



On Python and Tensors

Initial Considerations

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High performance computing (HPC)

- Use of supercomputers or computer clusters (grids) to tackle complex computation problems
- Will have guest lecture on basics of RIT research computing (RC)
 - RIT RC: https://www.rit.edu/researchcomputing/
 - (We will have a guest lecture / walkthrough on Sept 16 -- Viet -- on using RIT RC)
- Python is the "glue" (part of multilanguage model of HPC)
 - Ecosystem = NumPy, SciPy, and Matplotlib



The Oak Ridge Laboratory Frontier Supercomputer

Environments IPython console, Jupyter notebook, Spyder, ...

Python interpreter
Python 3, ...

Python packages numpy, scipy, matplotlib, ...

System and system libraries
OS, BLAS, LAPACK, ...

Your toolset

Some of the tools to engage with scientific computing

Python and development environments

- Vi / Vim, Emacs (simpler / bare-bones, classical)
- Atom, Gedit (GNOME Editor)
- Pycharm (an integrated development environment; IDE)

A Jetbrains
PyCharm view of
some ngclearn
source code!

(PyCharm community edition is free and available for multiple OS)

```
Project ~
                                                            data_loader.py
                                                                                                                                                                                 ⊕ 5 ♣ 1 ♣ 2 ½ 2 ^ >
  ngclearn C:\Users\ago10\IdeaProjects\beta-ngc-learn\ngc-learn
                                                                   class DataLoader(object): & Alexander Ororbia
  > a components
  > 

operations

✓ 
☐ utils

    > 🖻 density
    → i diffeq
     > 🖻 optim
     > 🗟 viz
       襣 __init__.py
       data_loader.py
       io_utils.py
       netric_utils.py
       nodel_utils.py
       patch_utils.py
        surrogate_fx.py
       weight_distribution.py
     .gitignore
     🦆 __init__.py
  Th External Libraries
                                                                       def __init__(self, design_matrices, batch_size, disable_shuffle=False, & Alexander Ororbia
  Scratches and Consoles
                                                                                     ensure_equal_batches=True, key=None):
                                                                           self.key = key
                                                                           if self.key is None:
                                                                                self.key = random.PRNGKey(time.time_ns())
                                                                           self.batch_size = batch_size
                                                                           self.ensure_equal_batches = ensure_equal_batches
```

Executing Python scripting code

- There are many ways to "run" code (execute Python interpreter)
 - Write / dynamically execute code "snippets" w/ Python interpreter directly
 - Use IPython interactive environment
 - Set up and iteratively build Python (Spyder) notebooks
 - Write Bash (terminal-level) scripts to call Python files (Linux-oriented)
- You will want to develop your own "workflow" as well as consider what your target audience will be
 - Notebooks can be useful for tutorials/demo(s), executable via web-browser
 - Interacting w/ Python interpreter can be helpful for quick sanity checks and personal self-study (good to do in this class)
 - Bash-scripting is old-fashioned but robust and reliable (it's what I do my research, because I'm old)

Version control

- Source code management (also known as "revision control")
 - Key software engineering practice of controlling, organizing, & tracking different versions of your software/scripts
 - Backbone: a history of computer files (e.g., Python text, supporting file types like images, etc.)
 - Useful for publicly "releasing" your code (to engender scientific reproducibility)
- Quality (free) tools:
 - Bitbucket
 - Github
 - Good to have, and very useful for team / multi-person projects
 - You should sign up for the "student developer pack" (gets you lots of important features like private repos)



Bitbucket

Github: One possible simple (work)flow



- 1) Git clone / set up your (local) repository (repo)
- 2) Write your code / folders (do things locally)
- 3) Git add / commit your code (differences) to the repo itself
 - git add <source_code_file/folder> // this points to what code is to be added
 - git commit -m "<insert message>" // this gets your code ready to upload
 - git push // this physically places your code (or changes) onto repo
 - git status

Developing some of the basics

import numpy as np

Vectorized operations / objects

- Vectors, matrices, tensors (> 2nd order arrays)
 - Essential tool for numerical computation
 - Useful data representation, especially for operations (ops) that are repeated for set of values
- Vectorization eliminates the need for explicit loops (batch operations applied to data)
 - In Python, ops often built on lower-level libraries (BLAS, LAPACK, XLA< etc.)
- Essentially what NumPy, i.e., numpy (and numpy. linalg), is for
 - Built on C (for processing/manipulating arrays)
 - All elements in a numpy (fixed-size) array are of the same type (homogeneous)
 - These arrays have in-built operations to be applied to them (along with functions/modules that work with these data structures)

Questions?

