

Installing R packages into Anaconda Navigator

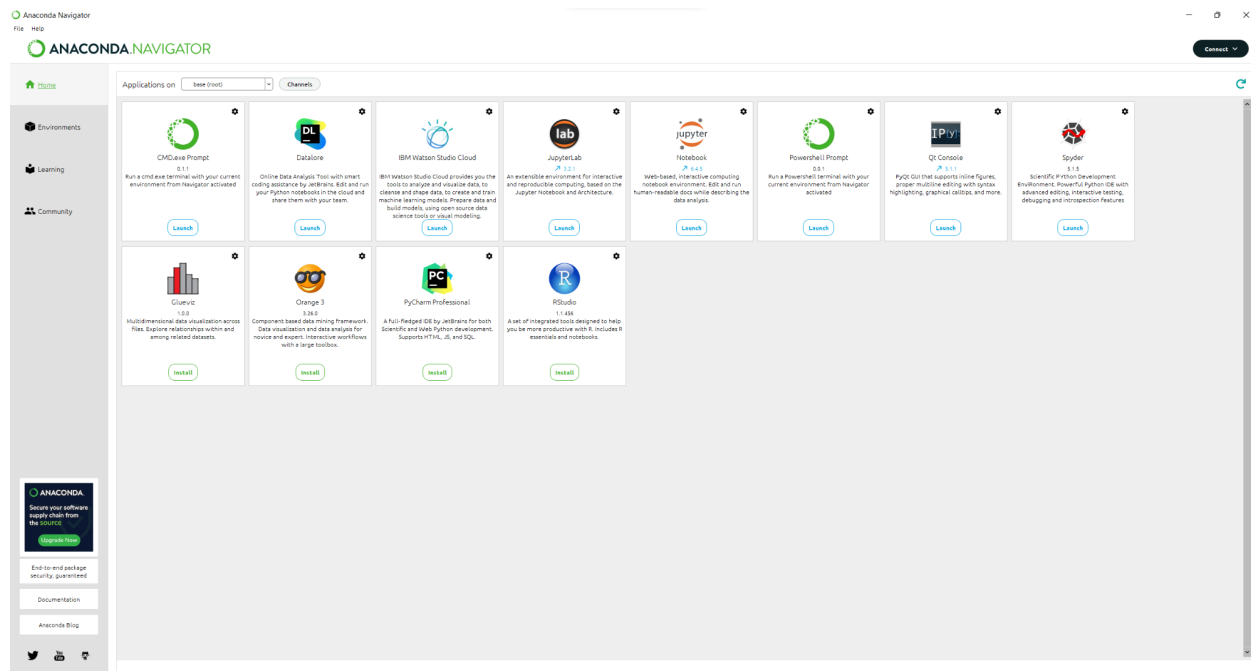
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Anaconda is a desktop application that allows the user to launch common python programs without using the command line. <https://www.anaconda.com/>

To install Anaconda on different OS: Windows, MacOS, Linux [Anaconda | Anaconda Distribution](#)

Installation steps: <https://docs.anaconda.com/anaconda/install/windows/>

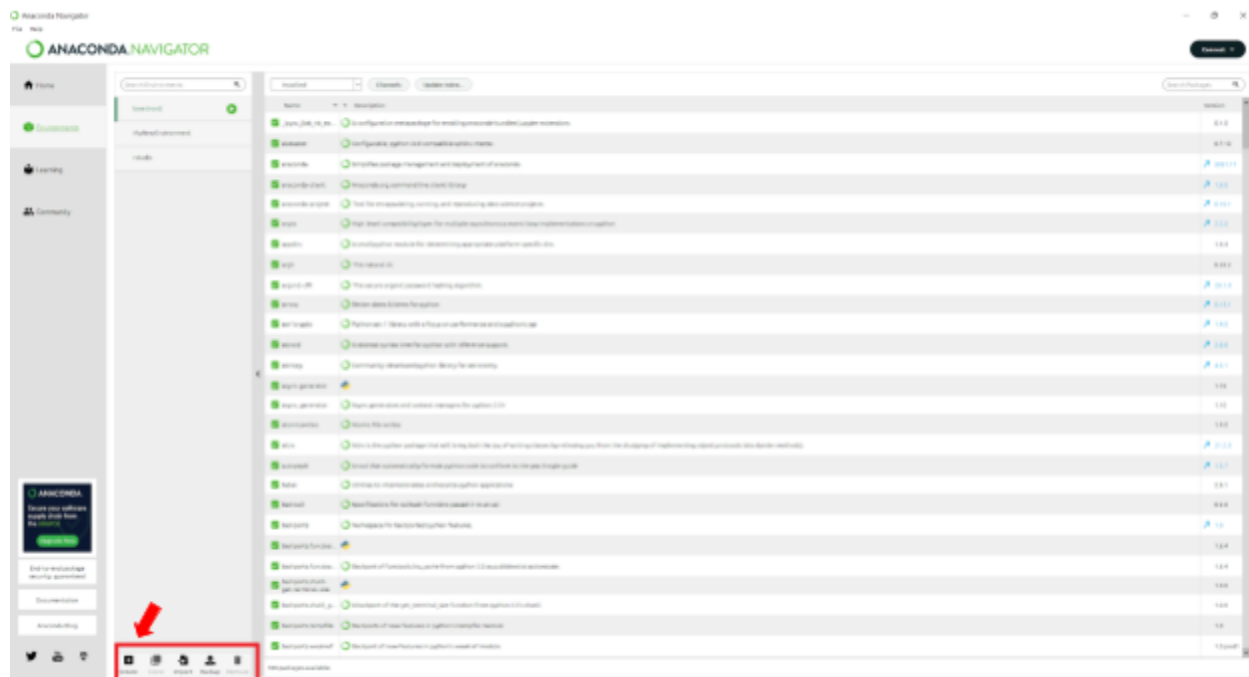
This is how the homepage of Anaconda looks like: You can launch Jupyter Notebooks directly from here.



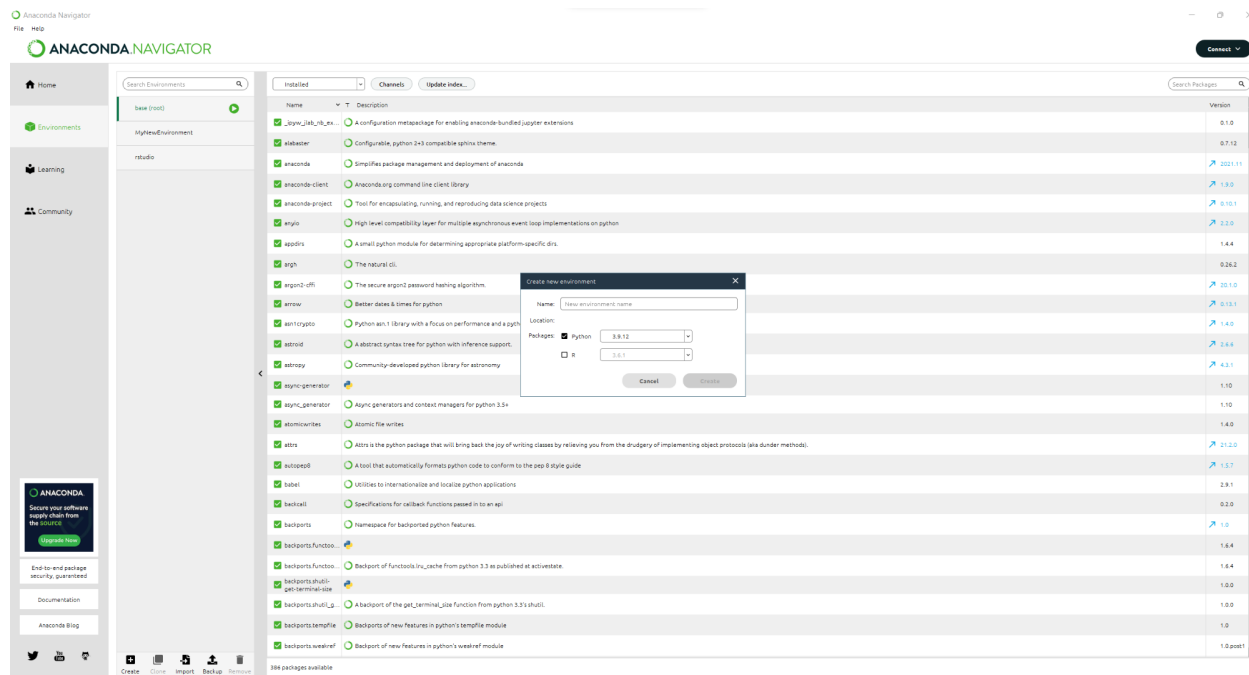
Anaconda, by default, works with Python kernels. In order to run Jupyter notebooks using R code, we need to install R Kernels onto our Anaconda environment.

To install R Kernels:

- 1) Go to the environment and click on 'create' shown on the lower right end of the page



- 2) A new dialog box would open as shown below. Select the R packages and provide a name for the new environment. After a while, the environment would be created.



The screenshot shows a JupyterLab environment with a notebook titled "Metabolomics_MultivariateDataAnalysis". The notebook content is as follows:

Multivariate analyses for untargeted metabolomics data

By M. Irwin (add your names here)

In this notebook we will perform a Principal Coordinate Analysis (PCoA), also known as metric or classical Multidimensional Scaling (MDS) to explore and visualize patterns in an untargeted mass spectrometry-based metabolomics dataset. We will then assess statistical significance of the patterns and dispersion of different sample types using permutational multivariate analysis of variance (PERMANOVA).

Data

The files used in this tutorial are a subset of an untargeted LC-MS/MS metabolomics dataset of bacterial cultures to which pooled antibiotics were added (sulphonamides, sulfamethoxazole, ciprofloxacin and ampicillin) to investigate potential bioconformations. (links to be replaced) Data were acquired on a Dionex Ultimate 3000 Thermo Fisher Scientific HPLC system coupled to a Thermo Orbitrap HD quadrupole ion of flight (Q/OF) mass spectrometer. MS/MS data were acquired in data-dependent acquisition (DDA) with fragmentation of the seven most abundant ions in the seven most abundant ions in the spectrum (links to be replaced). Data files were subsequently preprocessed using MZmine2 and the `bioconductor::normalizeLog2Abundance` function.

Questions

- Is there a difference in the metabolomic profiles of different bacterial species?
- Is there a difference in the metabolomic profiles of different sample types?
- Is there a difference in the bacterial metabolomic profiles across different dispensers?

Install and load libraries

```
In [1]: install.packages("magrittr")
install.packages("ggplot2")
library("magrittr")
library("ggplot2")
```

Specify where the data can be found by providing urls for the featuretable and metadata

```
In [2]: ft <- read.csv("https://raw.githubusercontent.com/robertmccormick/untargeted_metabolomics_SummerSchool_2022/main/data/featuretable.csv")
ft <- read.csv("https://raw.githubusercontent.com/robertmccormick/untargeted_metabolomics_SummerSchool_2022/main/data/metadata.csv")
ft <- read.csv("https://raw.githubusercontent.com/robertmccormick/untargeted_metabolomics_SummerSchool_2022/main/data/featuretable.csv")
ft <- read.csv("https://raw.githubusercontent.com/robertmccormick/untargeted_metabolomics_SummerSchool_2022/main/data/metadata.csv")
```

Load featuretable and metadata

A red box highlights the "Run" button in the JupyterLab toolbar, with a red arrow pointing to it.