report_executed

August 2, 2021

1 Statistics

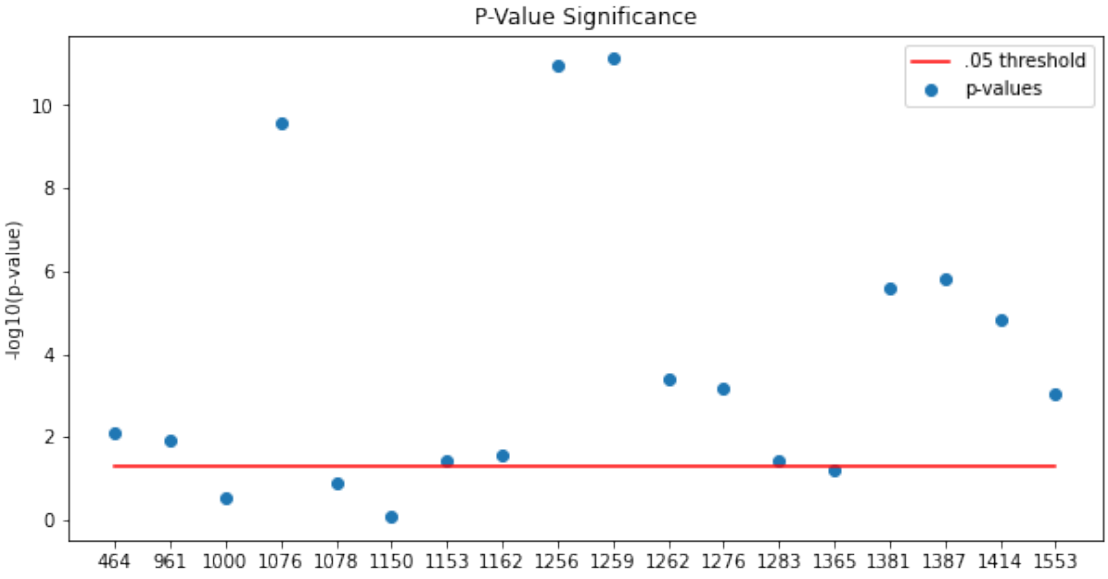
Describe the module blabla

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)
```

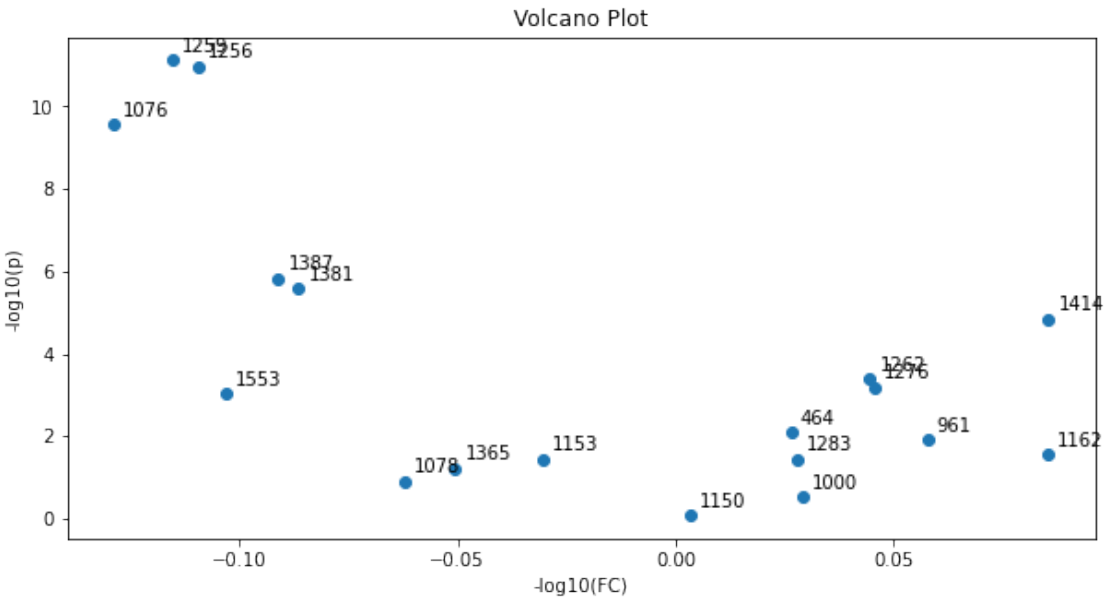
```
t_test.plot_logp_values(variables)
```



1.2 Volcano Plot

blabla

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



2 Dimension-Reduction

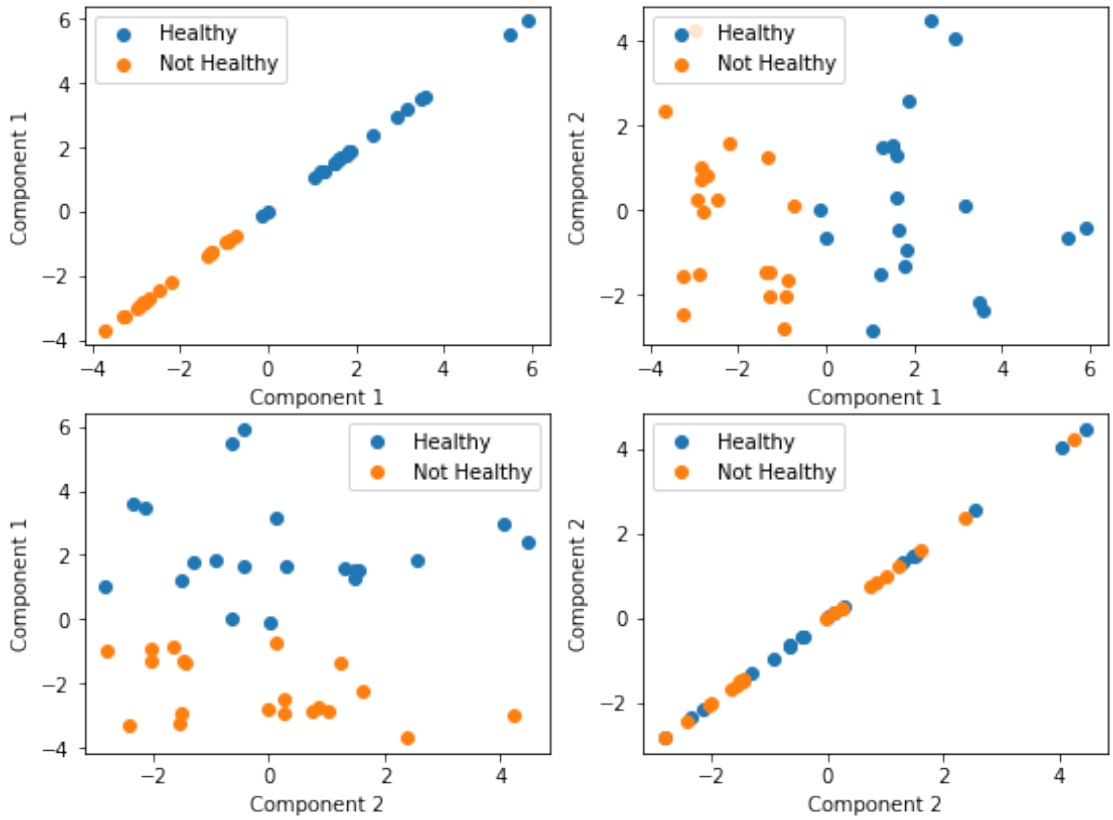
Dimension-reduction methods are used to condense high dimensional data down to dimensions which provide the most information. We have implemented the principal component analysis (PCA). It performs a change of basis and the new basis is chosen, such that the i-th principal component is orthogonal to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

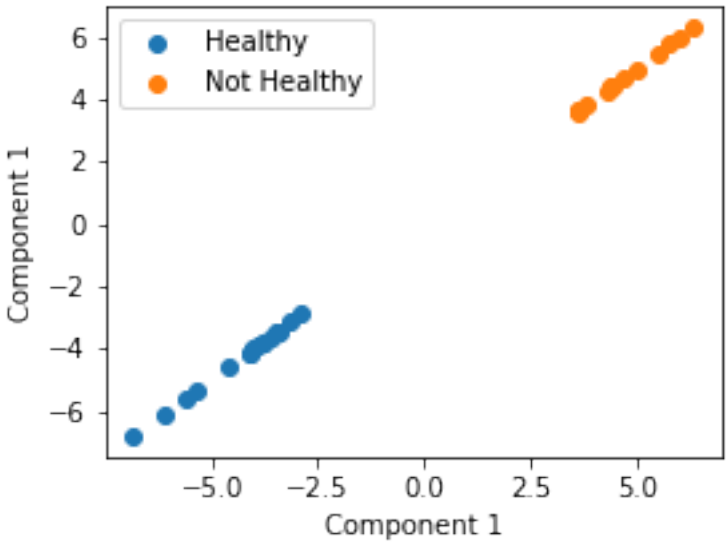


2.2 Linear Discriminant Analysis

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

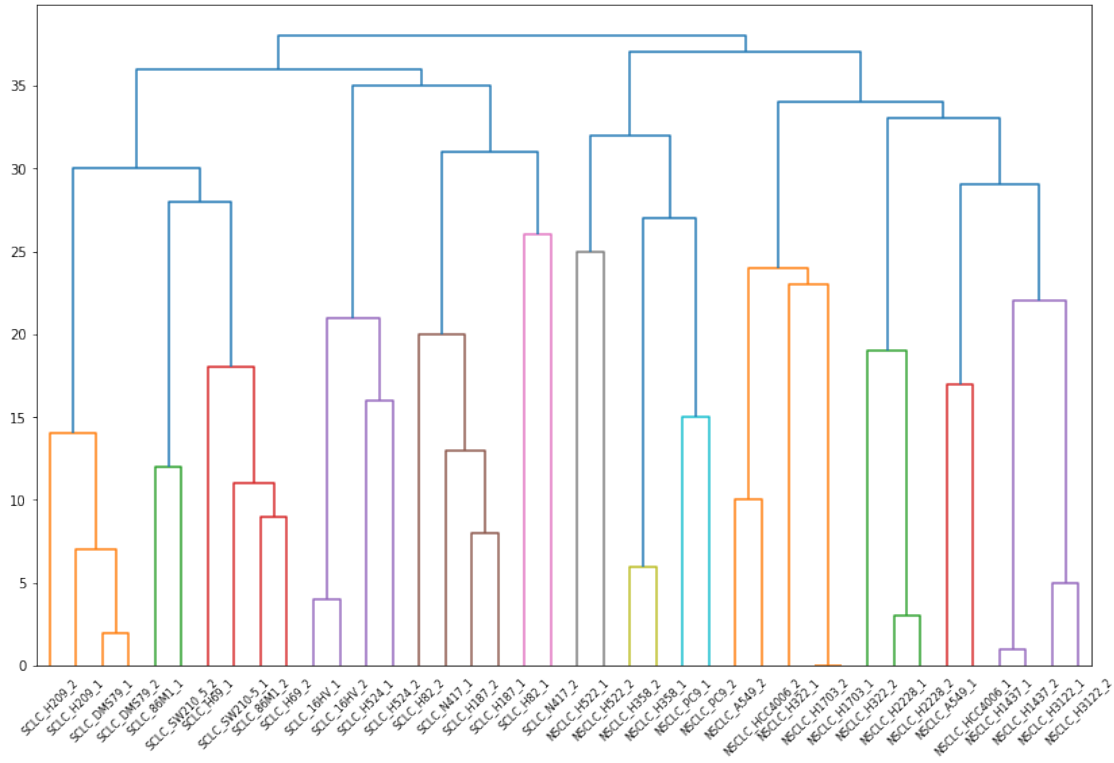
[5]:
```
kmeans_cluster = adapml_clustering.Clustering(data.data, 'kmeans', 3)
kmeans_cluster.getClusterResults(samples)
```

	Cluster 1	Cluster 2	Cluster 3
0	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

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

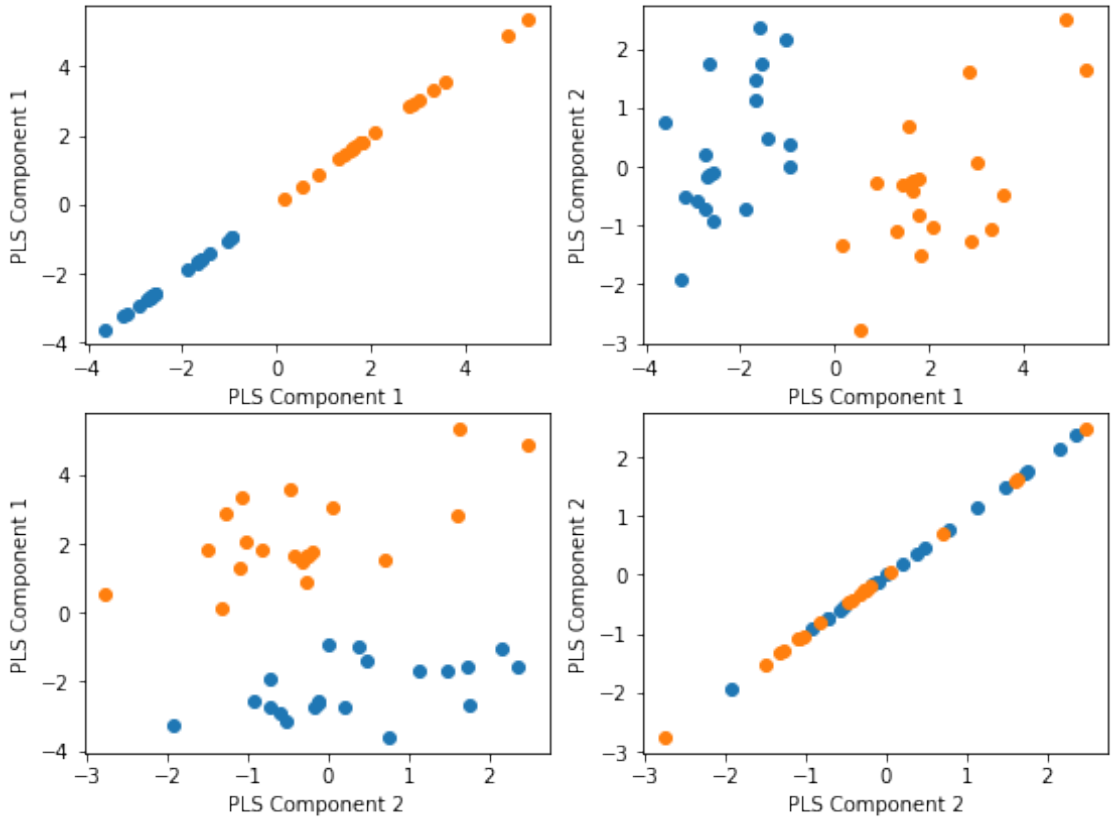


4 Classification

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:  {'gamma': 'scale', 'kernel': 'rbf', 'shrinking':
True}
SVM: R^2=1.0 Q^2=1.0
```

4.3 Random Forest

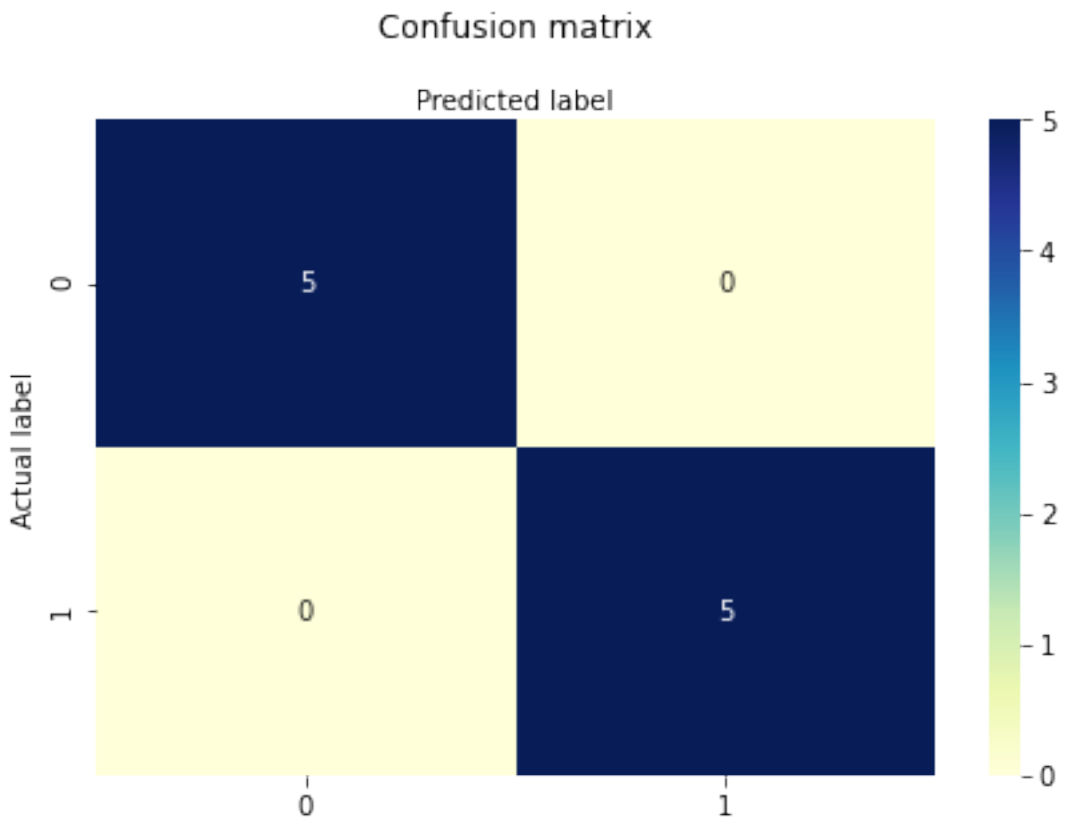
[9]:
```
data = adapml_data.DataImport(path_to_data)
rnf = adapml_classification.Classification(data.data, response1D,␣
 ↪'randomforest', .75, kfolds=3)

adapml_classification.print_model_stats(rnf, "RF")
```

```
Random Forest Validated Parameters:  {'criterion': 'gini', 'n_estimators': 50}
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)
```

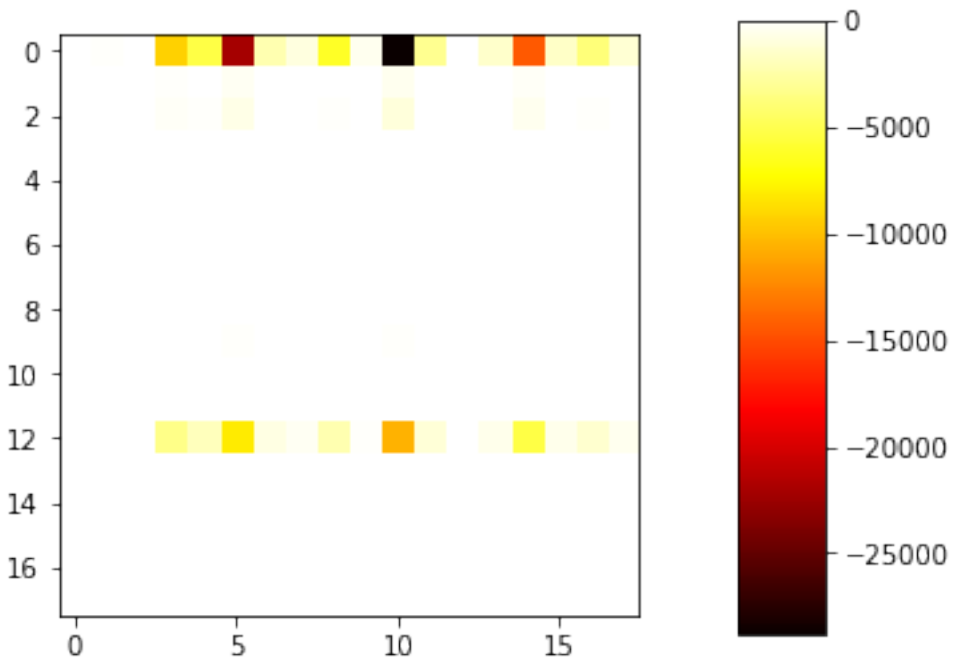
```
Accuracy: 1.0
<modules.adapml_classification.Classification object at 0x121a539d0>
```



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