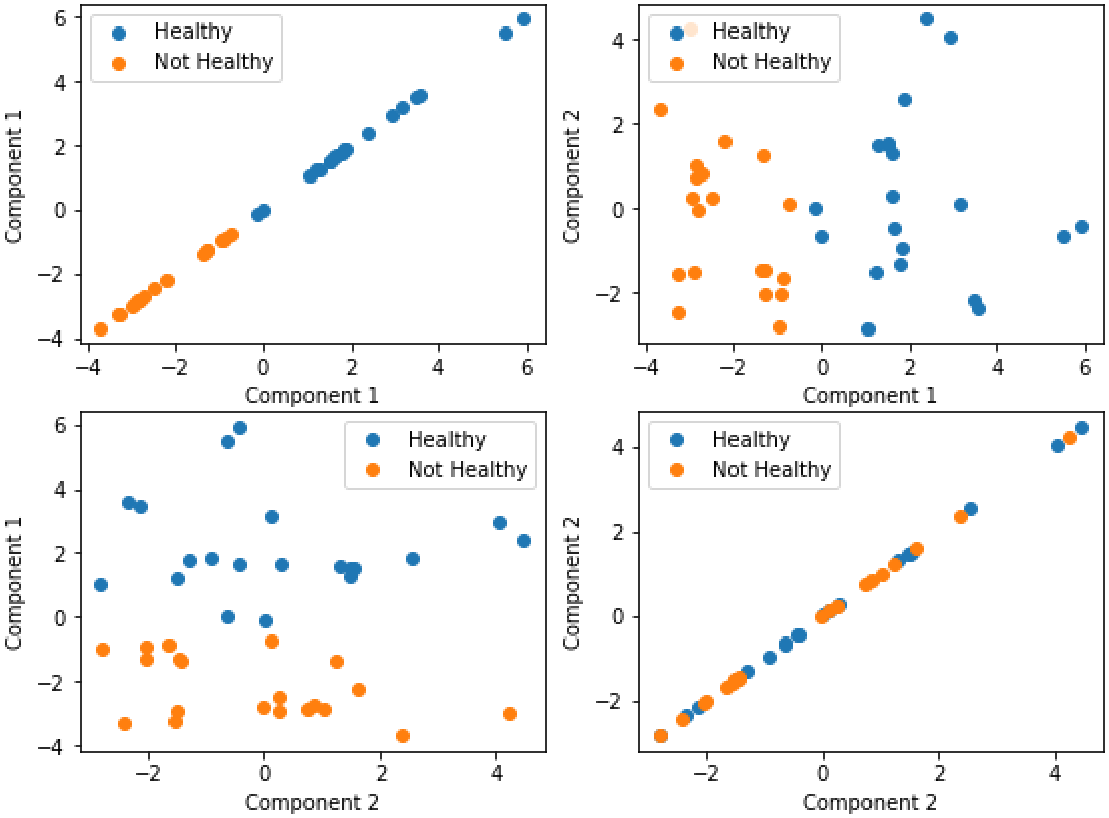
2.1 Principal Component Analysis

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
```

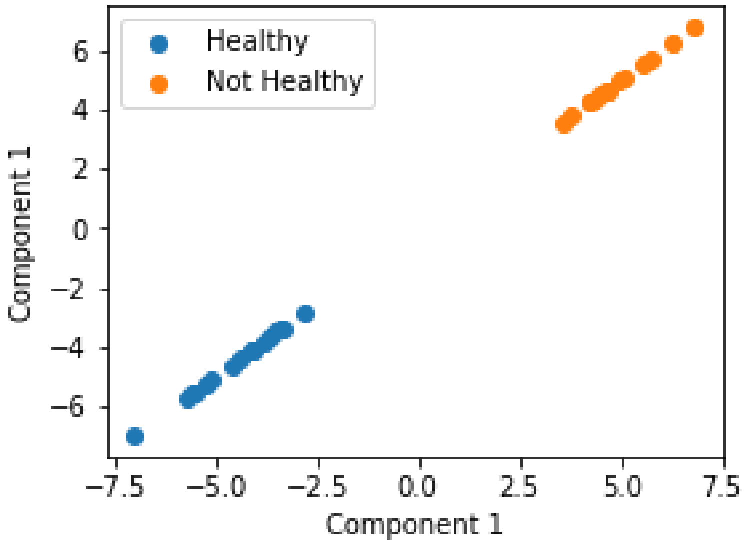


2.2 Linear Discriminant Analysis

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.

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.

[5]:

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

dbscan_cluster = adapml_clustering.Clustering(data.data, 'dbscan', 3)
dbscan_cluster.getClusterResults(samples)
```

```
        Cluster 1        Cluster 2     Cluster 3
0     NSCLC_H522_1     NSCLC_A549_1  NSCLC_H358_2
1      SCLC_86M1_2    NSCLC_H1703_2  NSCLC_H522_2
2      SCLC_86M1_1    NSCLC_H1703_1  NSCLC_H358_1
3      SCLC_16HV_1     NSCLC_A549_2   NSCLC_PC9_1
4      SCLC_16HV_2    NSCLC_H1437_1   NSCLC_PC9_2
5     SCLC_DMS79_1    NSCLC_H2228_1           NaN
```

```
6     SCLC_DMS79_2    NSCLC_H2228_2           NaN
7      SCLC_H187_2    NSCLC_H1437_2           NaN
8      SCLC_H187_1    NSCLC_H3122_1           NaN
9      SCLC_H209_1     NSCLC_H322_2           NaN
10     SCLC_H524_1     NSCLC_H322_1           NaN
11     SCLC_H209_2    NSCLC_H3122_2           NaN
12     SCLC_H524_2  NSCLC_HCC4006_1           NaN
13      SCLC_H69_1  NSCLC_HCC4006_2           NaN
14      SCLC_H82_1              NaN           NaN
15      SCLC_H82_2              NaN           NaN
16      SCLC_H69_2              NaN           NaN
17     SCLC_N417_2              NaN           NaN
18     SCLC_N417_1              NaN           NaN
19  SCLC_SW210-5_1              NaN           NaN
20  SCLC_SW210_5_2              NaN           NaN
Empty DataFrame
Columns: [Cluster 1, Cluster 2, Cluster 3]
Index: []
```

3.2 DBSCAN Clustering

```
[6]: dbscan_cluster = adapml_clustering.Clustering(data.data, 'dbscan', 3)
     dbscan_cluster.getClusterResults(samples)
```

```
Empty DataFrame
Columns: [Cluster 1, Cluster 2, Cluster 3]
Index: []
```

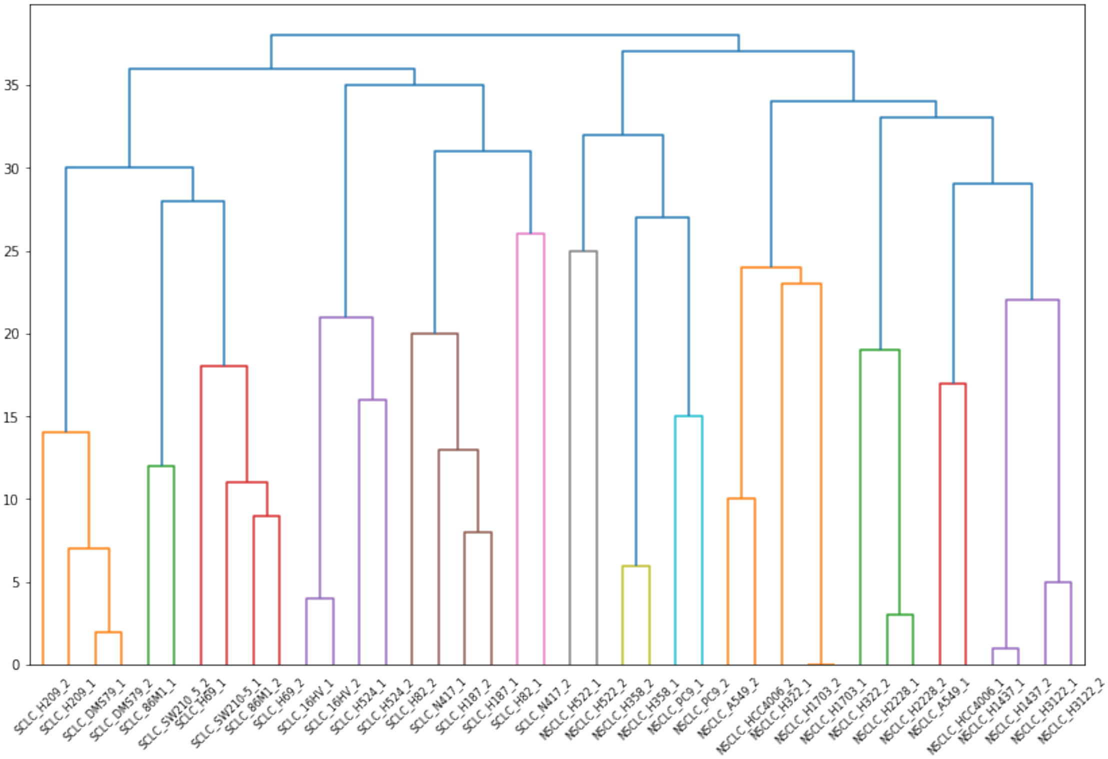
3.3 Hierarchical Clustering

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

```
[7]: 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  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
```



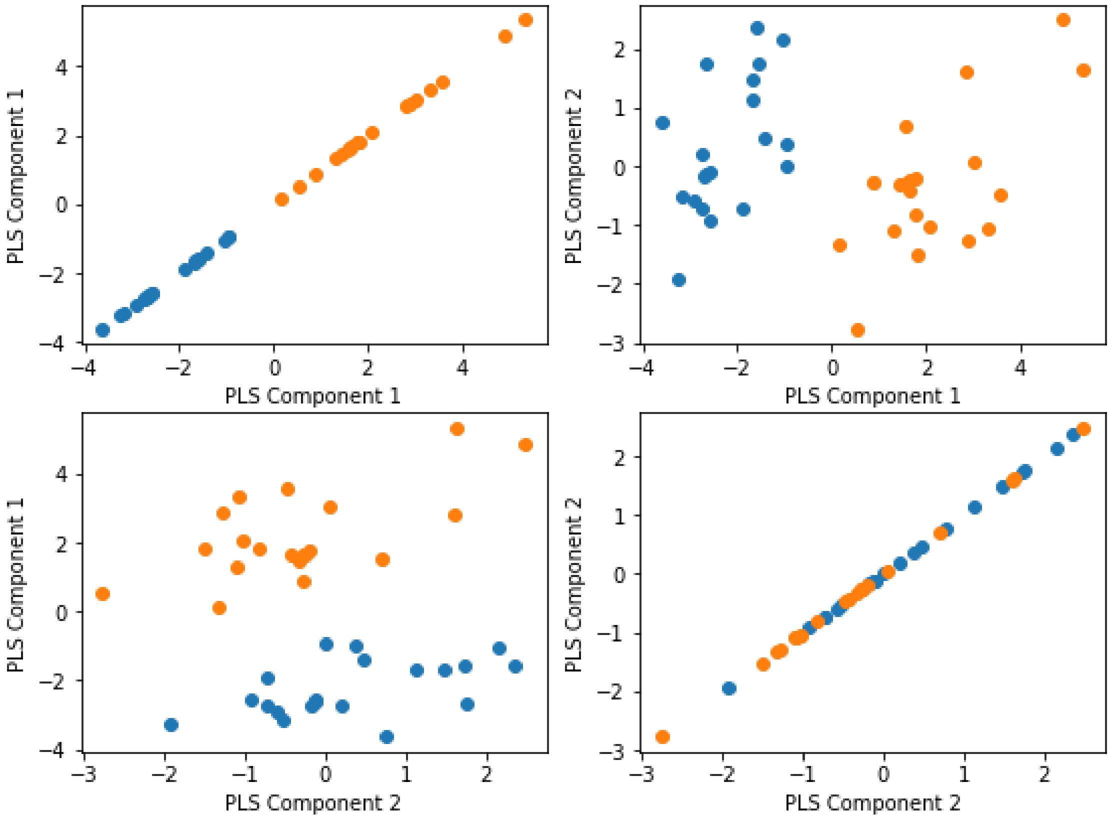
4 Classification

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

```
[8]: 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.

```
[9]: 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.

```
[10]: 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")
```

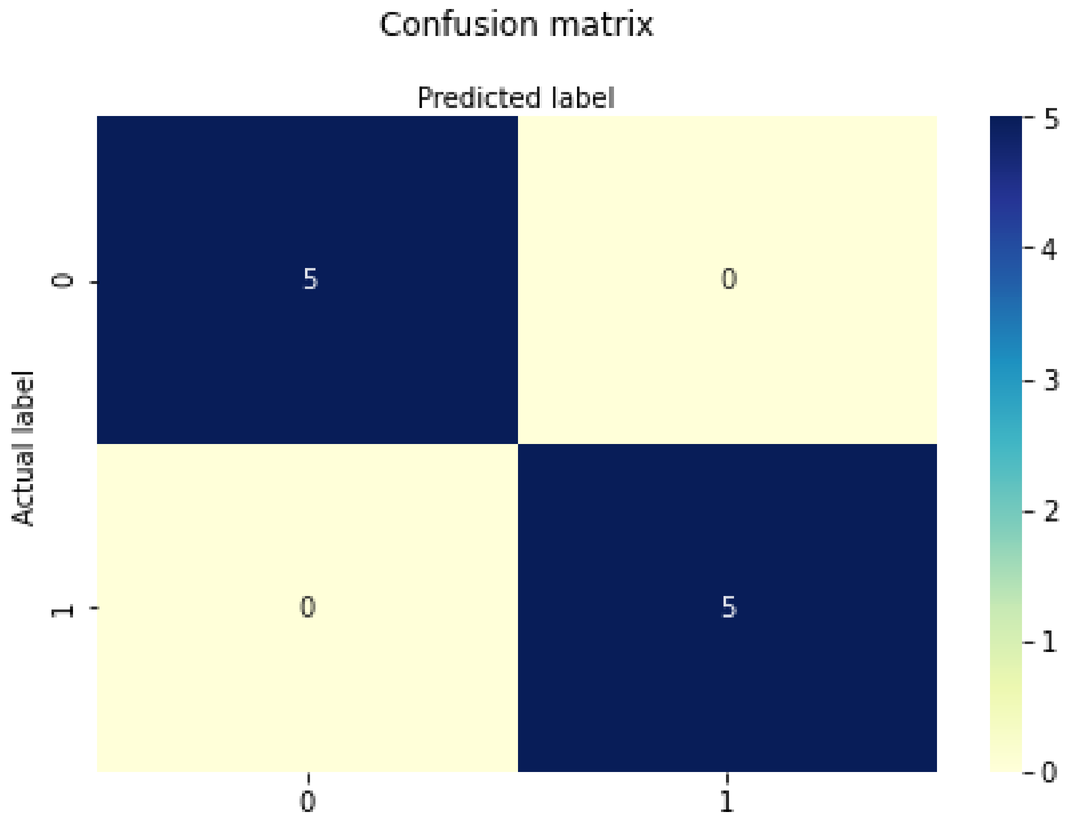
```
Random Forest Validated Parameters:  {'criterion': 'gini', 'n_estimators': 10}
RF: R^2=1.0 Q^2=1.0
```

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.

```
[11]: 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 0x7fac51706820>
```

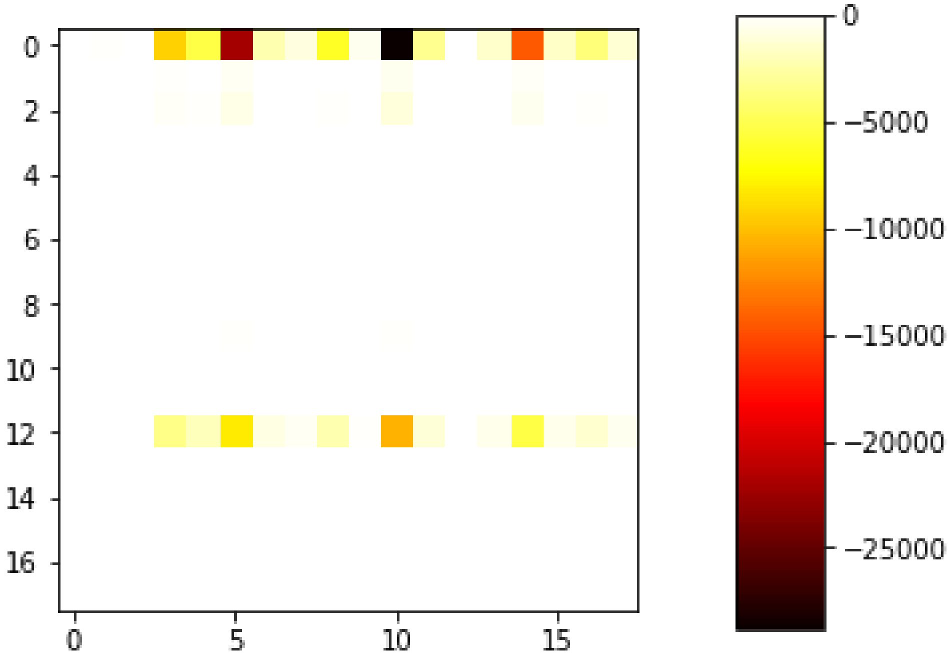


5 Regression

5.1 Linear Regression

[12]:

```
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