PHYS4038/MLiS and AS1/MPAGS

Scientific Programming in

python™

mpags-python.github.io

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An introduction to scientific programming with

python™

Session 3:

Staying organised

Session 3

In this session:

- Organising your python installation
- Version control
- GitHub tools and workflow
- How to submit coursework

Managing your environment

- **Some good things about Python**
  - lots of modules from many sources
  - ongoing development of Python and modules

- **Some bad things about Python**
  - lots of modules from many sources
  - ongoing development of Python and modules

- **A solution**
  - Maintain (or have option to create) separate environments (or manifests) for different projects

Managing your environment

- **Desirable**
  - long term stability of your programs
  - help others easily install same dependencies
  - benefit from latest features and bugfixes

- **Solution**
  - maintain separate environments for different projects
    - Anaconda: `conda`
    - native Python: `pip` and `virtualenv`

Managing your environment

- **conda** – http://conda.pydata.org
  - specific to the Anaconda Python distribution
  - install modules
    - automatically manage dependencies and compatibility
    - similar to 'pip', but can install binaries and not just for python
    - can use pip within a conda environment (but try conda first)
  - create and switch between environments
    - specific collections of compatible modules and executables

  - Windows: use Anaconda Prompt
  - Linux/Mac: use any terminal

Managing your environment

- conda basic usage

```
$ conda create -n python_course  # -n <name> or -p <path>
$ conda activate python_course   # <name> or <path>
$ conda install scipy matplotlib
$ ipython  # use the environment
$ conda deactivate
```

Managing your environment

- Saving your environment (to use on another machine or distribute)

```
$ conda env export -n python_course > environment.yml
$ conda create -n new_env -f environment.yml
```

  - environment.yml contains all dependencies and versions
  - maybe neater to manually maintain your own environment.yml

```
name: myenv
dependencies:
  - python
  - numpy
  - matplotlib
```

  - to make your environment match an environment.yml file:

```
$ conda env update -n myenv -f myenv.yml --prune
```

Managing your environment

- **virtualenv**
  - general Python solution – http://virtualenv.pypa.io
  - modules are installed with pip – https://pip.pypa.io

```
$ pip install virtualenv   # install virtualenv
$ virtualenv ENV1          # create a new environment ENV1
$ source ENV/bin/activate  # set PATH to our environment
(ENV1)$ pip install emcee  # install modules into ENV1
(ENV1)$ pip install numpy==1.8.2 # install specific version
(ENV1)$ python             # use our custom environment
(ENV1)$ deactivate         # return our PATH to normal
```

Managing your environment

- **virtualenv**
  - can record current state of modules to a 'requirements' file

```
(ENV1)$ pip freeze > requirements.txt
$ cat requirements.txt
emcee==2.1.0
numpy==1.8.2
$ deactivate
$ virtualenv ENV2
$ sourceENV2/bin/activate
(ENV2)$ pip install -r requirements.txt
```

Managing your environment

- **Updating packages**

```
$ conda update --all
$ conda update scipy emcee
OR
$ pip install --upgrade
$ pip install --upgrade scipy emcee
```

Jupyter kernel discovery

- Can install and run Jupyter notebook in an environment, but better to run from base environment and then select kernel within notebook
- Jupyter can autodiscover conda environments
- Just need to install nb_conda_kernels in notebook environment

```
$ conda install -n base nb_conda_kernels
```

- and ipykernel in any environments you want to use in notebook

```
$ conda install -n myenv ipykernel
```

Version control

- Keep a secure backup of your work
- Maintain a record of significant changes
- Undo mistakes
- Undo undone mistakes that turned out to not be mistakes
- Log the reasons why you made particular changes
- Separate your work on different features
- Collaborate more easily

- Distributed version control
  - everyone has a full copy of history

GitHub

- Where many projects keep and share code
  - particularly open-source projects
- Unlimited private repos for education and research:
  - https://education.github.com

Similar alternative:

Getting started with version control

- Create a GitHub account
- Join assignment to create a new repository

  `https://classroom.github.com/a/bsgUSS2H`
- Create README in the browser
- Brief intro to Markdown

  https://guides.github.com/features/mastering-markdown/
- Installing git (with conda)

```
$ conda install git
```

Getting started with version control

- Clone your repo locally

```
$ git clone <link_to_your_repo>
```

- Edit README.md locally, then check status and diff

```
$ git status
$ git diff  # show changes
```

- Add files to commit, perform commit and push commit to GitHub

```
$ git add README.md
$ git commit -m"Edited the readme"
$ git push
```

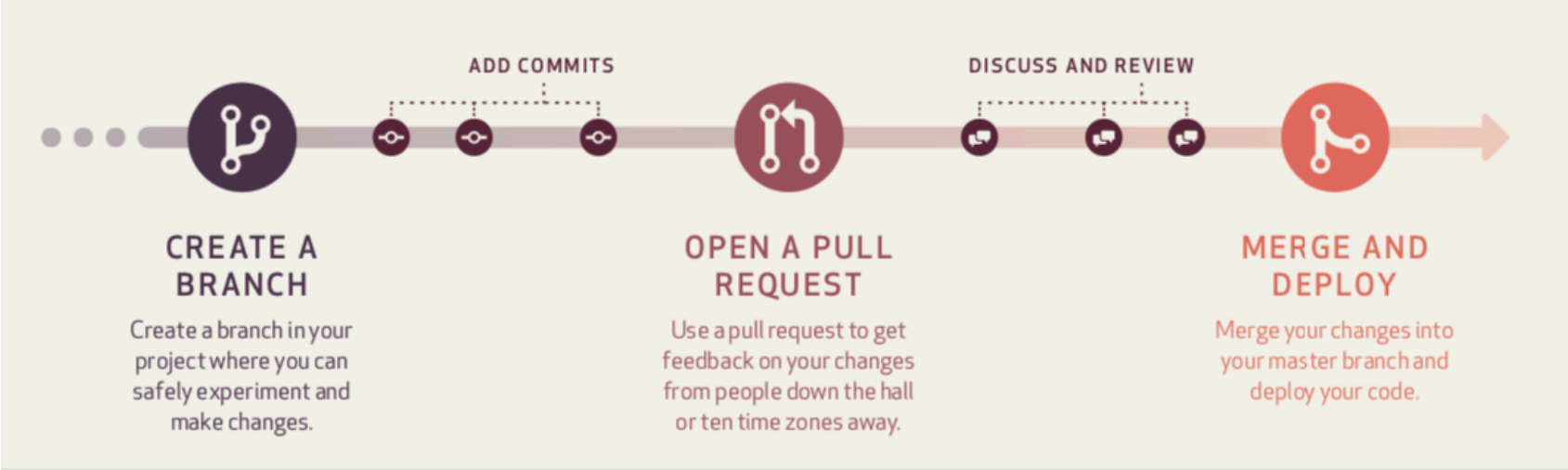
- If files changed on GitHub, fetch and merge the changes

```
$ git pull
```

https://guides.github.com/introduction/git-handbook/

Good practice and GitHub extras

- Using branches and tags
- Issues
- Pull requests



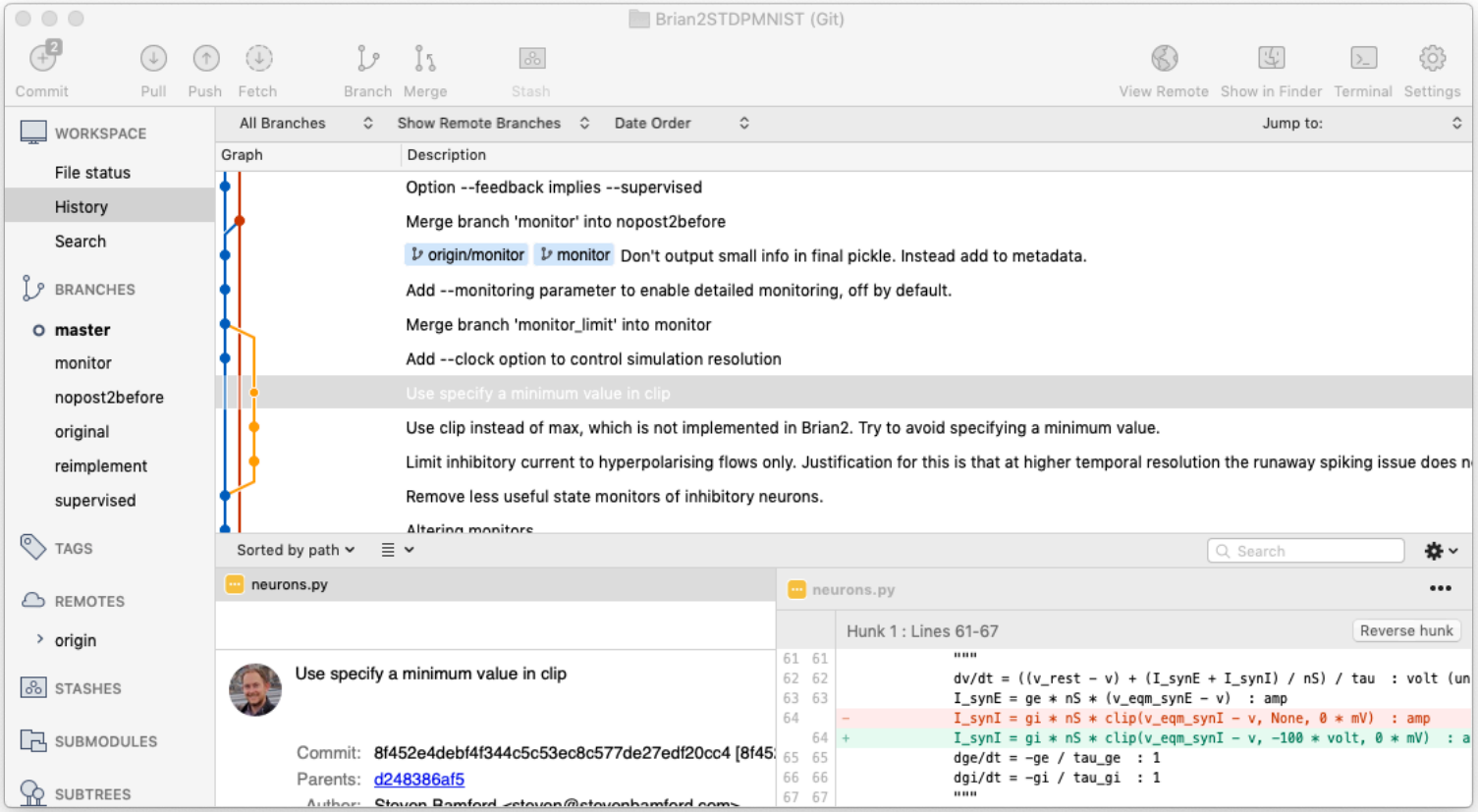
For more information:

- https://guides.github.com
- https://www.atlassian.com/git/tutorials
- https://lab.github.com

Git GUIs

Atlassian SourceTree — *GUI for Windows & Mac*

SmartGit — *GUI for Windows, Linux, Mac*



Assessment

For those taking this module for MPAGS credits

- Assessed by development of a Python program relevant to your interests
  - put course material into practice
  - opportunity to become familiar with Python
  - get feedback on your coding
- Your code should…
  - be written as an executable module (.py file) or Jupyter notebook (.ipynb)
  - do something meaningful: analyse real data or perform a simulation
  - define at least two user functions (but typically more)
  - make use of appropriate specialist modules
  - produce at least one informative plot
  - comprise >~ 50 lines of actual code
    - excluding comments, imports and other 'boilerplate'
  - contain no more than 1000 lines in total
    - if you have written more, please isolate an individual element

Code development

- Three stages (first two optional for MPAGS students)

1. hand-in by **28th October**
   - README describing what you intend your code to do
   - Rough outline of the code (classes, functions, snippets, comments, pseudocode)

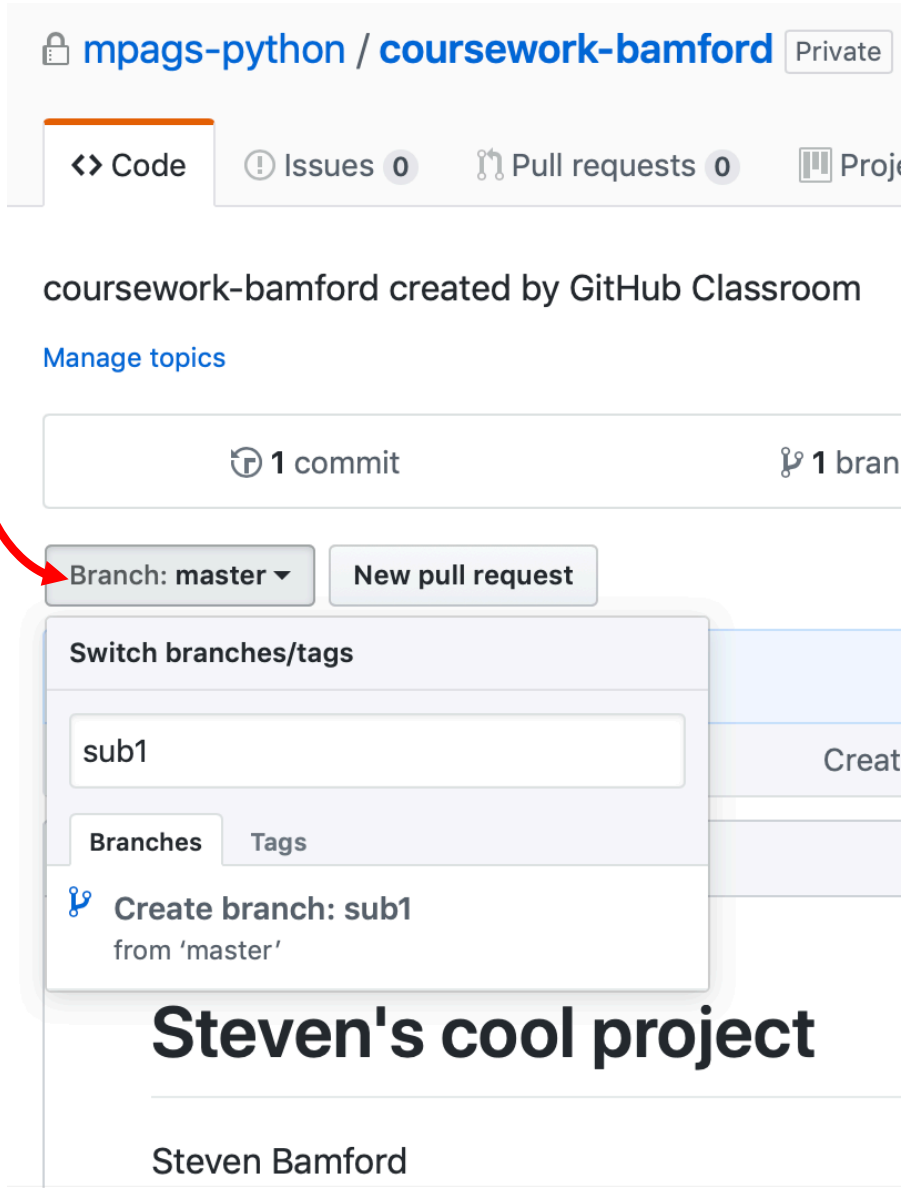
2. hand-in by **18th November**
   - Rough version of your code, may be incomplete, have bugs, although try to make it reasonable and easy to understand!

3. hand-in by **16th December**
   - Complete working version of your code

Deadlines are 3pm on Wednesdays.

Coursework submission

- Submission and feedback via your GitHub repository
- Mandatory for MLiS, optional for MPAGS
- Create a branch called `sub1`
- Should contain a README file including:
  - your full name and university
  - possibly some background (basic explanation, references, …)
  - an overview of the intended functionality of your program
  - ideas of the modules you plan to use
  - ideas of the structure of your code (functions, etc.)
  - possibly snippets or pseudocode
  - any remaining uncertainties or questions



Questions and exercises

Any questions?

- ask on the Slack channel (@Steven Bamford)
- email steven.bamford@nottingham.ac.uk
- ask in the next synchronous session

Exercises

Practice using conda and git