Metabolomics_analysis_tools Basics

Let's get started! First, import functions we will use for this demo from the package metabolomics_analysis_tools@import_functions.

```
import metabolomics_analysis_tools.data_preprocessing.data_reading as dr
import metabolomics_analysis_tools.data_preprocessing.normalization as dn
import metabolomics_analysis_tools.stats_analyses.analyses as sa
import warnings
warnings.filterwarnings('ignore')
```

1. Then we can use the data_reading module to read in the data, by default it will read in the data from the resources/test_dataset folder in the package.
   We can also use the data_reading module to read in the data from a custom path, by passing the path as an argument to the read_data_file function (file_path='path/to/file.csv').
   The read_data_file function will return a pandas dataframe.

```
df=dr.read_data_file()
```

```
data read successfully
the shape of the dataframe is:  (77, 65)
```

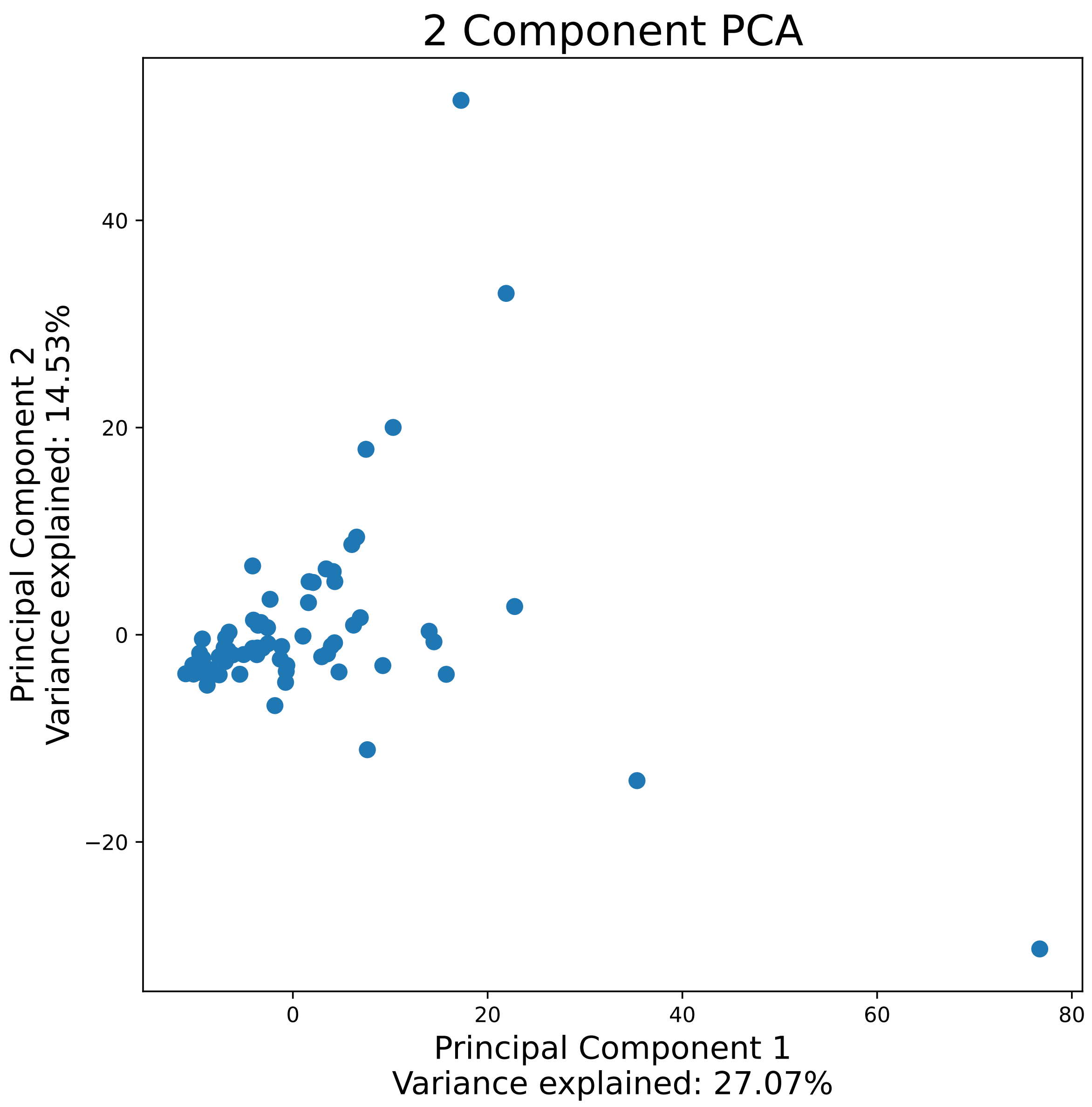
2. Next we can use the normalization module to normalize the data, here we will use the median normalization method normalized_data=dn.normalize_by_median(df).
   We can have a look at the first 5 rows of the normalized data normalized_data.head().

```
normalized_data=dn.normalize_by_median(df)
normalized_data.head()
```

	Patient ID	Muscle loss	1,6-Anhydro-beta-D-glucose	1-Methylnicotinamide	2-Aminobutyrate
0	PIF_178	cachexic	0.895833	1.786066	1.78551
1	PIF_087	cachexic	1.363596	9.299454	2.315539
2	PIF_090	cachexic	5.930482	1.768306	1.161106
3	NETL_005_V1	cachexic	3.3875	1.447541	16.43756
4	PIF_115	cachexic	0.486842	2.013661	1.490944

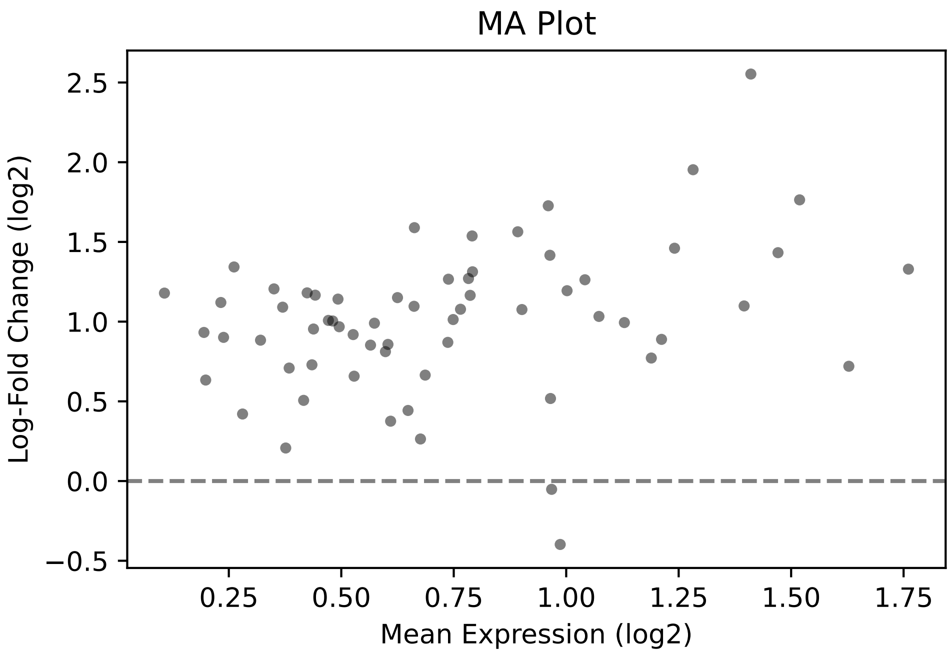
3. (a)We can use the analyses module to perform statistical analyses on the data.
   Here we will first perform a PCA analysis on the data to see if there are any patterns in the data.
   The PCA_analysis function will return a pandas dataframe containing the principal components principal_components=sa.PCA_analysis(normalized_data).

```
principal_components=sa.PCA_analysis(normalized_data)
```



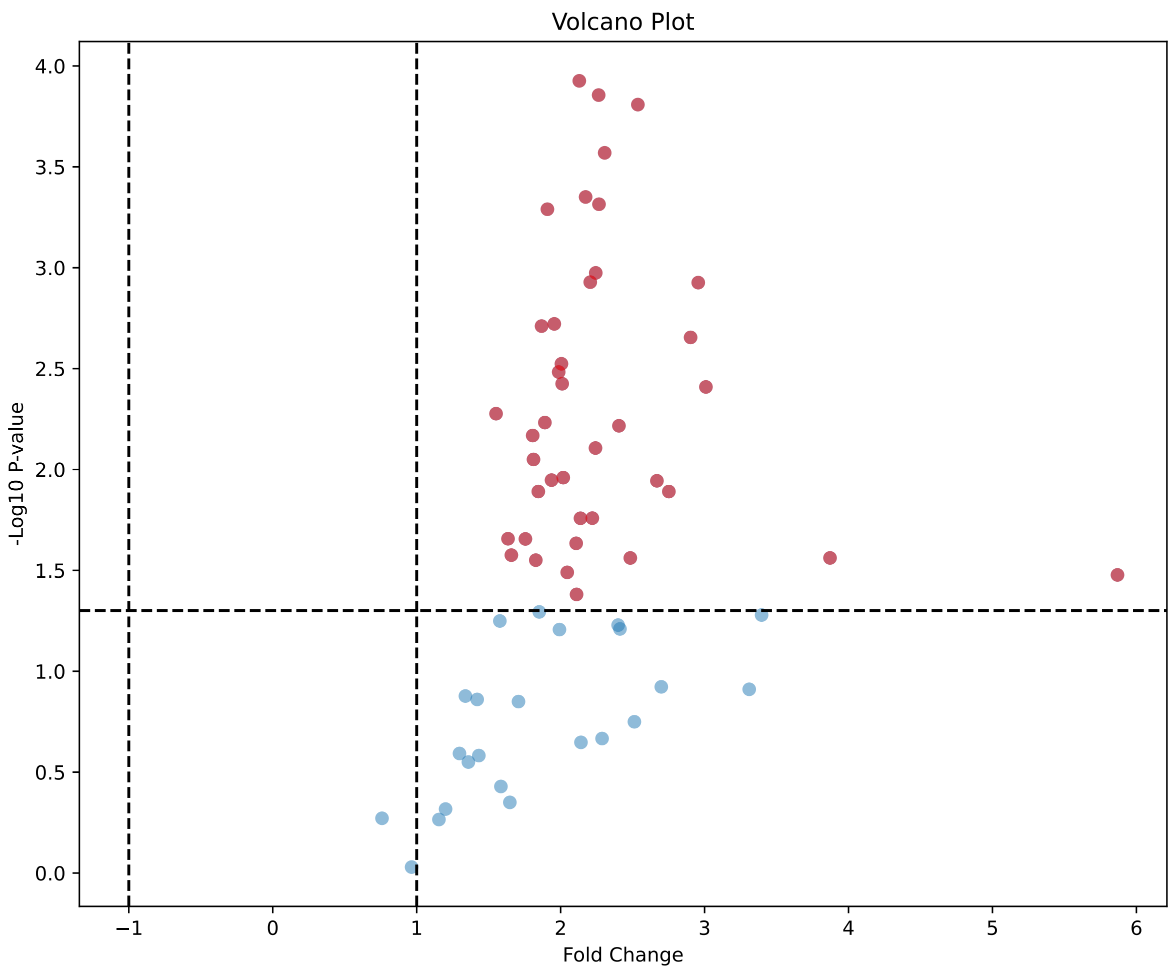
3. (b)Next, we can do the same for the MA plot.
   The MA_plot function will return a pandas dataframe containing the log2 fold change and the -log10 p-value

```
MA_plot=sa.ma_plot(normalized_data)
```



3. (c)We can also do a volcano plot, which can show us the significantly differentially expressed metabolites in the data.
   The volcano_plot function will return a pandas dataframe containing the log2 fold change and the -log10 p-value volcano_plot=sa.volcano_plot(normalized_data)

```
volcano_plot=sa.volcano_plot(normalized_data)
```


Volcano Plot
-Log10 P-value
Fold Change
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−1
0
1
2
3
4
5
6