report_executed

July 22, 2021

1 Statistics

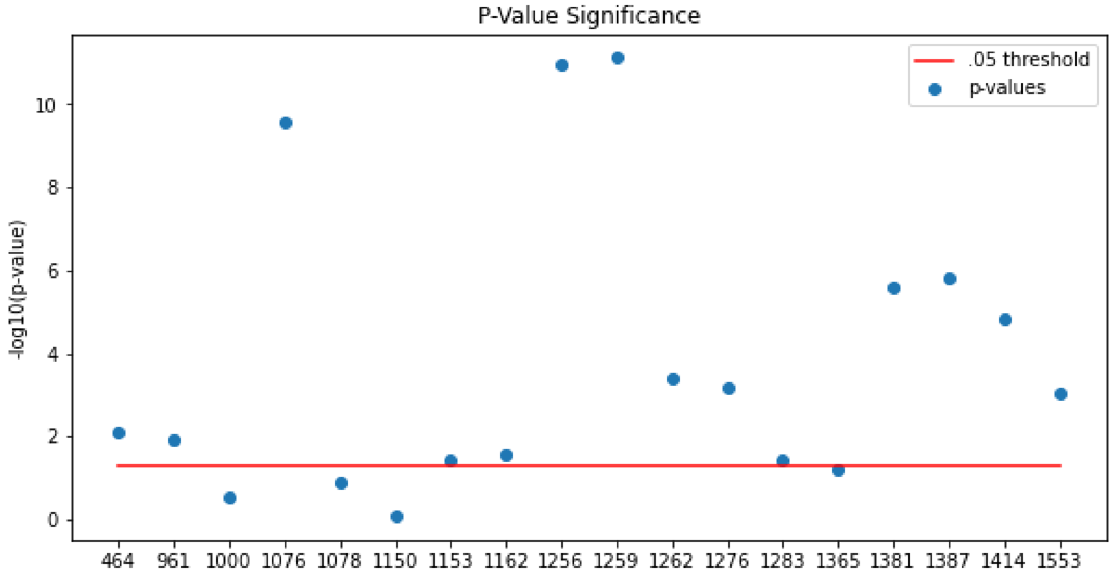
Describe the module blabla

1.1 T-Test

Explain the test labla

[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)
```

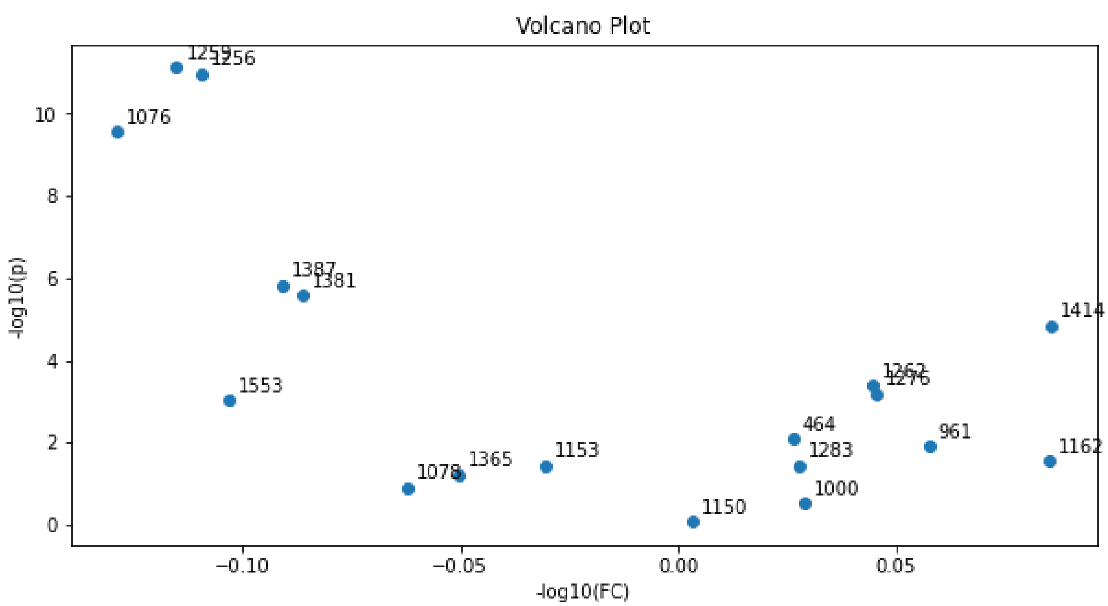
```
t_test.plot_logp_values(variables)
```



1.2 Volcano Plot

blabla

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



2 Dimension-Reduction

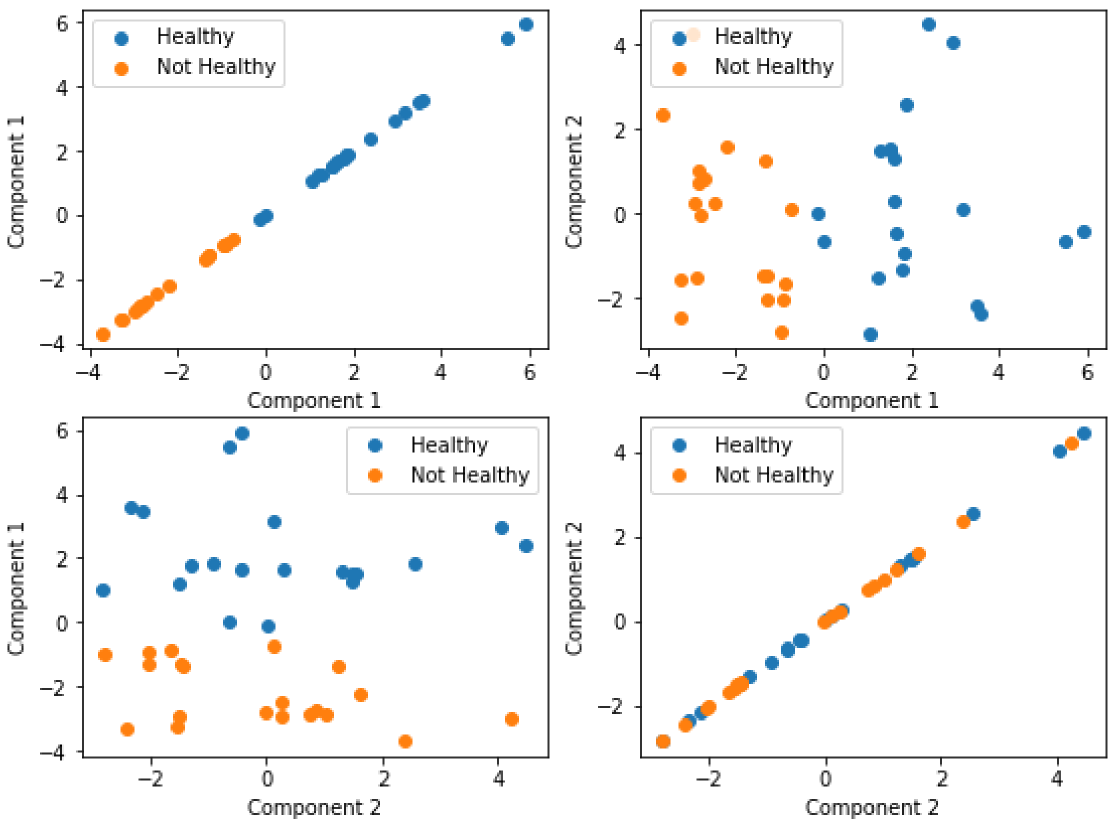
Dimension-reduction methods are used to condense high dimensional data down to dimensions which provide the most information. We have implemented the principal component analysis (PCA). It performs a change of basis and the new basis is chosen, such that the i-th principal component is orthogonal to 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
```

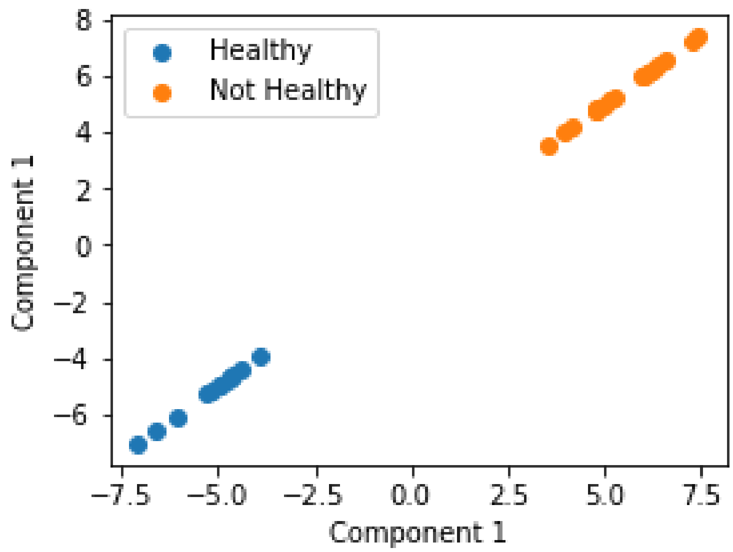


2.2 Linear Discriminant Analysis

bla

[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

3.1 K-Means Clustering

[5]:
```
kmeans_cluster = adapml_clustering.Clustering(data.data, 'kmeans', 3)
kmeans_cluster.getClusterResults(samples)
```

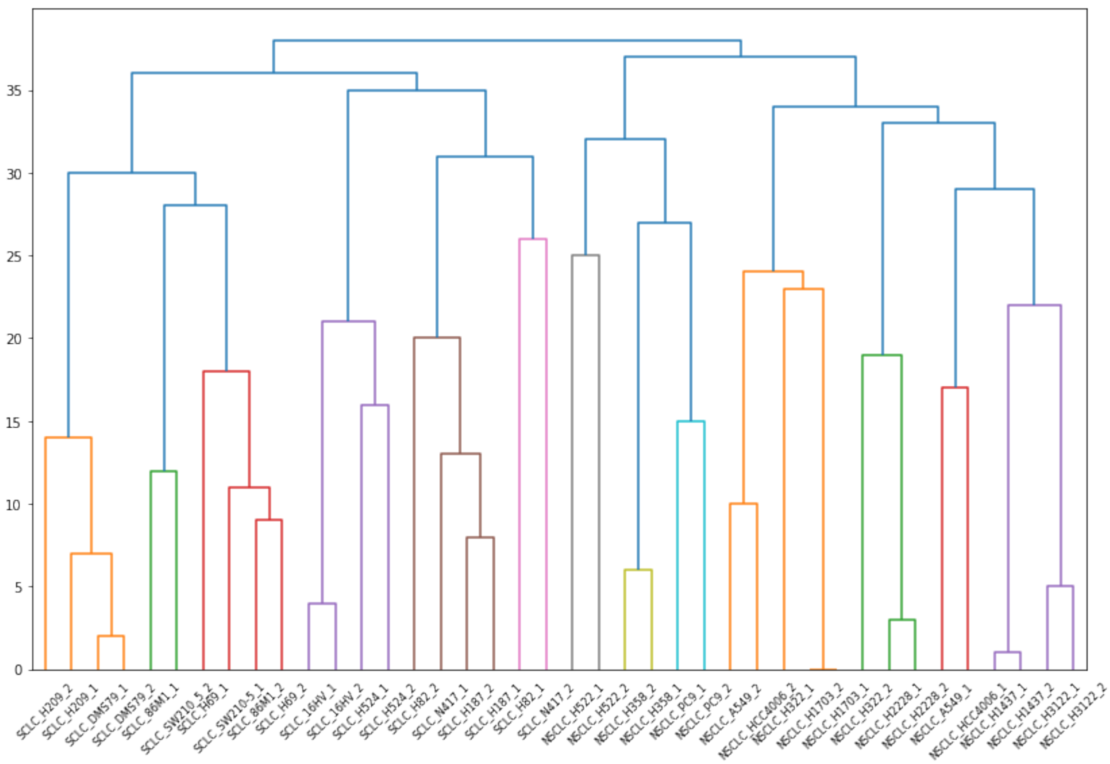
	Cluster 1	Cluster 2	Cluster 3
0	NSCLC_A549_1	NSCLC_H522_1	NSCLC_H1437_1
1	NSCLC_H1703_2	SCLC_86M1_2	NSCLC_H2228_1
2	NSCLC_H1703_1	SCLC_86M1_1	NSCLC_H2228_2
3	NSCLC_A549_2	SCLC_16HV_1	NSCLC_H1437_2
4	NSCLC_H322_1	SCLC_16HV_2	NSCLC_H3122_1
5	NSCLC_H358_2	SCLC_DMS79_1	NSCLC_H322_2
6	NSCLC_H522_2	SCLC_DMS79_2	NSCLC_H3122_2
7	NSCLC_H358_1	SCLC_H187_2	NSCLC_HCC4006_1
8	NSCLC_PC9_1	SCLC_H187_1	NaN
9	NSCLC_PC9_2	SCLC_H209_1	NaN
10	NSCLC_HCC4006_2	SCLC_H524_1	NaN
11	NaN	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
```

3.2 Hierarchical Clustering

[6]:
```
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
```

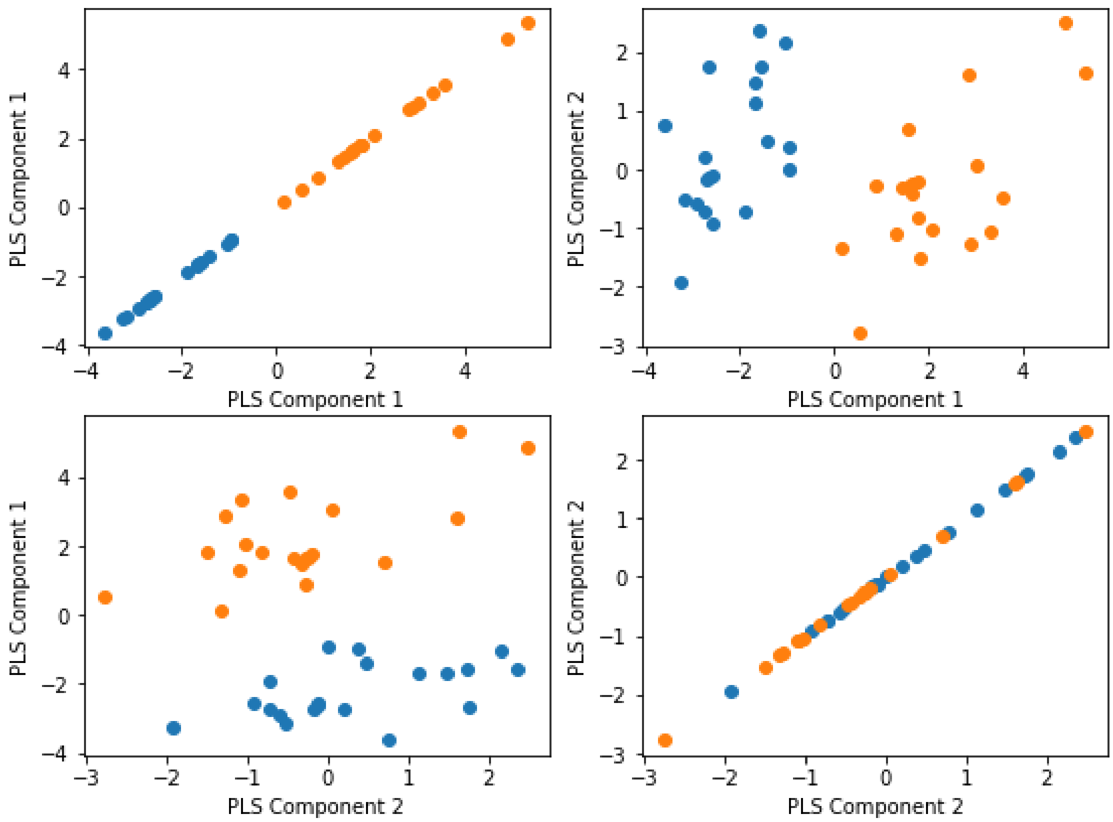


4 Classification

4.1 Partial Least Squares-Discriminant Analysis

[7]:
```
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

[8]:
```
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

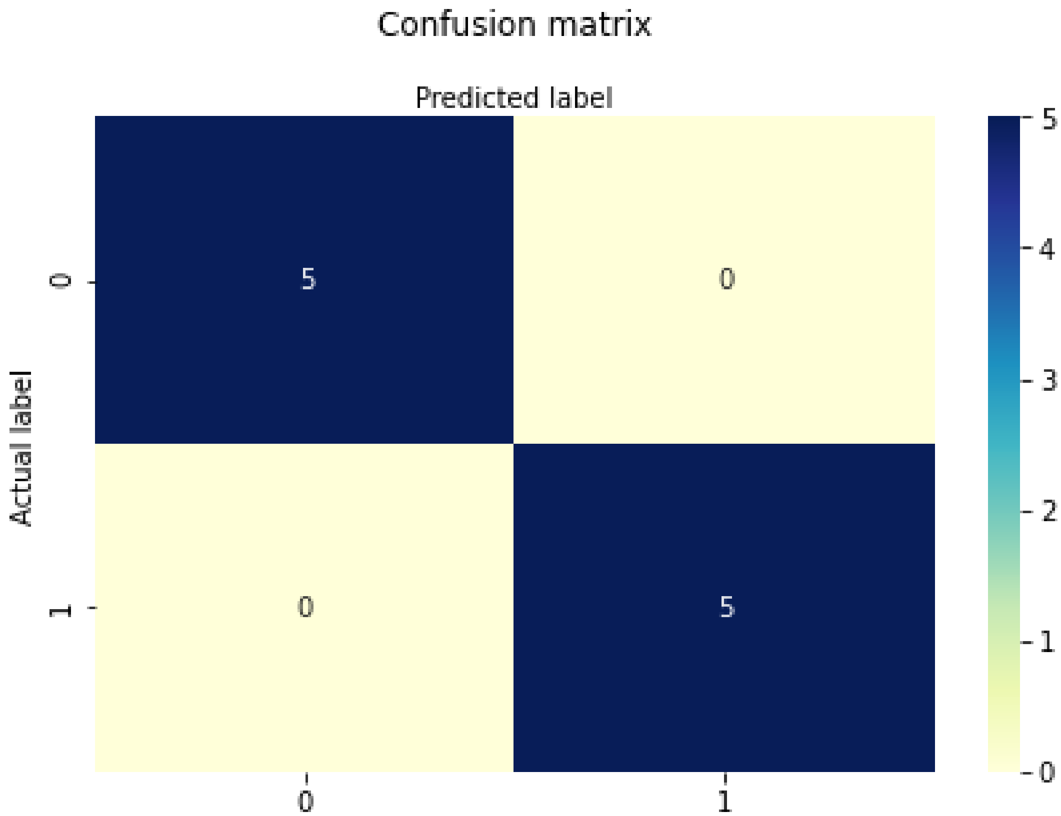
[9]:
```
data = adapml_data.DataImport(path_to_data)
rnf = adapml_classification.Classification(data.data, response1D,␣
 ↪'randomforest', .75, kfolds=3)

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

[10]:
```
data = adapml_data.DataImport(path_to_data)

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

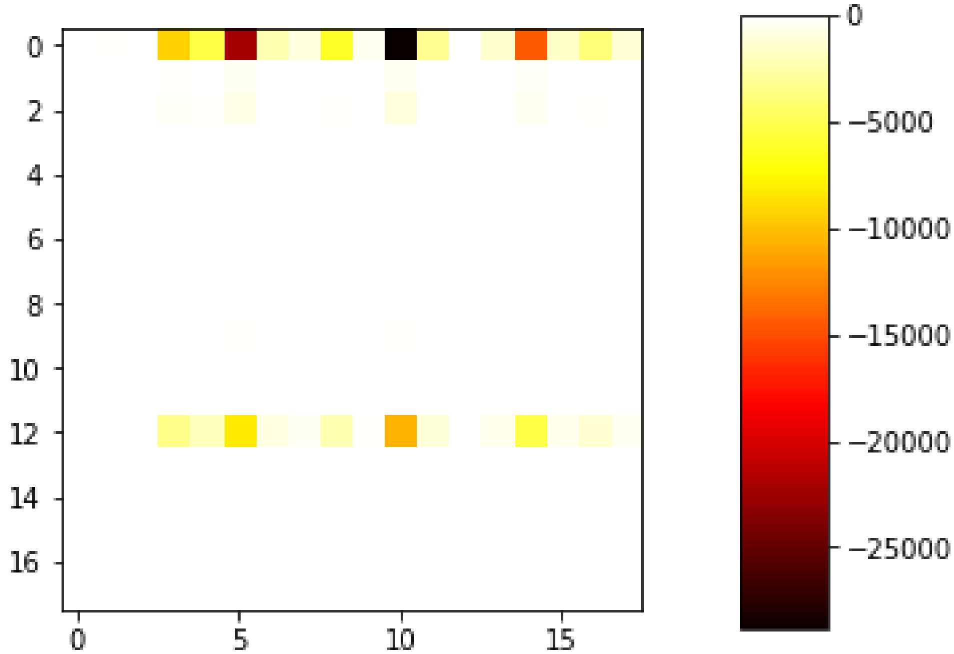
```
Accuracy: 1.0
<modules.adapml_classification.Classification object at 0x7fe7618d3250>
```



5 Regression

5.1 Linear Regression

[11]:
```
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