

# Introduction to Scientific Python

Blake Fleischer, PhD

Research Scientist

Partnership for an Advanced Computing Environment (PACE)

# Objectives :

- Showcase python as a viable alternative to scientific packages like R, MatLab
- Overview of some of Python's scientific functions



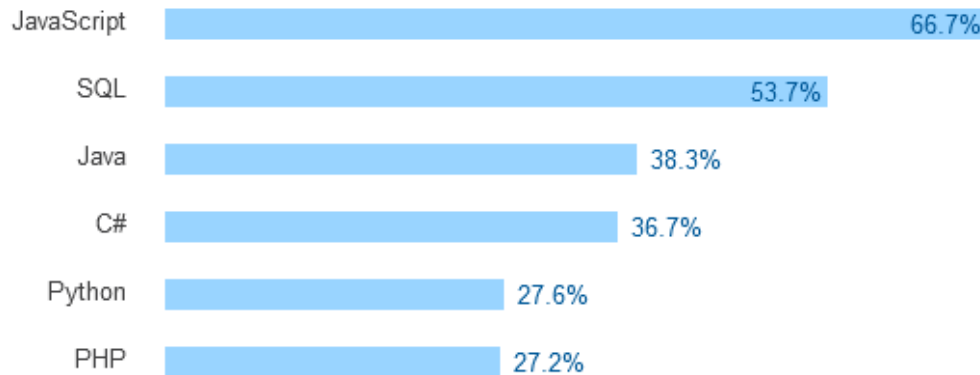
# Why python for Science?

- Easy to learn
- Well Supported
- Useful after graduation (free and open source)
- Extremely popular outside of academia



# People use Python

## 2017 StackOverflow Survey



## Google searches for language + 'tutorial' (PYPL)

Worldwide, Aug 2017 compared to a year ago:

Rank	Change	Language	Share	Trend
1		Java	22.7 %	-0.7 %
2		Python	16.3 %	+3.7 %
3		PHP	8.9 %	-1.1 %
4		C#	8.3 %	-0.5 %

# Python Packages

- Extending beyond simple programming, additional functionality comes from packages

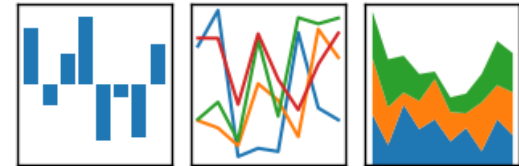


- Package discovery:
  - Finding the packages that suit your needs



pandas

$$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$$



# Tools of the Trade: Git

- “*Version control* is a system that records changes to a file or set of files over time so that you can recall specific *versions* later.”
- Git incorporates free web hosting for publicly visible files
- Backbone of the developer world
- Developed to support the Linux kernel
- <https://try.github.io/levels/1/challenges/1>
- <http://rogerdudler.github.io/git-guide/>
- How to undo things:
  - <https://github.com/blog/2019-how-to-undo-almost-anything-with-git>



# Tools of the Trade: Anaconda

- Package manager for python – useful for managing Python!
- From the author of Python's numpy and scipy packages
- To set up:
  - Download anaconda from <https://www.continuum.io/downloads>
  - Install packages for this course:
  - `conda install python=3 scipy numpy matplotlib jupyter notebook pandas pytables hdf5`



# Tools of the Trade: Jupyter

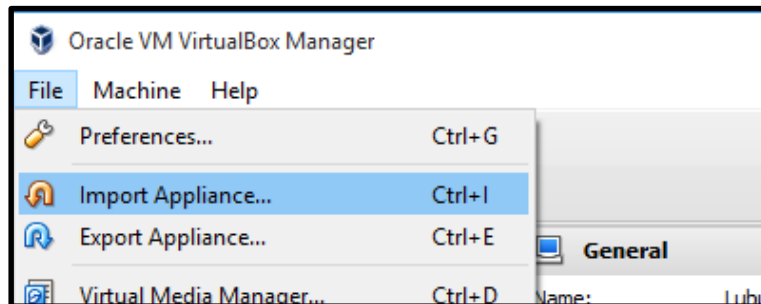
- Framework for interactive programming
- Jupyter Notebook: a web interface to interactive programming
  - Interface for coding, viewing data, and plotting
  - Reproducible science
- Uses ipython
  - Access docstrings (help on commands)
  - Tab completion





# Materials for this Course:

- Download VirtualBox (free)
  - <https://www.virtualbox.org/wiki/Downloads>
- Download the .ovf image for the course (1.8 GB compressed, + ~5GB when added to virtualbox)
  - <http://pace.gatech.edu/sites/default/files/Lubuntu32.ova>



- Alternatively, install anaconda on your local machine and pull the materials from:
  - <https://github.com/blakeflel/IntroScientificPythonWithJupyter>

# Overview

- Part I:
  - Jupyter Notebook overview
  - Input/Output in Python
  - Basic Math
  - Indexing/Array Operations
  - Plotting
  - FittingPlot
- Part II
  - Some basic statistics
  - Signal Processing
  - Ordinary Differential Equations
  - Pandas
  - Gotchas and Optmization

