Practical 1: Getting Started

Getting to grips with Jupyter, Git and Markdown

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This week's practical is focussed on getting you set up with the tools and accounts that you'll need to across many of the CASA modules in Terms 1 and 2. Outside of academia, it's rare to find a data scientist who works entirely on their own: most code is collaborative, as is most analysis! But collaborating effectively requires tools that: a) get out of the way of doing 'stuff'; b) support teams in negotating conflicts in code; c) make it easy to share results; and d) make it easy to ensure that everyone is 'on the same page'.

0.1 Learning Outcomes

- You will have finished installing the tools needed to work on *Foundations* and *Quantitative Methods*.
- You will have a GitHub account enabling you to synchronise 'local' and 'remote' work.
- You will have seen how code is synchronised using the Command Line.

You *will* find things confusing this week, but they will start to make more sense as we move further into the module. The key is to keep trying things out and to ask for help when you get stuck.

1 Key Concepts/Tools

I wasn't sure where else to put these, but they *do* need to be written down so that you have a chance to learn them! Also note that, if you haven't done this already, you need to finish installing all of the tools listed on on the CASA Computing Platform web page. This process will take time, so please keep reading or work on other things while you wait!

1.1 Some Terminal Basics

Throughout *Foundations* we will make regular use of the 'Terminal', also known as the 'Command Line' (CLI), on both Mac and PC. There will be a whole lecture on the CLI and why/how we use it, but becoming comfortable with text commands is like gaining a bonus super-power alongside your new programming skills: need to change a line of text or code in thirty files? No problem! Need to start up a new Podman container? Done! Need to see how much free memory your server has? Yep!

There are many different types of terminal out there, but we are currently recommending that you use the following:

- Windows users: you are very strongly encouraged to use the Windows Terminal instead
 of the 'Power Shell', though the latter will also work in a pinch. The 'Command Prompt'
 (cmd) does not work for our purposes.
- **MacOS** users: please try to use **iTerm2** in preference to the built-in Terminal because it is easy to add additional usability features such as OhMyZSH, but it's not essential that you do so.

In fact, you can also run OhMyZSH on Windows but it looks like you're in for a bit of a long haul and might want to leave it for when you've done everything else this week.

If you need help understanding how to use the Command Line or want to be able to do *much more* there are a wide range of tutorials available.

Here are some starting points for learning more:

- **I need help understanding**: Software Carpentries is your friend! They have an entire tutorial titled The Unix Shell.
- I *still* **need help understanding**: the Programming Historian is another good place to look! And they *also* have an entire tutorial titled An Introduction to Bash.
- **I want to do** *more* **on the Command Line**: O'Reilly has produced an online book called Data Science at the Command Line that will take you much, much further.

Two more things:

- 1. Pressing the 'up' arrow on your keyboard moves you back one step in your command history. This is *massively* useful when you want to run the same command again (e.g. the one to run Podman!) since it saves you looking it up or copy+pasting.
- 2. To close a Terminal window you can run the exit command. If you make changes to the Terminal configuration file you often need to open a new window to see your changes take effect.

1.2 Following Convention

A common convention in programming is to use the <some text or other> to indicate that you should replace the text between the < and > with something that makes sense in your context. For example, if you see cd <directory> (cd means change directory) then if you want to change to the Documents directory you should type cd Documents. If you see <your username here> you should type jreades if that's your username. And so on. You do not include the < or > characters!

So, for example, if you see cd ~<your username> then you should type cd ~jreades (or whatever *your* username is). If you don't know your username you can type whoami. After each of these commands you need to hit the Enter/Return key () in order to run the command.

2 Running Podman

One of the most confusing things about starting up a new container (i.e. jreades/sds:2025) with a "local mount" (i.e. a location on your computer that Podman *connects* to the container) is that it seems like magic and it's often hard to understand why you're seeing what you are under the work directory.

2.1 Starting Up 'Right'

So *before you do anything else* please spend a minute in the Terminal (macOS) or Windows Terminal (Windows) learning how to get to your home directory and, within that, to a CASA directory where you can store your work and keep the virtual machine from accessing data that it shouldn't.

What we are doing is creating a directory on your computer that you can access from the virtual machine. This is where you will store your notebooks, data, and any other files that you need to work with. The ultimate structure we'll produce this:

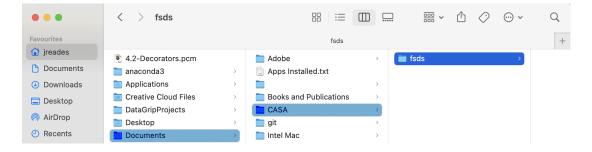


Figure 1: 'Target' Directory Structure

On both a Mac and a PC you should be able to run the following:

 cd \$HOME - this will change directory to your home directory (on a Mac it will be /Users/<your username>, on a PC it will be something like C:\Users\<your username>). Hint: cd means 'change directory'!

- 2. cd Documents this will move you into your 'Documents' folder. Note: on Windows this might be called My\ Documents (the \ is not a mistake, you need it when there's a space in the name), in which case it's cd My\ Documents! If you have set up your computer in another language this might be called something else, but the Terminal should still 'know' which folder contains your documents.
- 3. mkdir CASA this will create a CASA folder in your home directory.
- 4. cd CASA you are now changing into the CASA directory.
- 5. echo \$pwd (PC) or pwd (Mac) this should show you the 'full path' to your new CASA directory (e.g. /Users/<your username>/Documents/CASA or something like that).

Leave the Terminal window open! You will need it in a moment.

2.2 Configuring the sds2025 Image

During the 'install festival/social' you should have installed Podman and, time permitting, 'pulled' the image appropriate to your system. If you haven't, then you should do so as a priority now.

2.3 Running Podman

By default, the best way to start the sds2025 virtual machine (also called a 'container') is from the Terminal or Power Shell.

2.3.1 On Windows

Using the *same* Power Shell copy and paste the following **all on one line**:

```
podman run --rm -d --name sds2025 -p 8888:8888 -v "$(pwd):/home/jovyan/work" jreades
```



Windows Commands

\$ (pwd) is actually a *command*, you are asking the Power Shell to use the *current working* directory (pwd == print working directory) as the 'mount point' for the work directory. The Command Prompt doesn't support pwd, but the Power Shell should. You can check this by simply typing pwd and hitting enter () to see if you get an error.

2.3.2 On macOS

Using the same Terminal copy and past the following (change the image to jreades/sds: 2025amd if using an older Intel Mac):

```
podman run --rm -d --name sds2025 -p 8888:8888 \
  -v "$(pwd):/home/jovyan/work" \
  jreades/sds:2025-arm start.sh jupyter lab \
  --LabApp.password='' --ServerApp.password='' --NotebookApp.token=''
```

No work directory or Permission Denied?

On some macOS machines we are seeing (or, rather, not seeing) problems with the work directory as well as 'permission denied' errors whenever you try to make changes to this directory. In this case the answer appears to be that you need to change part of the run command:

- From: -v "\$(pwd):/home/jovyan/work"
- To: -v "\$(pwd):/home/jovyan/work:rw,z,U"

This can still have a few issues with files that you add to the work directory *after* starting up podman but we'll run you through this issue (and how to deal with it) in class.

2.4 How do I Know it Worked?

With the virtual machine running, you will *mainly* interact with Python through your browser. To check if it's running, we just have to visit the web page and see what happens: http://localhost: 8888/lab/tree/work/. We'll talk more about exactly what is going on over the next few weeks, but this should show you a page that looks something like this (probably with fewer files listed on the left-hand side):

File Edit View Run Kernel Tabs Settings В C Filter files by name Q work/fsds/practicals m / ... / fsds / practicals / Name Last Modified Notebook data a year ago dtools a year ago img 2 hours ago Practical-01-Getti. an hour ago ■ Practical-02-Fou... 6 days ago Practical-03-Fou Practical-04-Obje... 6 days ago >_ Console Practical-05-Num... 6 days ago Practical-06-Spat... 6 days ago Practical-07-Text... 6 days ago Practical-08-Dim... 6 days ago Practical-09-Visu... Practical-10-Grou... Practical-10-Grou... 2 years ago Practical-10-Grou... 2 years ago \$_ Other Practical-10-Grou... 6 days ago ■ Practical-Supple... a year ago ■ Practical-X-Air_Q... a year ago M \$_ a year ago Practical-X-Classi... 2 years ago Markdown File Practical-X-Correl... a year ago Practical-X-Merge...

Figure 2: Screenshot of Jupyter Lab

See the Container Run (and Run)...

Simple 0 5 0 6

Once you have started a container, the machine will continue running until you either restart the computer or stop the container. This *can* consume memory and battery power indefinitely.

Launcher

3 Setting Up GitHub

Understanding how to use Git and GitHub effectively is a core element of learning to code. So one of the *first* things that we are going to do is set you up with an account and a new repository.

3.1 Your New GitHub Account

It doesn't really matter which way you do this, but we recommend that you set up your new GitHub account with *both* your personal and your UCL email addresses. GitHub 'knows' about educational users and will give you access to more features for free if you associate a .ac.uk email address to your account. So choose one email address to start with and then add the other one later.

From a security standpoint you should *also* enable 2-factor authentication so that you receive a text message when you log in on a new machine and are asked to confirm a code.

So in order to complete this task you need to do the following (**more detailed explanations below**):

- 1. Create a login with GitHub (if you've not done so already).
- 2. Create a new **private** repository on GitHub (see below).
- 3. Edit the README.md and .gitignore files for your new repository (see below).
- 4. Save the changes (this is called a 'commit') and explain in a general way what edits you did (see below).
- 5. Work out how to compare the original and edited versions of any file in your browser.

3.2 Creating a Private Repository

To create a repository, click on the + at the upper-right corner of the GitHub web page and select New Repository. You might as well call your 'repo' fsds or foundations since that's a lot shorter than foundations_of_spatial_data_science.

! Your 'Repo' Name

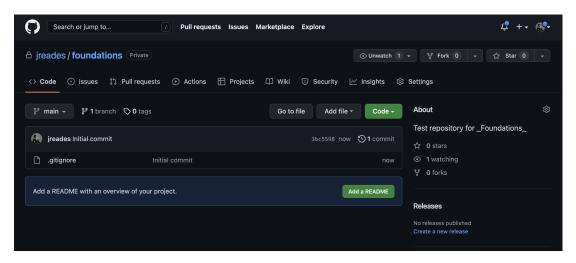
For the purposes of this tutorial (and all subsequent tutorials) I will assume that your repository is called fsds. You can call it whatever you like, in which case you will *always* need to substitute the name that *you* chose wherever you see me write fsds.

It's always helpful to provide some basic information about what's in the project (*e.g.* your notes and practicals for the *Foundations* module). And finally, make sure you:

- 1. Change the visibility from Public to Private,
- 2. Tick Add a README file,
- 3. Change Add .gitignore from None to template: Python.

Click Create Repository and you should end up on a page that looks like this:

Figure 3: Repository created



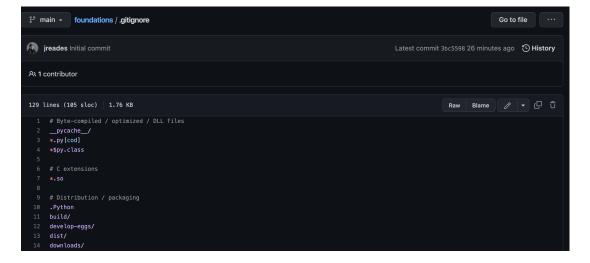
Your new repository has been created (on GitHub)! The README is a file – written in Markdown – that explains the purpose of a repository and any other notes you care to add.

4 Updating the .gitignore File

The .gitignore file tells Git what files to ignore by default. Unless you *force* Git to add an ignored file it will happily coexist in your *local* repository alongside files that are version-controlled and 'shared' with GitHub. Why would you want this? Because data does *not* belong in Git: large files especially will totally screw up your repository and they are really hard to remove. So we want to tell Git that it should leave those alone.

The Python template for .gitignore includes a lot of useful files and folders that we wouldn't want Git to track for us. But it *doesn't* include data. In your web browser, click on the .gitignore file and then the 'pencil' icon on the right to edit it on GitHub. You should see something like this:

Figure 4: Editing the .gitignore file



4.1 Exclude Data Files

We want to make it hard to accidentally add a large data file to our repository. Git/GitHub isn't designed for large, binary files (you can't 'read' a Parquet file) and we assume that data is backed up or available elsewhere, but our *code* is not! So as a first step we want to exclude files that are likely to just be 'data':

File Type	Extension
CSV	.CSV
Excel	.xls, .xlsx
Zip	.zip
GZip	.gzip
Parquet	<pre>.parquet, .geoparquet</pre>

Maybe look to see how files are already done to help you figure out how to exlcude .zip, .gz, and .csv files... but as a hint: * means 'any sequence of characters' so *.py means any Python script file ending in .py.

4.2 Exclude a Data Directory

To make it even *less* like that we accidentally include data, let's also exclude a data directory from our repository. As a clue, nearly everything in the Distribution / packaging section of the .gitignore file is a directory to be excluded from Git.

So how would you indicate that data is a directory? Once you're sure, add the data directory!

When you are done, don't forget to add a 'commit message' (e.g. 'Added file types to exclude to .gitignore') at the bottom and then click Commit changes.



Quick Answer

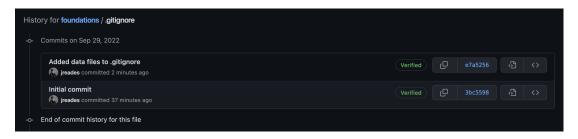
I don't want you to get hung up on this one thing in Practical 1, so if you just can't make sense of what you're being asked to do here, have a look at the Answers at the bottom of this page.

4.3 Check Your Changes

Once you have committed your changes, you should be back to the default view of the .gitignore file but there should be a message to the effect of Latest commit <some hexadecimal number> 10 seconds ago and, next to that, a History button.

Click on 'History' and let's go back in time!

Figure 5: The Gitignore history



On the history page you can browse every edit to your file. Whenever you commit a file, this like taking a snapshot at a point in time. Using the 'History' you can compare two different snapshots in order to see what has changed. This would help you to work out how you broke something, check that requested changes have been made, or see how an error might have been introduced.



Viewing Your Commit History

You can mouseover the buttons to see what they do. Why don't you try to find See commmit details and check what edits you made to the .gitignore file? You should see at least three plusses in the history view representing three new lines in the .gitignore file.

5 Creating Your First Remote File

To get some practice with Markdown let's write up some notes directly into our GitHub repository (aka 'repo'). You'll notice that we've not yet hit the BIG GREEN BUTTON marked Add a README... Let's do that now!

This will take you to an editing page for the new README.md file. You can type directly into this web page and it will update the repository, but only once you commit your edits.

5.1 Working on Your Markdown

Write your README file using at least the following Markdown features:

- A level-1 header (#)
- A level-3 header (###)
- Italic text (_this is italicised_)
- Bold text (**this is bold**)
- A link ([link text](url))
- An image (![Alt text](image_location))

If you're unsure how these work, just double-click on this text and you'll see Markdown in a Jupyter notebook. Here's some sample text to get you started:

```
### Foundations of Spatial Data Science
This repository contains practicals and notes from the _Foundations_ module.
```

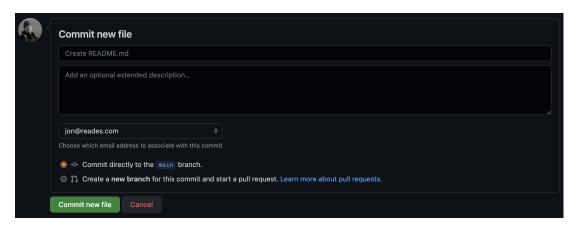
```
You can find the original [here](https://jreades.github.io/fsds/).
```

Don't forget to check out the "Preview" tab!

5.2 Commiting a Change

Once you're happy with how your text looks and works, it's time to commit! Scroll down to where you see something like this (you will see your *own* GitHub username, not mine):

Figure 6: GitHub Commit



You can just accept the description (e.g. Create README.md) or you can write your own. You can also provide an extended description if you choose. Then click Commit new file and you will see your new README appear.

6 Setting Up Git Locally

OK, so now we have our Git repository set up remotely and want to create a local *clone* so that we can easily syncrhonise changes between GitHub and our computer. Free backups and collaboration!

6.1 Configuring Defaults

The first thing to do is set up the default username and email for GitHub. These can be changed on a project-by-project basis, but to begin with it's best to set up the *global defaults*. Using the Terminal, enter the following (replacing <...> with *your* details):

```
git config --global user.email '<your GitHub email address>'
git config --global user.name '<your GibHub username>'
```

Recall: Convention!

As a reminder, <...> is a convention in programming to indicate that you should replace the text between the < and > with something that makes sense in your context. For example, if you see '<your GitHub email address>' you should type, for example,

6.2 Creating a Personal Access Token

For copying changes up to/down from GitHub, you *must* use a Personal Access Token. This is like issuing special passwords that allow only limited access to parts of your GitHub account.

To create a Personal Access Token:

- Visit *your* GitHub User Page (e.g. github.com/jreades)
- Click on your user icon (at the top-right corner of the page) and click the Settings link (near the bottom on the right side of the page).
- Scroll down the settings page until you get to Developer settings (near the bottom on the *left* side of the page).
- Click the Developer settings link to reach the 'apps' page and then click on the Personal access tokens link.
- Select Tokens (classic) from the left-hand menu and then click the Generate new token button.

Types of Personal Tokens

You now need to choose the type of token to generate. I personally find the old type of tokens easier to work with because the 'new' fine-grained tokens are intended to support complex workflows when all we're trying to do is allow one computer to push/pull from Git.

- Generate new token (classic) for general use token and then specify the following:
 - I'd suggest writing FSDS Token or something similar in the Note section.
 - Set the expiration to 90 days
 - Click the repo tickbox for 'Full control of private repositories'.
- Save the resulting token somewhere safe as you will need it again! (e.g. a Note on your phone, a password manager, etc.).



🛕 Keep your Personal Token Safe

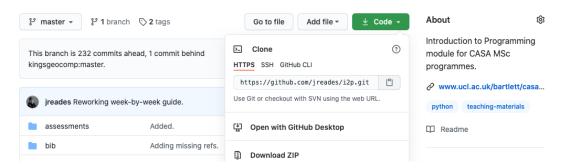
You will need it at least twice in this tutorial and may want to use it again on other computers. You can always create a new one, but then you'll need to update every computer where you access your GitHub repositories.

6.3 Cloning Your Repository

Now we are going to clone (i.e. copy) the repository that you just created on to your own computer. This is surprisingly straightforward provided that you have installed the command line tools.

On your private repository page, click on the green button labeled Code visible in the screenshot below:

Figure 7: Screenshot of cloning interface



You should then copy your HTTPS URL (in my screenshot it's https://github.com/jreades/i2p.git).

Now go back to the Terminal or PowerShell that you left open earlier and type the following (replacing <the_url_that_you_copied_from_the_browser> with the URL that you copied from GitHub):

```
git clone <the_url_that_you_copied_from_the_browser>
```

The first time that you do this, you will need to provide login information. Use your GitHub username and the Personal Access Token that you just created. On your computer you should now see a new directory with the same name as your repository. For example: Documents/CASA/fsds.

6.4 Storing Credentials & 'Pulling'

You can now activate the credtial helper that will store your Personal Access Token (though you should *still* keep your secure note!):

```
cd fsds
git config credential.helper store
git pull
```

When you type git pull you should be asked again for your username and password. You should (again) use the Personal Access Token as your password. You should not be asked again for pushing or pulling data into this GitHub repository. If you are *not* asked for your Personal Access Token then this likely means that your token is already saved and ready to use on all future 'actions'.

6.5 Jupyter < - > Your Computer

If you now go back to Jupyter, you should now see that the work directory is actually the same as the CASA directory that you created earlier; you know this because you can now see an fsds directory that wasn't there before.

This is because Podman is 'mounting' the work directory in the container to the CASA directory on your computer. This means that you can save files in the work directory in Jupyter and they will be saved in the CASA directory on your computer.

i Organising Your Work

There are any number of ways to organise your CASA work, what's important is that you are logical about things like names and hierarchy. This will make it much easier to access files and notebooks using Podman, Quarto, and Python.

6.6 Adding a Local File to Your Repository

In order to tie together the different concepts covered above, we are now going add Practical 1 (this practical) to your GitHub repo. The easiest way to do this is to download the notebook by clicking on the Jupyter link on the right side of this page. So the process is:

- 1. Click on the Jupyter link to save this file to your computer as a notebook with the extension .ipynb.
- 2. Move the file to your new repository folder (e.g. \$HOME/work/Documents/CASA/fsds/).



It is highly likely that your browser automatically added a .txt extension when you saved the Notebook file to your computer. You need to remove that ending to your file name or Jupyter won't be able to run it. You can rename a file by either doing it directly in the Finder/Windows Explorer, or by *moving* (mv) the file:

```
mv <notebook_name>.ipynb.txt <notebook_name>.ipynb
```

In the Terminal/PowerShell we now need add this file to Git so that it knows to keep track of it. Unlike Dropbox or OneDrive, just putting a file in a repo directory does not mean that Git will pay attention to it:

```
# Assuming that you are 'in' the 'fsds' directory...
git add Practical-01-Getting_Started.ipynb
git commit -m "Adding notebook 1 to repo."
```

🛕 Add, Commit, Push, Repeat

Unless you have *added* and *committed* a file to Git then it is *not* version controlled. Unless you have *pushed* your committed files to GitHub they are only backed up locally.

6.7 Status Check

We now want to check that the file has been successfully added to Git. We do this with a status check in the repository directory (i.e. cd \$HOME/work/Documents/CASA/fsds/):

```
git status
```

You should see something like:

```
On branch master
Your branch is ahead of 'origin/master' by 1 commit.
  (use "git push" to publish your local commits)
```

This is telling you that your local computer is 1 commit (the one that you *just* completed) ahead of the 'origin', which is on GitHub. GitHub doesn't *have* to be the origin (nor does the repository have to be one that we created in order to be an origin) but conceptually and practically it's easier to create new repositories on GitHub and clone them to our computer.

6.8 Keep Pushing

To synchronise the changes we just made, let's follow Git's advice:

```
git push
```

You should see *something* like the below series of messages (the exact details will differ, but the 'Enumerating, Counting, etc' messages will be the same):

```
Enumerating objects: 5, done.
Counting objects: 100% (5/5), done.
Delta compression using up to 8 threads
Compressing objects: 100% (3/3), done.
Writing objects: 100% (3/3), 306 bytes | 306.00 KiB/s, done.
Total 3 (delta 2), reused 0 (delta 0), pack-reused 0
remote: Resolving deltas: 100% (2/2), completed with 2 local objects.
remote: This repository moved. Please use the new location:
         https://github.com/jreades/fsds.git
To https://github.com/jreades/fsds.git
   7410d0e..45aa80a master -> master
```

If you now go over to your browser and visit your GitHub repo page (e.g. https://jreades.github.io/fsds/) — pressing the Reload button if you had the page open already — then you should see that the file you added *on your computer* is also showing up on the GitHub site as well! This means it's now fully version-controlled and backed-up.



🛕 Keep Pushing

Unless have *pushed* your commits to GitHub they are *only* stored on *your* computer. So your files can be properly version-controlled, but without a *push* if you lose your computer you *still* lose everything!

6.9 More About Git

From here on out you can keep changes made either directly on GitHub or locally on your computer (or any other computer to which you clone your repository) in synch by using git push (to *push* changes from a local computer *up* to the origin on GitHub) and git pull (to *pull* changes available on the origin *down* to the local computer).

That said, you can do a *lot* more than just push/pull to your own repository and this Twitter thread leads to a lot of useful additional resources to do with Git:

- Introduction to Version Control with Git on the Programming Historian web site is written for digital humanities researchers so it's intended to be accessible.
- Oh My Git is an 'open source game' to help you learn Git.
- Git Meets Minesweeper? is apparently a 'thing'.
- Visual Git Reference if you think visually or just want to check your understanding.
- Version Control with Git is a Software Carpentries lesson that takes you quickly through the important elements of getting set up and started. It would be a good refresher.
- Altassian's Documentation provides more detailed explanations of the commands and options.
- Learn Git Branching focusses on a key concept for software *collaboration*.
- Git Immersion provides a 'guided tour' of the fundamentals.



For the Group Work every member of your group will need to make contributions to a GitHub repository. This will require learning how to invite others to be contributors, how to merge changes, and how to deal with conflicts of the coding kind.

7 Setting up a GitHub Web Site



Bonus Content

It is not core to this module, but if you'd like to really make the most of Git, why not create a GitHub.io web site? Using Markdown (for the most bare bones effect) or code (via Quarto), you can render and push a web site to <your GitHub username>.github.io/. You might find this useful for creating a simple portfolio, blog, or other collection of 'outputs' that you can use to demonstrate to employers that you know your way around.

Rather than create a GitHub.io site using your *Foundations* repository, we'd recommend building one in the separate 'main' repository so that, for example, jreades.github.io, returns a web page.

To do this, the steps are detailed here, but read on to get an overview:

- 1. On the GitHub web site, create a new repository called <your username>.github.io (where <your username> is whatever your github username is). So for us, it would mean creating a *new* repository called <code>jreades.github.io</code>.
- 2. For your first web site, try setting up GitHub pages without specifying a branch: this way, anything that you put into your GitHub repository will show up on the public web site. Later, when you are more comfortable with GitHub, you may wish to switch to using a branch so that you can do work without always and immediately updating the web site.
- 3. One you've followed the GitHub instructions for publishing a web site, you should clone the site to your computer.
- 4. After cloning the site to your computer, try making a change to the README.md file and pushing the change back to GitHub. After a minute or two (possibly up to 10 minutes) you should see your web page update!

Congratulations, you can now publish a web site using nothing more than Markdown.

As you develop your Markdown, coding, and Quarto skills, you might also want to look into publishing to GitHub pages from Quarto. That's how we build the entire *Foundations* web site, so there's a *lot* further that you can go with this...

7.1 Other Useful Resources

- · GitHub Markdown Guide
- Common Mark
- · Markdown Guide, which helpfully includes do's and don'ts.

Finally, these are a bit overkill but the bits about setting up and installing git, bash/zsh, and so on may come in handy later:

- Setting Up a New Mac
- Beginner's Guide to Setting Up Windows 10
- Setting up Windows without Linux
- Microsoft Python Setup Guide

8 Answers

Normally, we will provide 'answers' later in the week, but for *this* week it makes sense to provide them right away if you need them...

8.1 .Gitignore

The main thing you should notice is the pattern: * means 'anything', while / at the end of a line implies a directory. So the following four lines should be added to your .gitignore file:

```
*.zip
*.gz
*.csv
*.gzip
*.feather
*.geofeather
*.parquet
*.parquet
data/
```

That's it.