Metabolomics_analysis_tools Tutorials

Introduction to the Metabolomics analysis tools

The goal of this project is to implement a Python based pipeline or package related to metabolomics data analysis. I am currently working with targeted metabolomics data in my lab, and it will be helpful with my work to develop a package that contains some very common metabolomics data analysis tools, including:

data transformation data normalization data scaling common statistical analyses including PCA, MA plot and Volcano plot. Even though there are lots of packages available for the functions mentioned above, implementing them myself will help me understand those functions better and help me do a better analysis job hopefully.

Goal of the tutorial

The goal of this tutorial is to show step by step how to install and use this package to perform data processing and statistical analyses functions in this tool, and also a bit on how to read the results generated from the analyses functions.

Example data description

Targeted metabolomics data Retrieve metabolites concentration data from (https://www.metaboanalyst.ca/Meta
or from https://www.ebi.ac.uk/metabolights/search?) (Metabolights)

A data file with metabolites concentration profile will contain a matrix with metabolites names and metabolites concentrations on each row for each sample. This file will be provided by the user, I will have data for testing

Step by step installation and running

Let's get started! First, we need to install the package.
Steps: 1. Git clone or download the github folder;
2. Open the terminal, and go to this folder;
3. Enter
`pip install dist/metabolomics_analysis_tools-0.1.0.tar.gz` to install the package locally;

Then, we can import functions we will use for this demo from the package metabolomics_analysis_tools@import_

```
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()
df.head()
```

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

	Patient ID	Muscle loss	1,6-Anhydro-beta-D-glucose	1-Methylnicotinamide	2-Aminobutyrate
0	PIF_178	cachexic	40.85	65.37	18.73
1	PIF_087	cachexic	62.18	340.36	24.29
2	PIF_090	cachexic	270.43	64.72	12.18
3	NETL_005_V1	cachexic	154.47	52.98	172.43
4	PIF_115	cachexic	22.2	73.7	15.64

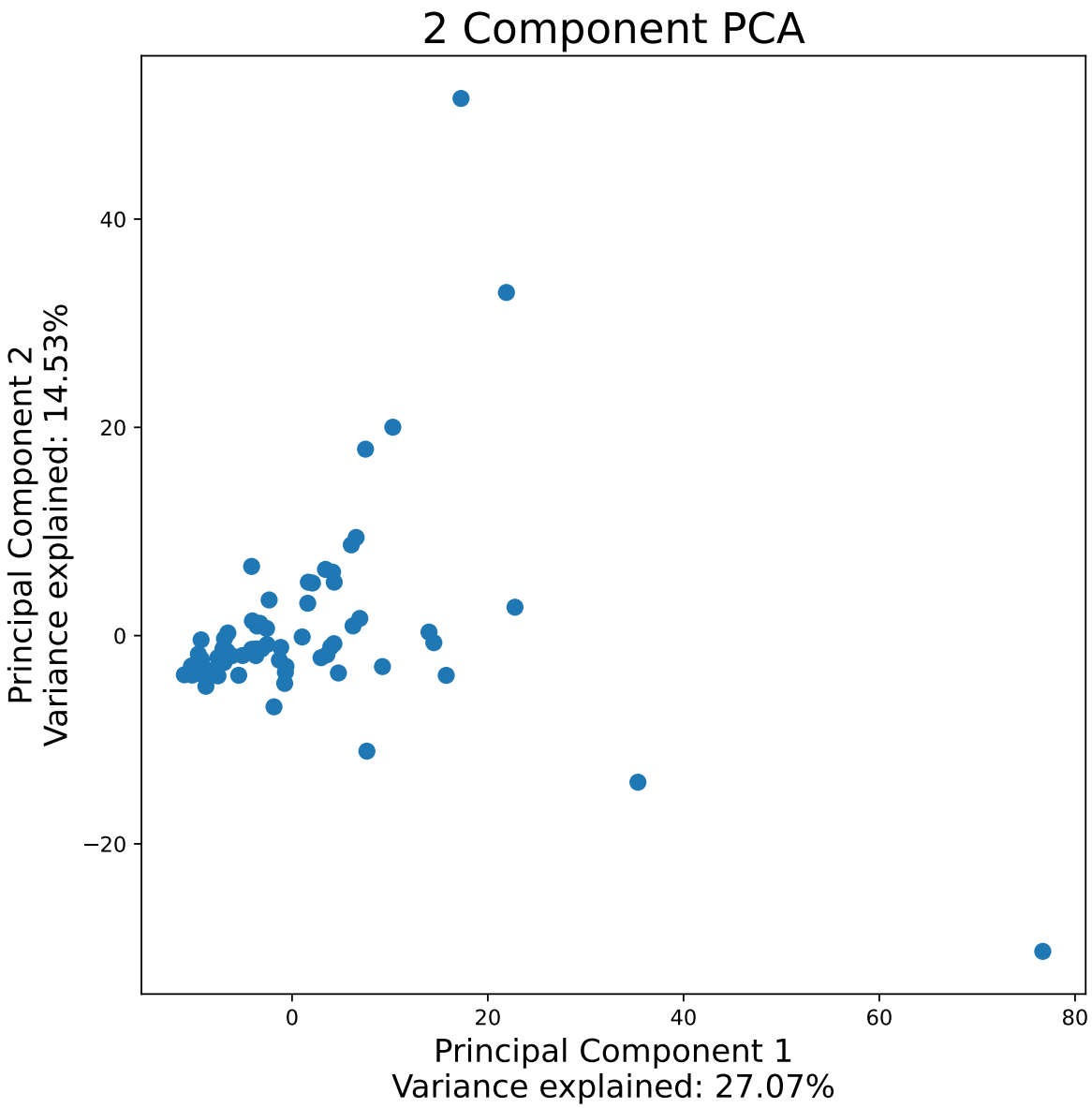
2. Next we can use the normalization module to normalize the data, here we will use the median normalization method normalized_data=dn.normalize_by_median(df).
   We can have a look at the first 5 rows of the normalized data normalized_data.head().

```
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

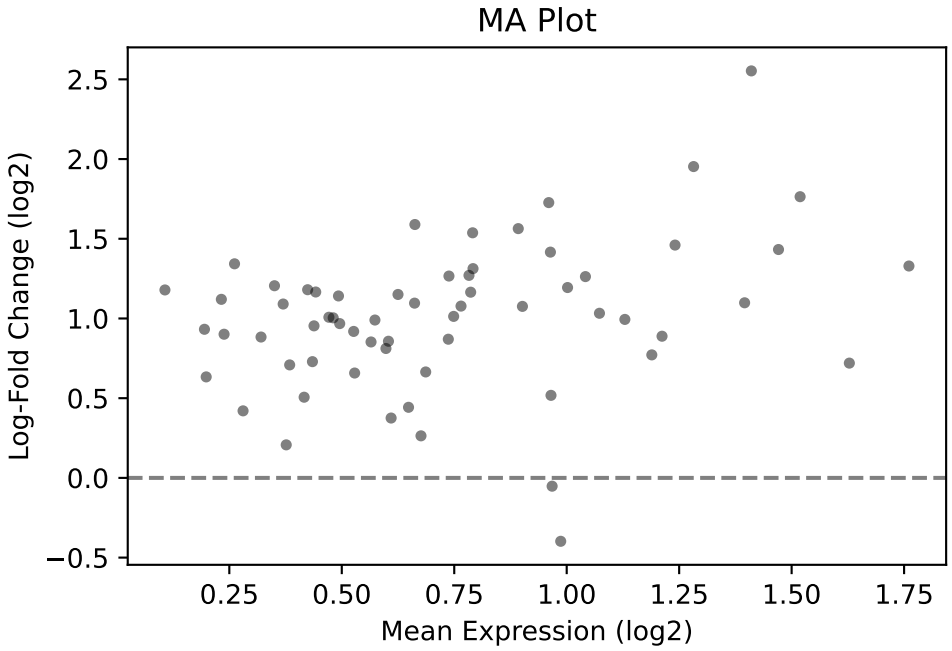
3. (a)We can use the analyses module to perform statistical analyses on the data.
   Here we will first perform a PCA analysis on the data to see if there are any patterns in the data.
   The PCA_analysis function will return a pandas dataframe containing the principal components principal_components=sa.PCA_analysis(normalized_data).

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



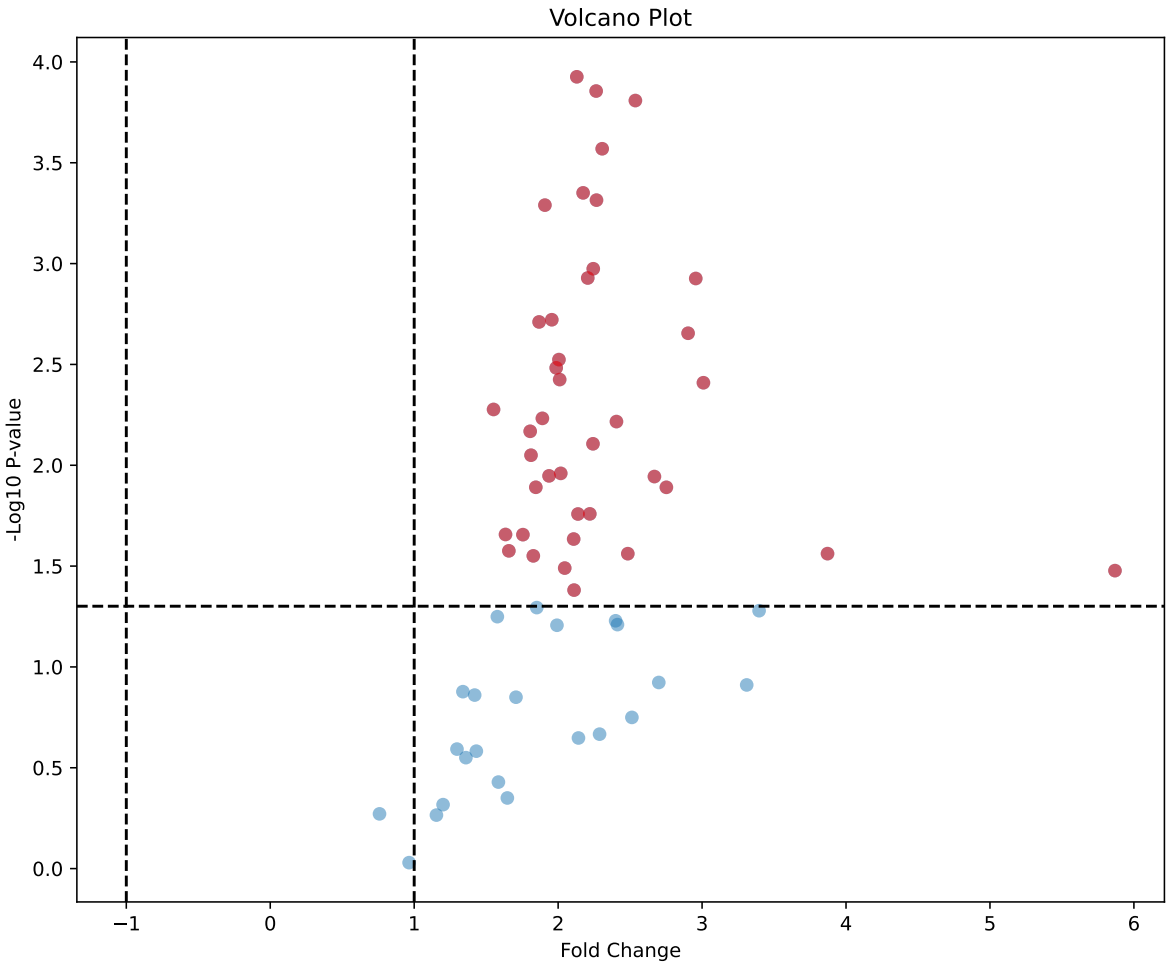
3. (b)Next, we can do the same for the MA plot.
   The MA_plot function will return a pandas dataframe containing the log2 fold change and the -log10 p-value

```
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