Setup Instructions

The following code segments set up a python environment that jupyter notebook can use as its kernel.

Mac & Linux

1. Copy-paste commands from `install_1.txt` file
2. Close the terminal and run commands from `install_2.txt` file in a fresh terminal. This next part will create a directory "tequila" with the tequila installation in the working directory, so make sure you're in a directory where you wish for this to be installed.

Windows

Windows currently does not support some packages like PyScf which are integral part of the jupyter notebooks 1-5. So, we recommend you to set up Windows

Subsystem for Linux(WSL)

Instructions

1. Open settings
2. Open Apps
3. At the top right, click on 'Programs and Features' (under 'Related Settings')
4. At the top left, click on 'Turn Windows features on or off'
5. Scroll down, and click on 'Windows Subsystem for Linux'
6. Click Ok
7. Follow the instructions to Restart your computer
8. Once your computer is back on, go to Microsoft Store and search 'ubuntu'
9. Install the ubuntu app

10. Launch Ubuntu, and create your username and password. This password will be used when you install a package using the sudo command

11. Install conda in WSL

12. Install conda using the Miniconda installer. Enter the following commands in ubuntu shell:

    ```
    wget https://repo.continuum.io/miniconda/Miniconda3-latest-Linux-x86_64.sh
    bash Miniconda3-latest-Linux-x86_64.sh
    ```

13. Accept the licence terms.

14. When asked 'Do you wish the installer to initialize Miniconda3 by running conda init?' type 'yes'

15. You've successfully installed Miniconda3. Now you can complete instructions under 'Mac & Linux' in the ubuntu shell.

Caution: Do not try and access any Linux files from your Windows File Explorer; do not go into your AppData folder to open linux files. This could potentially corrupt your linux distro. Whenever using WSL, simply open the ubuntu app, and access files from there. Note: When starting jupyter notebook, you will need to copy one of the URLs into your internet tabs.