

Python for Research Computation: An Intermediate Workshop

Adam Fine

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1 Introduction



Brendan Dolan-Gavitt
@moyix

...

My objection to Rust, OCaml, Haskell, etc. is that I am a bad programmer who wants to write bad programs. Python is naturally suited to this task

2:37 PM · Jan 6, 2022



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This workshop is a five-part series on various aspects of Python I wish I had known at the beginning of graduate school. Some familiarity with programming is assumed; familiarity with Python (as well as modules such as NumPy, matplotlib) will be helpful but not strictly necessary.

2 Rationale

Python has somewhat of a bad reputation. It's slow. It's badly designed - who thought duck typing was a good idea? why does the Global Interpreter Lock exist? Many people internalize these criticisms and resign themselves to writing bad, slow Python code. This workshop is intended as a defense of Python for research computing - in my opinion, Python is just enough of a programming language to be extremely powerful, while avoiding a lot of baggage that scientists don't care about. Also, it can be fast. Seriously.

3 Learning Objectives

By taking this workshop, students will be able to:

- Code in a manner that reduces and simplifies the debugging of errors.
- Implement computational pipelines in a rigorous and reproducible manner.
- Recognize potentially slow code and implement faster alternatives.
- Produce highly customized figures in `matplotlib` and `Seaborn`.
- Manipulate non-numerical data with `pandas`.

4 Schedule

1. Th 9/11 - Why Python? + Introduction to base Python
2. F 9/12 - Defense: defensive programming, reproducibility, creating workflows with `argparse` and `snakemake`, using `git` for research.
3. M 9/15* - Offense: Introduction to `NumPy` + how to write fast code.
4. T 9/16 - Figure... Tuesday? - plotting numerical data using `matplotlib`
5. F 9/19 - Handling categorical data with `pandas` and plotting it with `Seaborn`

All lectures other than Monday will take place from 2:30-3:30 PM in GCIS W105. Monday's lecture is at 10:30 AM, also in GCIS W105.

5 Assignments

One Jupyter notebook's worth of homework per lecture. Optional. Each homework is intended to take 1-2 hours. I intend to provide feedback on all submitted homework.

6 Github

All lectures, homework, and miscellaneous files can be found on my github here: <https://github.com/enifmada/research-python-workshop/tree/main>