

report_executed

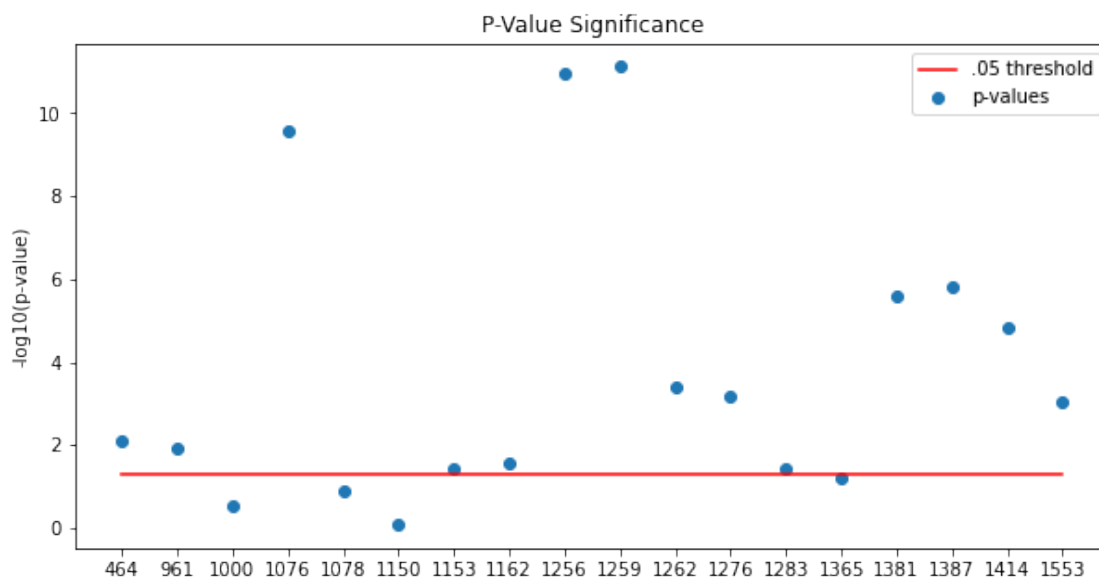
August 5, 2021

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.

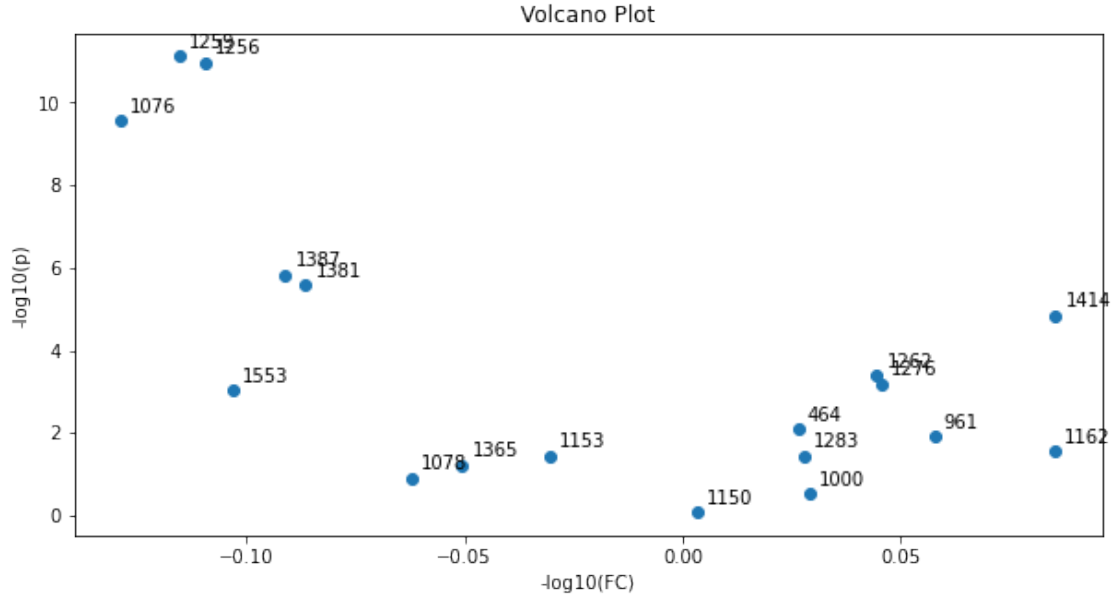
1.1 T-Test

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, \dots, x_n and y_1, \dots, 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.



1.2 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 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.

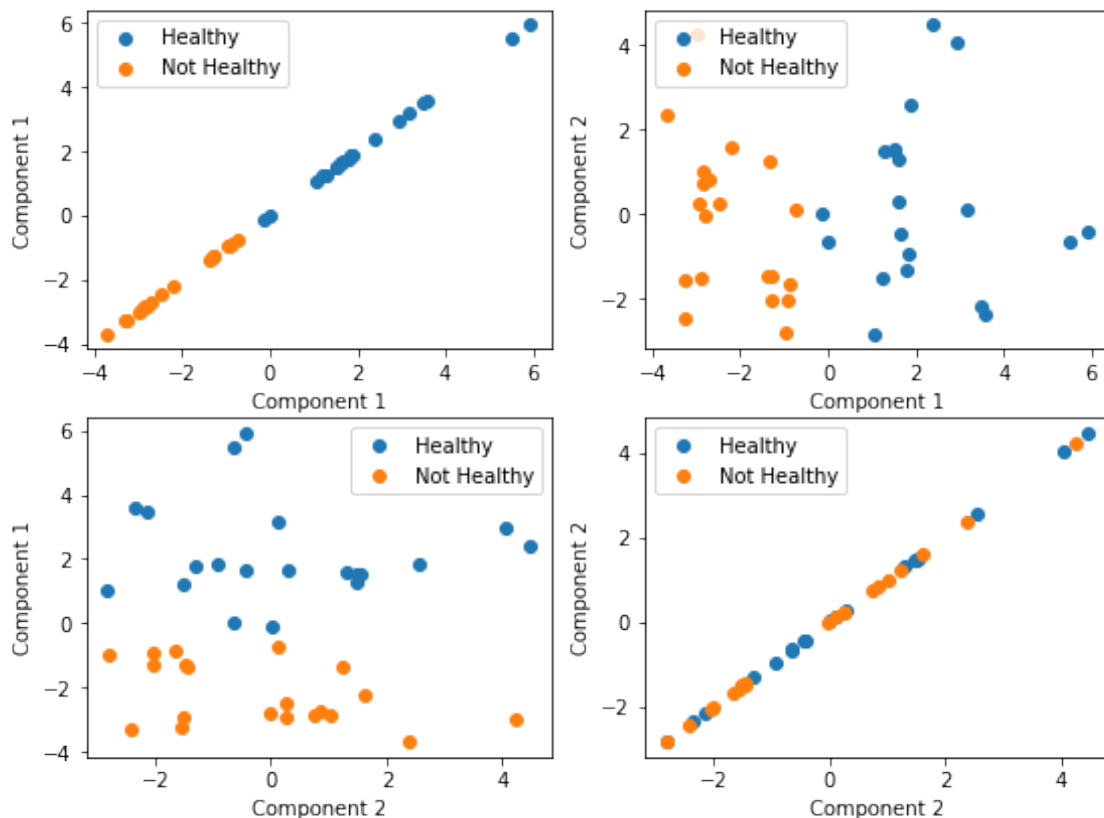
2.1 Principal Component Analysis

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.

PCA Projections

Projections of data into latent space.

Data is colored by response



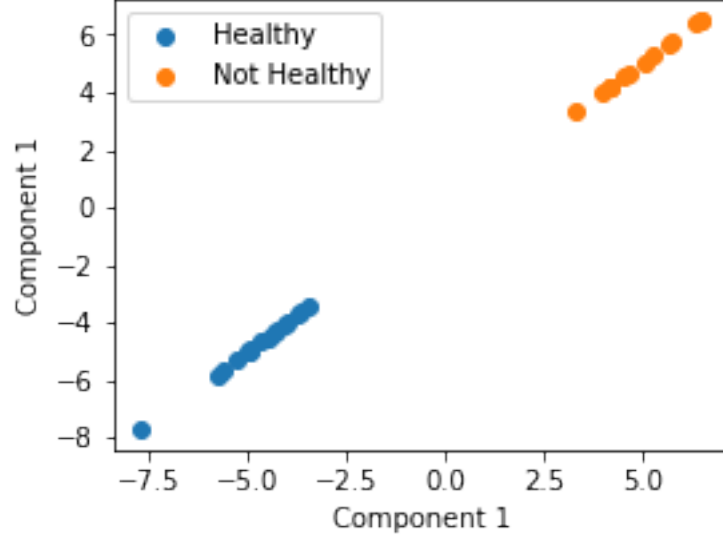
2.2 Linear Discriminant Analysis

Linear discriminant analysis is a classifier with a linear decision boundary. We assume normality and fit conditional densities $p(x | y = 0)$ and $p(x | y = 1)$ 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.

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 within-cluster sum of squares (WCSS)

$$WCSS = \sum_{i=1}^k \sum_{x_j \in C_i} \|x_j - \mu_i\|^2$$

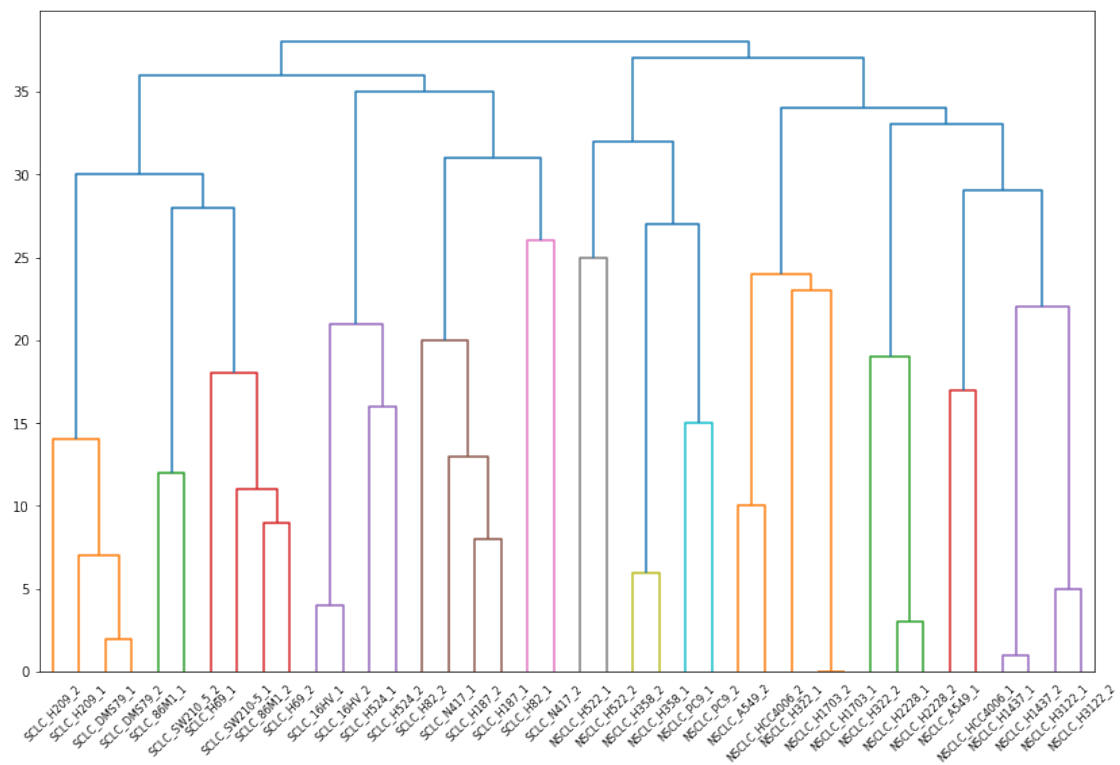
where x_1, \dots, x_n is the data and μ_i is the centroid of C_i cluster. It is solved by either Lloyd's or Elkan's algorithm and we use sklearn module in Python.

	Cluster 1	Cluster 2	Cluster 3
0	NSCLC_H358_2	NSCLC_A549_1	SCLC_86M1_2
1	NSCLC_H522_1	NSCLC_H1703_2	SCLC_86M1_1
2	NSCLC_H522_2	NSCLC_H1703_1	SCLC_16HV_1
3	NSCLC_H358_1	NSCLC_A549_2	SCLC_16HV_2
4	NSCLC_PC9_1	NSCLC_H1437_1	SCLC_DMS79_1
5	NSCLC_PC9_2	NSCLC_H2228_1	SCLC_DMS79_2
6	NaN	NSCLC_H2228_2	SCLC_H187_2
7	NaN	NSCLC_H1437_2	SCLC_H187_1
8	NaN	NSCLC_H3122_1	SCLC_H209_1
9	NaN	NSCLC_H322_2	SCLC_H524_1
10	NaN	NSCLC_H322_1	SCLC_H209_2
11	NaN	NSCLC_H3122_2	SCLC_H524_2
12	NaN	NSCLC_HCC4006_1	SCLC_H69_1

13	NaN	NSCLC_HCC4006_2	SCLC_H82_1
14	NaN	NaN	SCLC_H82_2
15	NaN	NaN	SCLC_H69_2
16	NaN	NaN	SCLC_N417_2
17	NaN	NaN	SCLC_N417_1
18	NaN	NaN	SCLC_SW210-5_1
19	NaN	NaN	SCLC_SW210_5_2

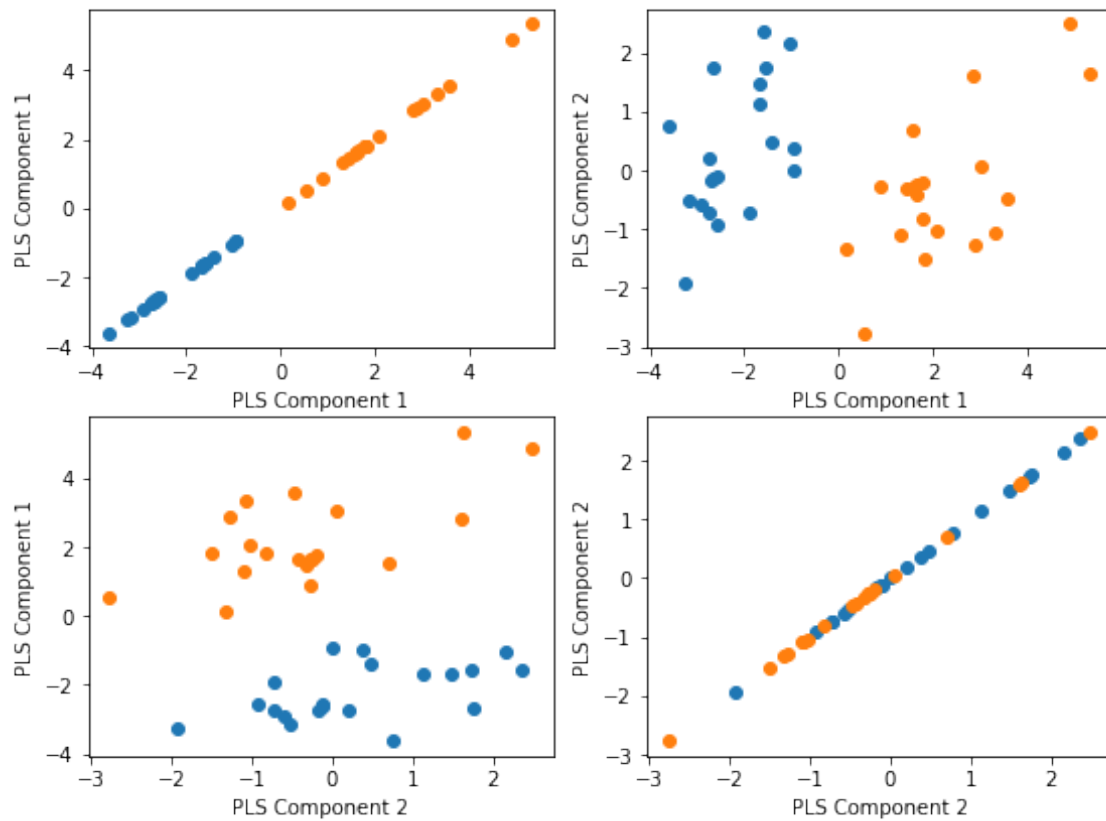
3.2 Hierarchical Clustering

	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



4.2 Support Vector Machines

SVM Validated Parameters: `{'kernel': 'linear', 'shrinking': True}`

SVM: $R^2=1.0$ $Q^2=1.0$

4.3 Random Forest

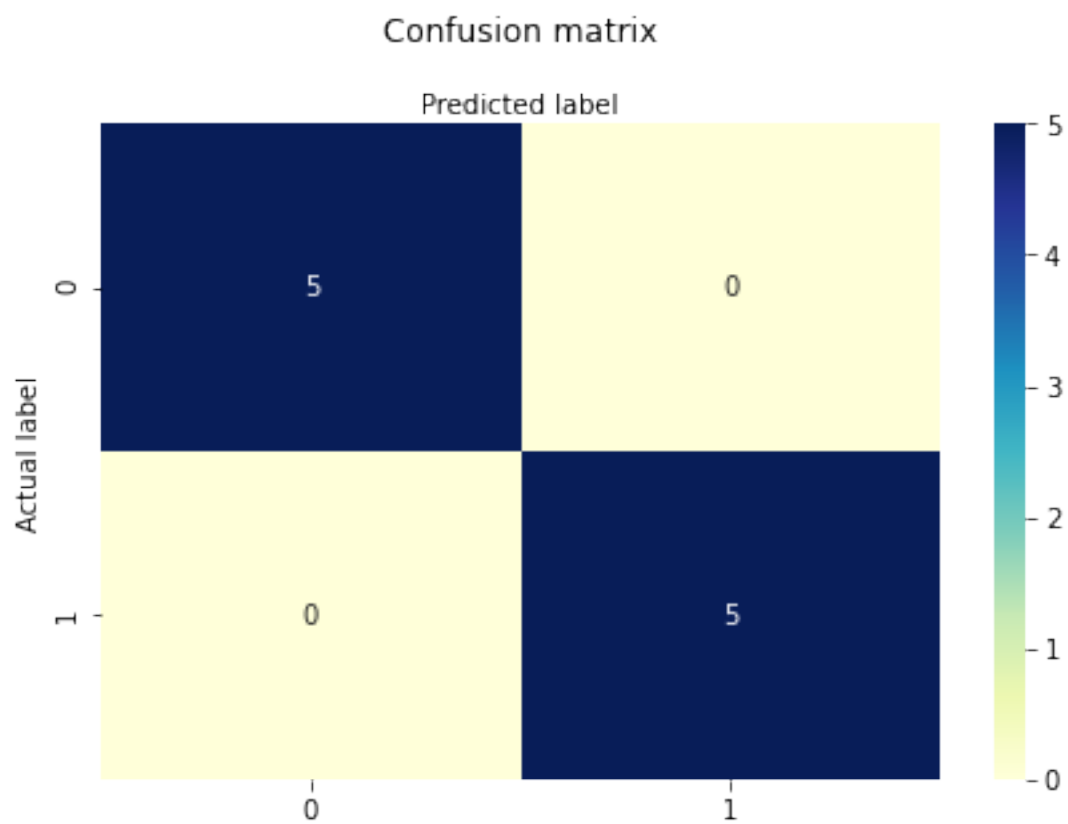
Random Forest Validated Parameters: `{'criterion': 'gini', 'n_estimators': 10}`

RF: $R^2=1.0$ $Q^2=1.0$

4.4 Logistic Regression

Accuracy: 1.0

<modules.adapml_classification.Classification object at 0x11eaf24c0>



5 Regression

5.1 Linear Regression

