

STA YOUNG RESEARCHERS WORKSHOP 2019

Friday, January 11, 2019
1530-1730

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Agenda

15:30 to 15:45 Introductions

15:45 to 16:30 Introduction to Predictive Modeling in Python Workshop -Christine

A brief overview of utilizing commonly used data science tools like numpy, Pandas, and sci-kit learn to perform predictive modeling on clinical data.

16:30 to 17:15 Introduction Molecular Dynamics Workshop -Tom

A brief overview of molecular dynamics in anesthesia research, followed by a hands-on Python workshop on determining the primary interacting residues of a ligand in a simulation of a GPCR.

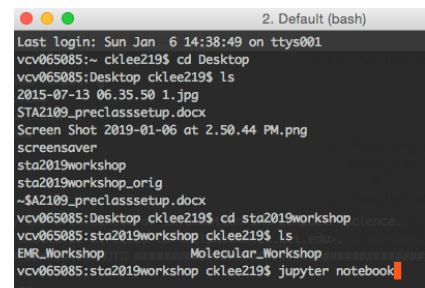
17:15 to 17:30 Free discussion on current and future anesthesia research

Pre-Workshop Setup/Installation:

1. Please bring a laptop to the workshop!
2. Please go to the following link to download workshop materials:
 - <https://qux.us/sta2019workshop.zip>
3. Install the free distribution of **Anaconda - Python 3.7 Version** on your laptop BEFORE the workshop: <https://www.anaconda.com/download/>
4. If you already have the Anaconda Python distribution or have just installed a fresh copy, please update it by running the following commands from a command prompt or terminal:

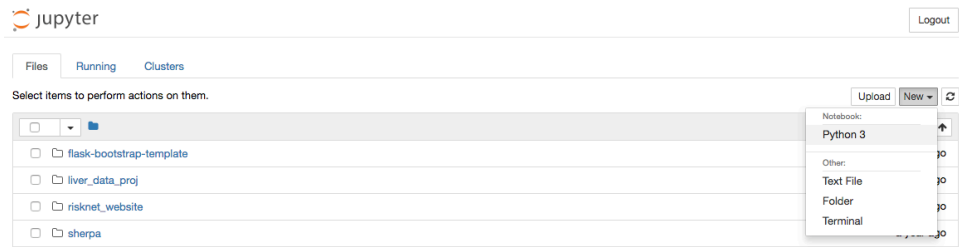
```
conda update conda
conda update anaconda
```

5. Finally, launch jupyter Notebook by either typing “jupyter notebook” in your terminal OR directly launching it from the Anaconda application.
 - If you have already downloaded the workshop materials, make sure to go into your workshop directory first before launching.



```
2. Default (bash)
Last login: Sun Jan 6 14:38:49 on ttys001
vcv065085:~ cKlee219$ cd Desktop
vcv065085:Desktop cKlee219$ ls
2015-07-13_06.35.50_1.jpg
STA2109_preclasssetup.docx
Screen Shot 2019-01-06 at 2.50.44 PM.png
screensaver
sta2019workshop
sta2019workshop_orig
~$A2109_preclasssetup.docx
vcv065085:Desktop cKlee219$ cd sta2019workshop
vcv065085:sta2019workshop cKlee219$ ls
EMR_Workshop      Molecular_Workshop
vcv065085:sta2019workshop cKlee219$ jupyter notebook
```

6. A web page should have opened in your default browser and will look like the following. Go to New > Python 3 to create a new notebook.



7. In this blank notebook, type the following commands in the grey box. Click in the grey box, and run the cell by going to Cell > Run Cells. OR hold SHIFT and ENTER.
- If you've already downloaded the workshop materials, simply run the Test Notebook.ipynb.

```
Click into the grey part of the following cell. The side bar should be green indicating the active cell. Then run it by clicking "Cell >> Run" or the play button up above.
```

```
In [1]: import numpy; print('numpy: ', numpy.__version__)
import scipy; print('scipy: ', scipy.__version__)
import pandas; print('pandas: ', pandas.__version__)
import sklearn; print('sklearn: ', sklearn.__version__)

numpy: 1.15.4
scipy: 1.1.0
pandas: 0.20.3
sklearn: 0.19.1
```

8. Install molecular dynamics package by going to your terminal and typing:

```
conda install -c conda-forge mdanalysis
```

Python Tutorials:

If you're new to Python or a little rusty, here are two tutorials which you can work through before class:

· [LearnXinYMinutes' Python Tutorial](#) - Teaches basic Python and assumes you already know how to program. Shorter.

· [A Crash Course in Python for Scientists](#) - Teaches basic Python and basic programming concepts. Longer.