JOHNS HOPKINS
WHITING SCHOOL
of ENGINEERING

EN.540.635
Software Carpentry

Lecture 8
Git, Version Control, and Python Modules

Have you ever…

- Overwritten a file by accident?
- Deleted a file by accident?
- Worked on a project with others, but had issues whenever you had to merge your work?
- Made a lot of edits to something until you thought:

  "Huh… what I had in that first version was much better than what I have now…"?

What is Version Control?

- It stores changes to your work over time, so that you may always retrieve what you had lost.
- It allows you to make edits without breaking everything.
- It allows several people to work together without annoying one another.
- The most popular platforms for version control are:

Git

SVN

Git and Github

- Git was originally created by Linus Torvalds in 2005, originally for use in the Linux kernel. It is free, open-source, and available for all common operating systems (Windows, macOS, Linux).

- Github is a website that has Git functionalities and other features useful for hosting source code.

- In concept, any project you are working on that involves files (source code, Word documents, PowerPoint slides, etc.) can be managed with Git and Github.

- Git Website: https://git-scm.com/
- Github Website: https://github.com/

Git and Github

- In practice, pretty much any large software project that requires collaboration between team members needs to use version control.

- For this class, Git and Github will be our way to learn about it and incorporate version control into your work.

- It is important to note that you do not NEED Github in order to use Git - everything can technically be done from the command line.

Command Line Interface (CLI) vs. Graphical User Interface (GUI)

- If we can do everything we need to do with a GUI (which Github does provide), why should we learn how to do things from the command line?

- Using the command line can be faster than using a GUI at the expense of being a bit more complicated to learn and use.

- If you work in tech or software development, there may be many times where you will have to use the command line because a GUI is not available.

Your Profile on Github

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Why GitHub? Enterprise Explore Marketplace Pricing Search / Sign in Sign up

Henry Herbol
hherbol

PRO

Postdoctoral Researcher in the field of Computational Chemistry and Machine Learning with a Ph.D. in Materials Science and Engineering from Cornell University.

Block or report user

Overview Repositories 12 Projects 0 Stars 6 Followers 16 Following 9

Popular repositories

neigh
C code for python - Generate neighbour list
C ★1 1

clancelot
Forked from jminuse/clancelot
A set of computational chemistry Python libraries and tools developed by the Clancy Group, Cornell University
Python

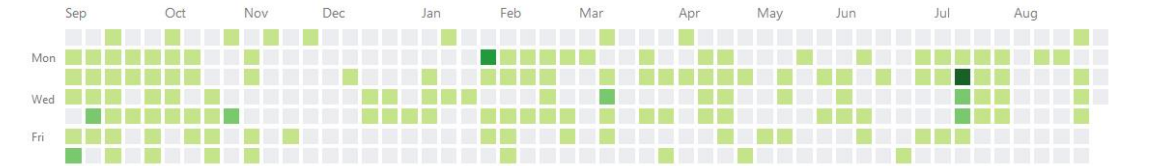
Grad-MCSMRFF
Forked from jminuse/lammps-min-params
A LAMMPS min_style for parameterizing force fields
Python

frazier-pipeline
Pipeline for submitting solubility simulations. Bonus output may include Unsaturated Mayer Bond Order amongst other things.
Python

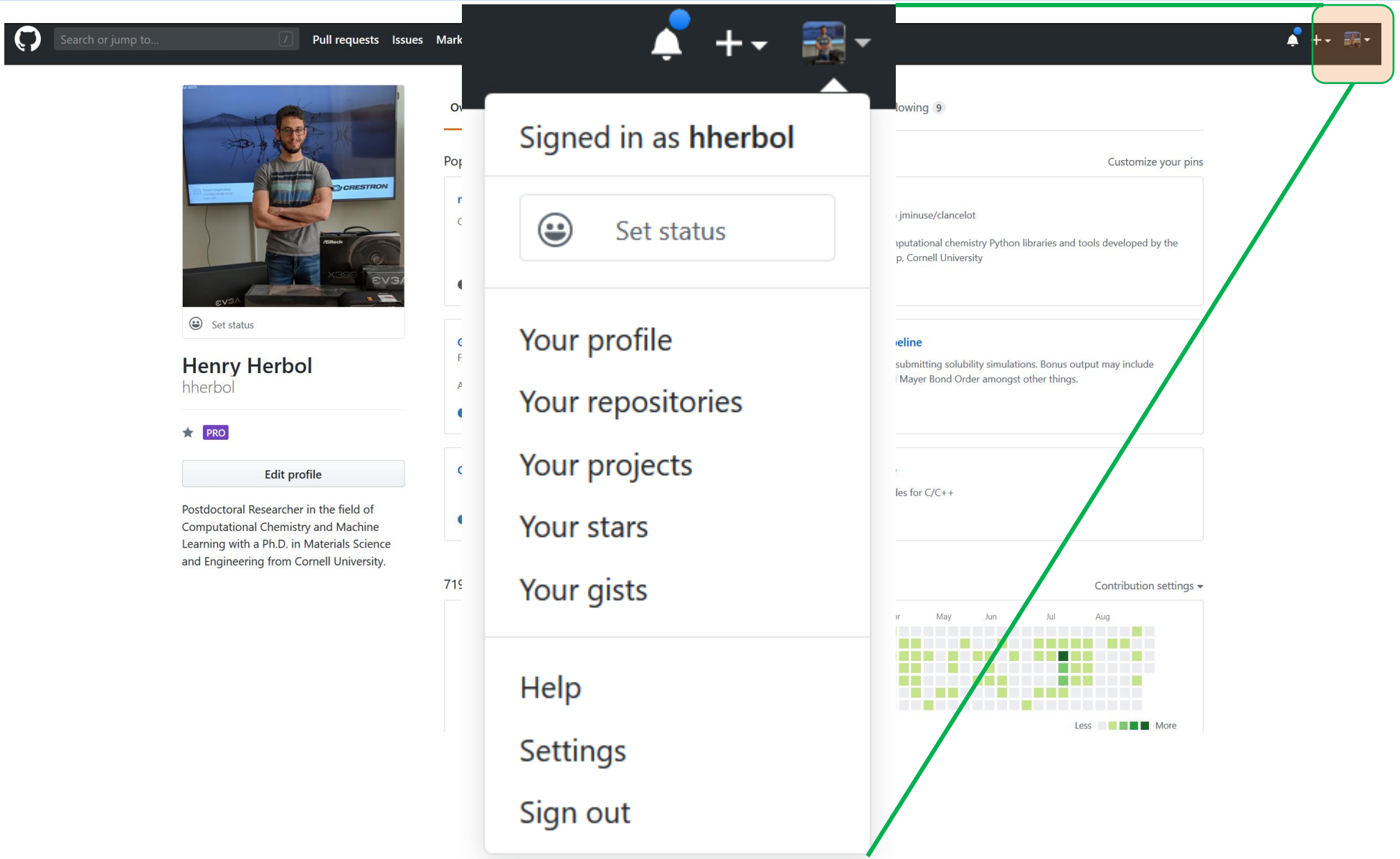
ColourEdit
Python

C_Practice
Practice Codes for C/C++
C

719 contributions in the last year



Sidebar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Pull requests
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PRO
Edit profile
Postdoctoral Researcher in the field of Computational Chemistry and Machine Learning with a Ph.D. in Materials Science and Engineering from Cornell University.
Customize your pins
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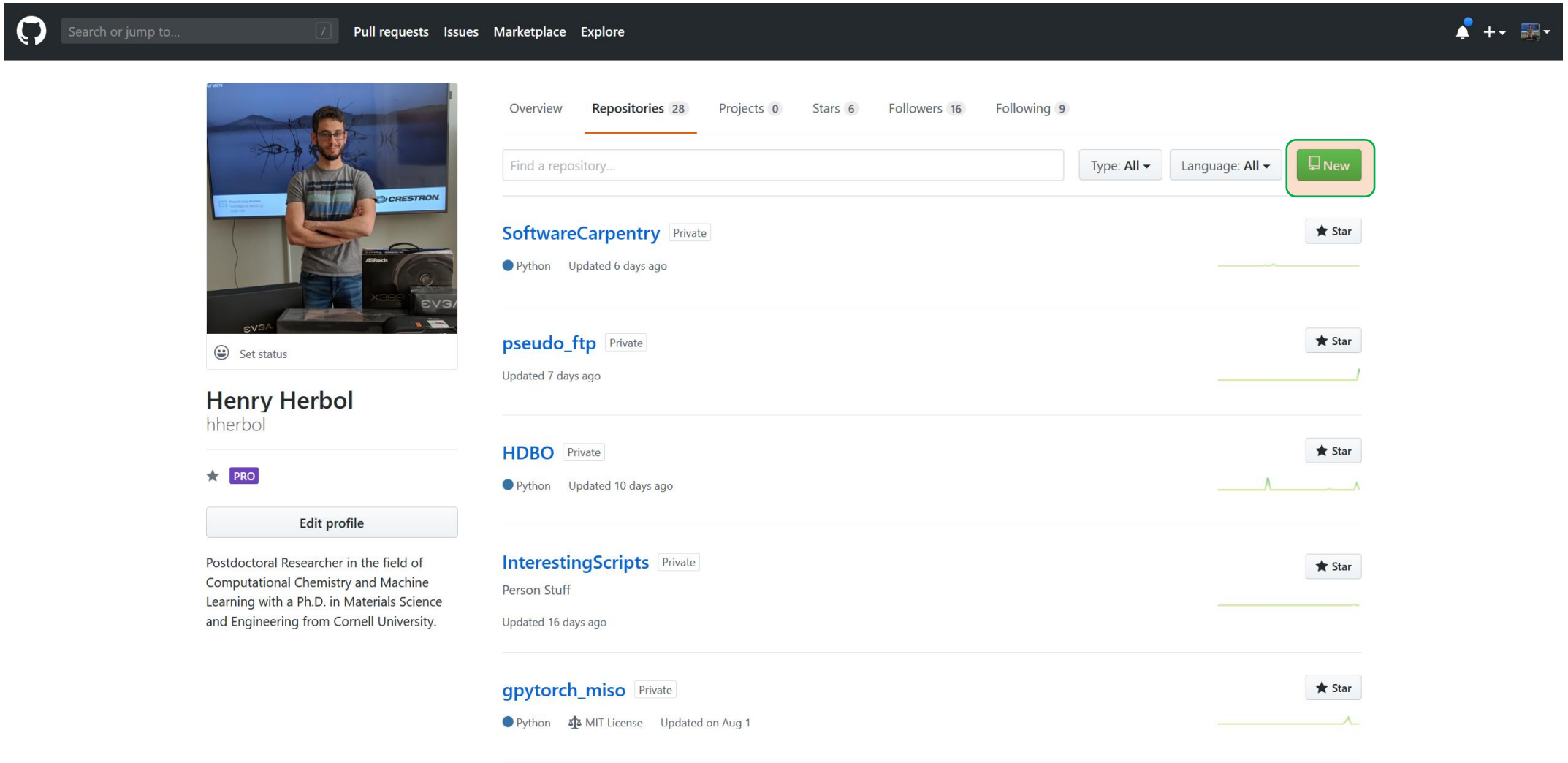
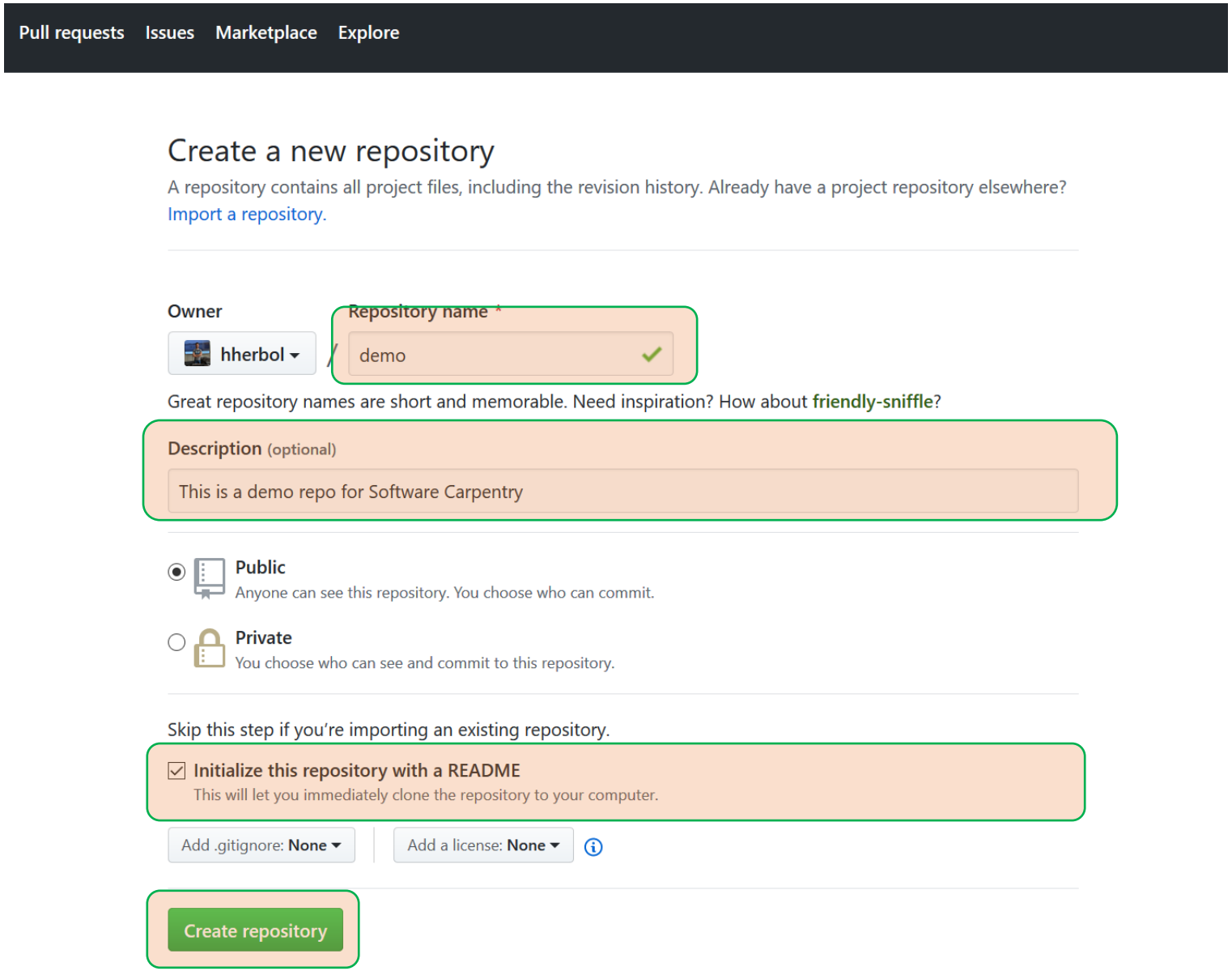
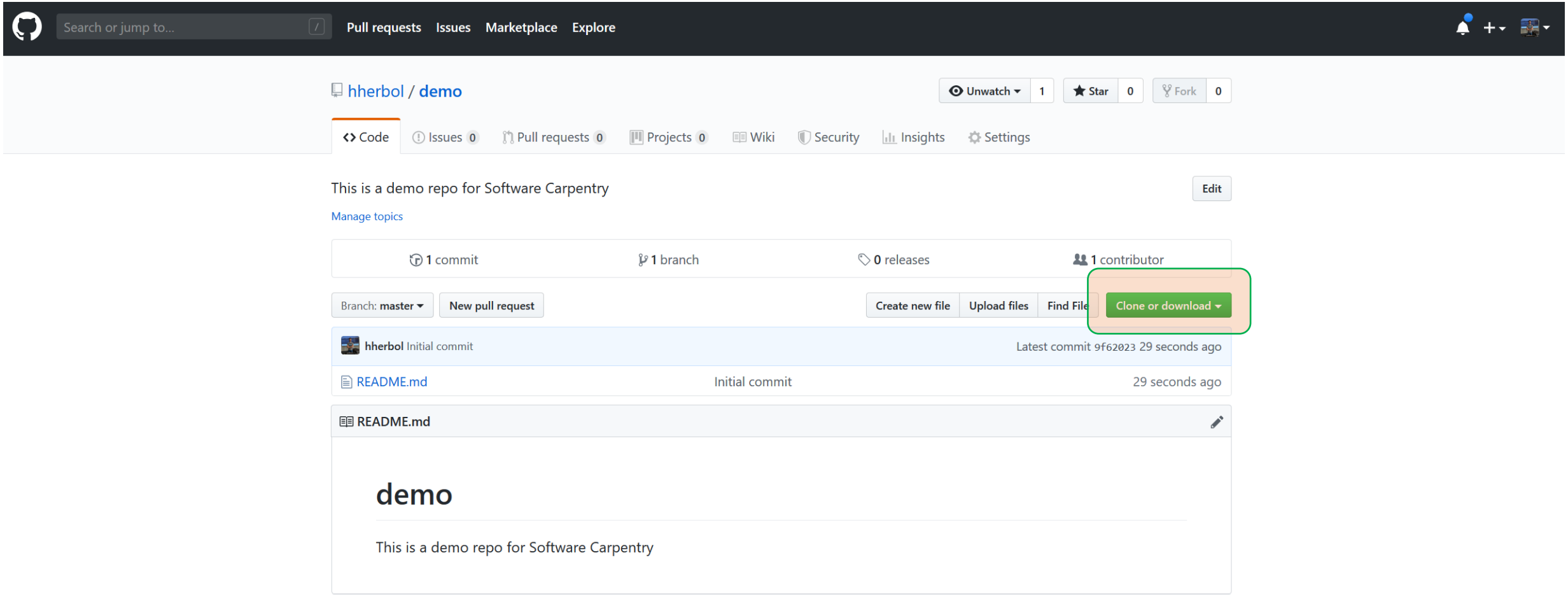
Your Repositories



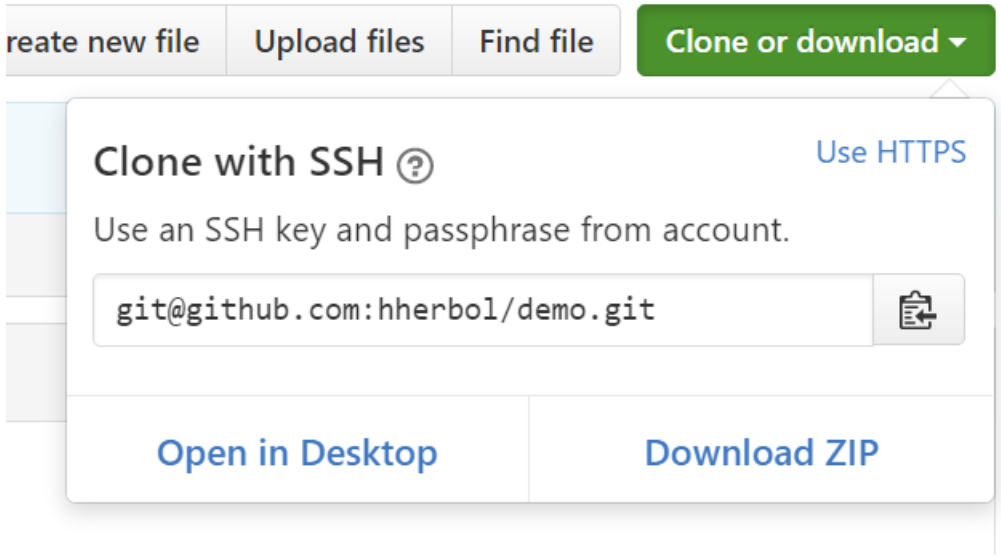
Creating a New Repository

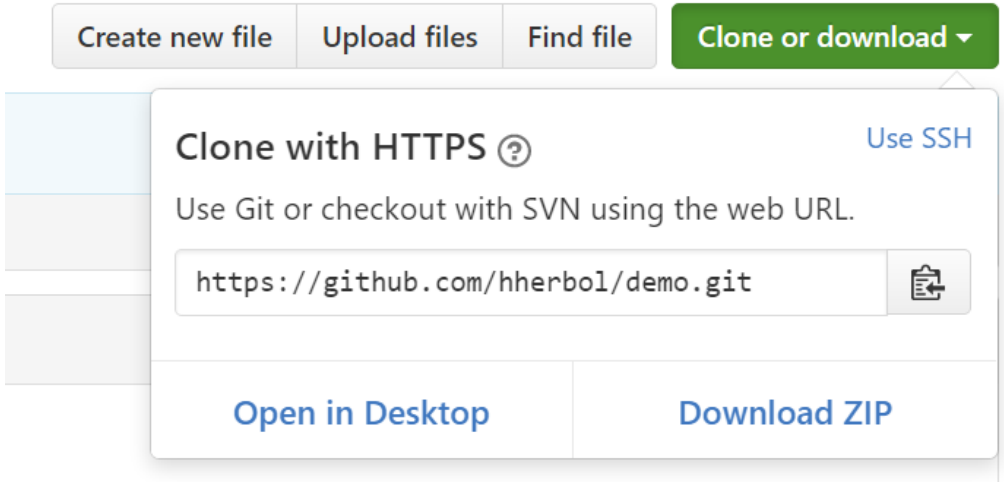


Creating a New Repository



Cloning from Github





README and .gitignore

- README.md is a markdown file that should contain text that acts as a ”user manual”. It should cover some/all of the following things:
  - Configuration/installation instructions
  - Operating instructions
  - File manifest
  - Troubleshooting (known errors and bugs)
  - Credits and acknowledgments

- .gitignore is a special file that you can use to specify files that git should ignore. Any files that appear in your repo that you don’t need (or are too large), you should list them in this file.

Git Command Summary


```
usage: git [--version] [--help] [-C <path>] [-c <name>=<value>]
           [--exec-path[=<path>]] [--html-path] [--man-path] [--info-path]
           [-p | --paginate | -P | --no-pager] [--no-replace-objects] [--bare]
           [--git-dir=<path>] [--work-tree=<path>] [--namespace=<name>]
           <command> [<args>]

These are common Git commands used in various situations:

start a working area (see also: git help tutorial)
   clone      Clone a repository into a new directory
   init       Create an empty Git repository or reinitialize an existing one

work on the current change (see also: git help everyday)
   add        Add file contents to the index
   mv         Move or rename a file, a directory, or a symlink
   reset      Reset current HEAD to the specified state
   rm         Remove files from the working tree and from the index

examine the history and state (see also: git help revisions)
   bisect     Use binary search to find the commit that introduced a bug
   grep       Print lines matching a pattern
   log        Show commit logs
   show       Show various types of objects
   status     Show the working tree status

grow, mark and tweak your common history
   branch     List, create, or delete branches
   checkout   Switch branches or restore working tree files
   commit     Record changes to the repository
   diff       Show changes between commits, commit and working tree, etc
   merge      Join two or more development histories together
   rebase     Reapply commits on top of another base tip
   tag        Create, list, delete or verify a tag object signed with GPG

collaborate (see also: git help workflows)
   fetch      Download objects and refs from another repository
   pull       Fetch from and integrate with another repository or a local branch
   push       Update remote refs along with associated objects

'git help -a' and 'git help -g' list available subcommands and some
concept guides. See 'git help <command>' or 'git help <concept>'
to read about a specific subcommand or concept.
```

- To check if you have Git installed on your computer, you will see a display like this if you type git into your command line.
- This menu has all the common commands listed (and they are grouped based on their function).
- There are also tutorials and help functions built in.

The Help Function

- The ***single most important thing*** to remember is that if you ever have any questions about a certain Git command, you can always use the help flag.

- For example:

```
git <command> --help
```

- This will take you to a screen that displays the documentation for the command you are using. To exit this screen, press the q key.

Repositories

- A repository, or *repo* for short, is a data structure that stores all the metadata for a set of files in a directory.

- To simplify, you can think of it as a place where we store all our files and keep track of the history of the files themselves.

- To create a new repo locally, you would make a new directory, change to it, and use the command:

```
git init
```

Cloning

- If we have an existing repo, we can easily create a copy of it using git *clone*.
- Cloning works both locally and remotely.
- Local:

```
git clone /path/to/repository
```

- Remote:

```
git clone username@host:path/to/repo
```

This can also be replaced with an HTTPS or SSH URL

- Most of the time, we start a remote repo (on Github) and then clone a local version to our computer.

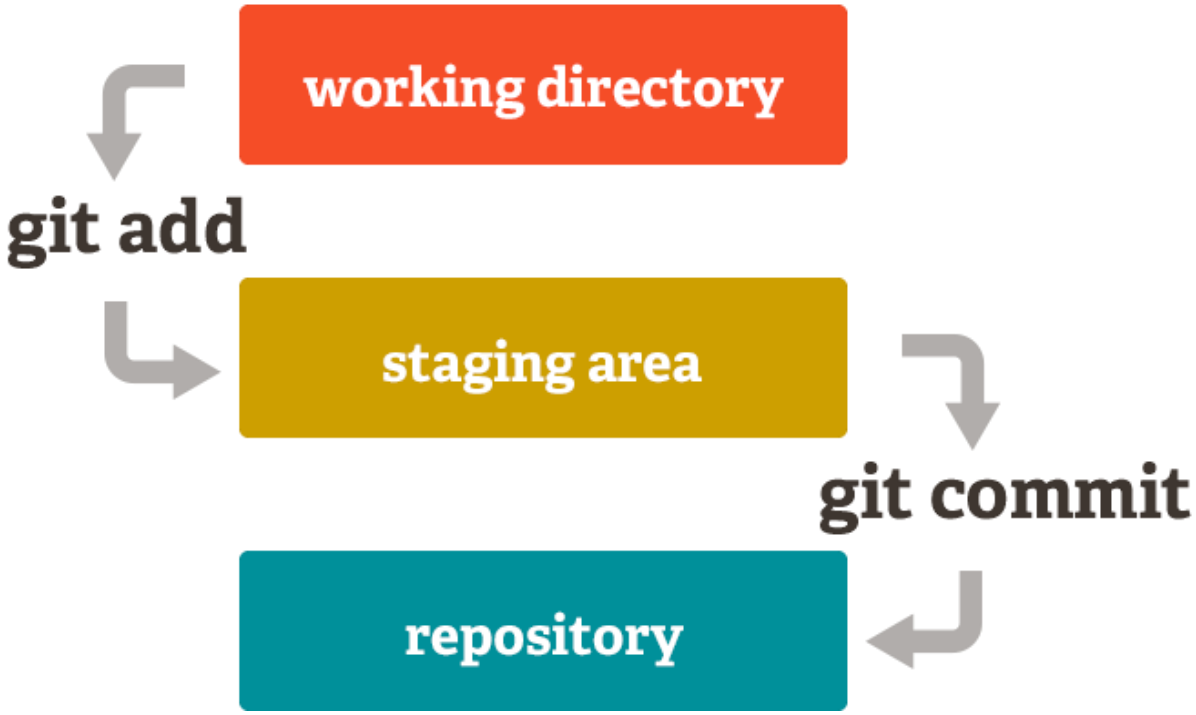
Workflow

In the local repo on your computer, there is a certain workflow as to how you make changes and "save" them:

1. *Working Directory* – this is where the actual files are located.

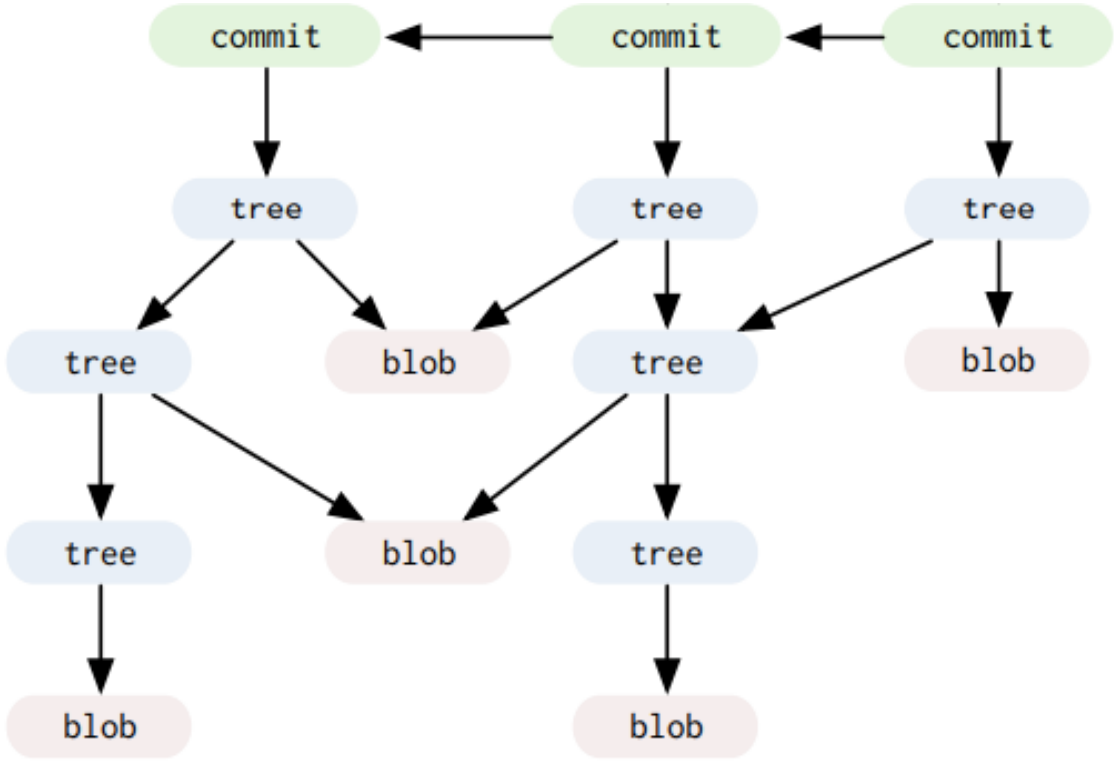
2. *Index* – this is basically a staging area where you add all the changes you've made.

3. *Head* – this points to the last commit that was made. Once you've staged all the changes you want to make, you commit them and update the head.



How Exactly Does Git Work?

- Git stores the content of your files in objects (here, they are called “blobs”).
- Your folders turn into objects called “trees” that contain other trees and blobs.
- A commit is a type of object that contains a tree. Once created, objects cannot change.



From David Gohberg’s “The Biggest Misconception About Git”

Adding Files to the Index

- First, you will *add* files to your local repo and make edits to them.

- Once you've made all the changes you want to make and you want to update your repo, you must add those changes to the index.

  - To add a specific file, use the command: `git add <filename>`

  - If you changed multiple files and you want to add all of them, use the command:

```
git add *
```

- Even if you have files from a previous commit, you must add them again if you've made any edits to them.

Removing Files

- If you have previously added a file, but now you want to remove it from your working directory and index, you can use the command:

```
git rm <filename>
```

- To remove a file just from the index, but keep it in your working directory, you can use the *rm* command with an appropriate flag:

```
git rm --cached <filename>
```

Committing

- So now, we have staged all the changes we want to make. The next step is to *commit* all those changes with the following command:

```
git commit -m "Commit message"
```

- For every commit you make, you need to include a message that quickly describes all the changes you made. If you ever want to go back to a previous version of your code, you can find a version of your project you want based on the commit message you used.

- At this point, we have basically “saved” our changes in our local repo on our computer.

Pushing to a Remote Repository

- Normally, we have a remote repo that we keep separate from our local repo (especially when we are collaborating on a project with other people).

- To properly update the remote repo, we need to *push* our local changes to it with the following command:

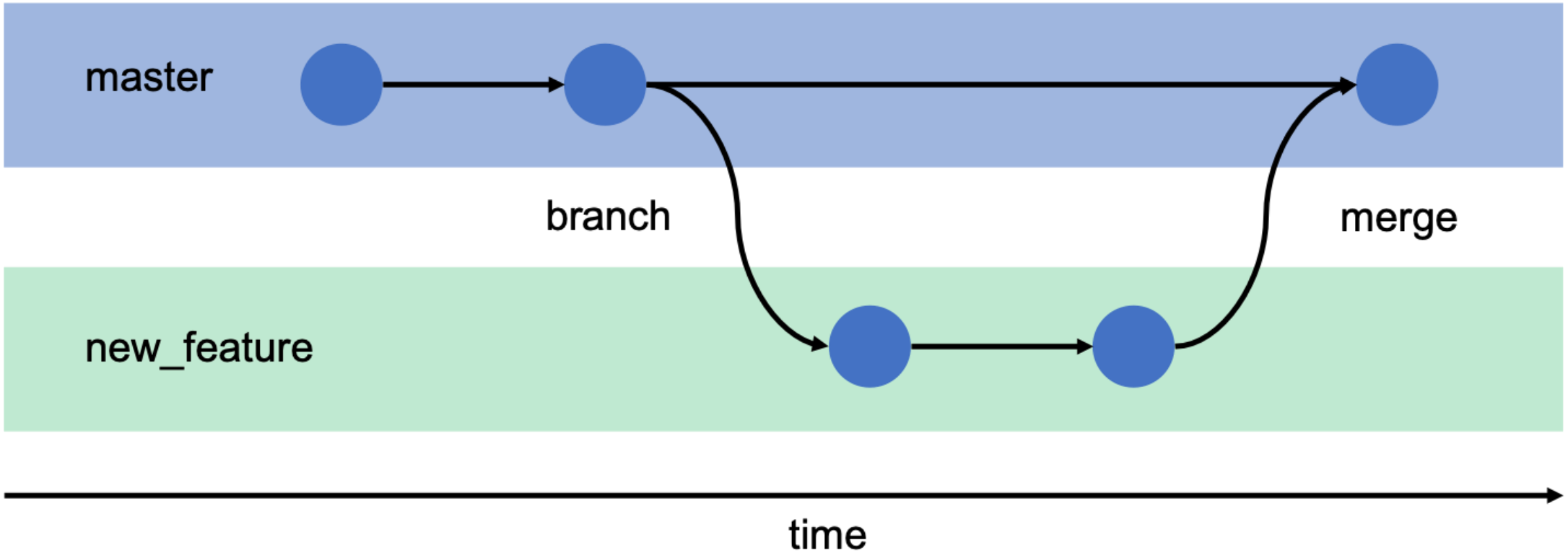
```
git push origin <branch_name>
```

- For this to work, we need to have cloned our repo from an existing remote repo.

Branching

- *Branches* are used for working on different files/parts of code that are isolated from each other.
- The default branch is called the *master* branch. Every repo will start with a master branch when initialized.
- If you are collaborating with other people, you will probably be working on different parts of the code and you may want to have different branches for each part.
- Once you have finished work on a certain branch, you can *merge* it back into the master branch.

Branching



Branching

- To create a new branch:

```
git checkout -b <branch_name>
```

- To switch to an existing branch:

```
git checkout <branch_name>
```

- To delete a branch:

```
git branch -d <branch_name>
```

- A branch is not available to collaborators unless you first push it to the remote repo.

Updating and Merging

- If there have been changes made to the remote repo (by other people) and we want to update our local repo with those changes:

```
git pull
```

- Once we have finished working on a different branch and we want to update our master branch, we *merge* those changes:

```
git merge <branch_name>
```

Merging

- Git will try to automatically reconcile the changes when you merge branches.
- If there are any conflicts (ex. if you and another person both edited the same lines of code in the same file, but in different branches), you will have to manually edit the files to resolve conflicts.
- Once you've made the appropriate changes, you'll have to add/commit them again.
- Before merging, you can preview those changes with the following command:

```
git diff <source_branch> <target_branch>
```

Software Versions and Tagging

- It is common for software releases to have numerical identifiers to distinguish between different versions.

- The most common format for this numbering is called *semantic versioning:*

4.2.1

MAJOR *Minor* patch

- In Git, you can label software releases with *tags:*

```
git tag 1.0.0 9fbe0a5613
```

This string should be the first 10 characters of the commit tag you are referring to

Repository History

- To look back at the history of a repo, we can use Git's *log* command:

```
git log
```

- This will display the history of commits and who made them.

- There are many different parameters for displaying the history in different ways:
  - See all commits from a certain author.
  - Modify the display (lists, ASCII trees).
  - See changed files.
- To see all the different parameters available, use: `git log --help`

Replacing Local Changes

- There many be times where you accidentally mess up your local repo (accidentally delete a file, made a small change somewhere and now your code doesn't work at all, etc.).

- To replace a file with the version from your previous commit:

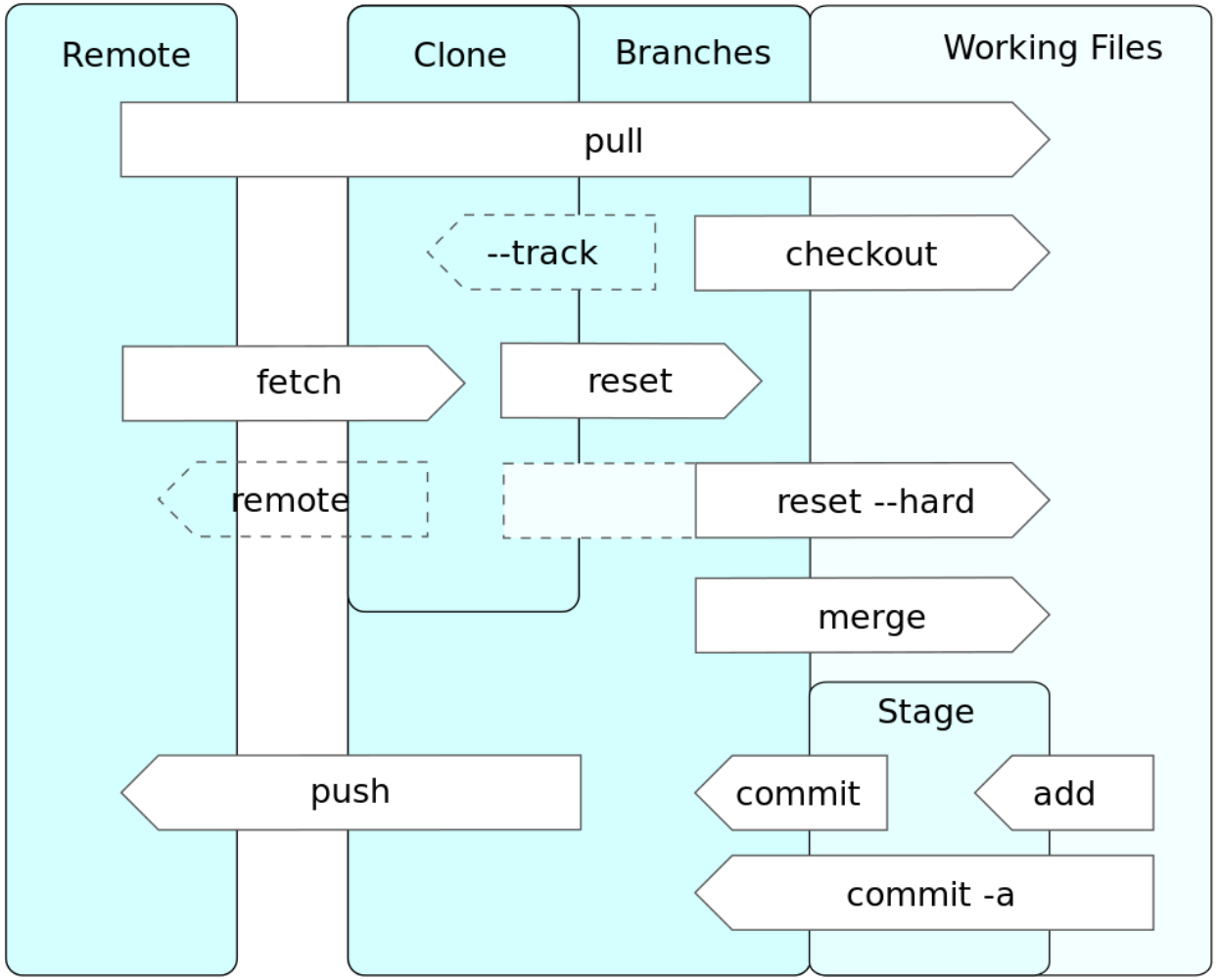
```
git checkout -- <filename>
```

- If you want to drop all the changes you've made since a previous commit, you can use the following commands:

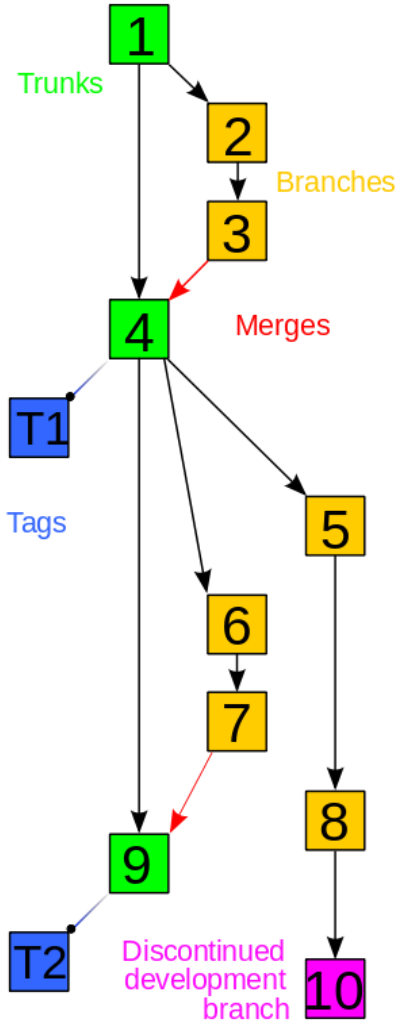
```
git fetch origin
```

```
git reset --hard origin/<branch_name>
```

Overall Workflow



Command Workflow



Example of Project History Tree

Python Modules

- We've seen several different Python libraries that have useful functions:
  - random
  - math
  - PIL
  - Matplotlib

- The ability to import existing functions and classes from other Python scripts is very important for complex programs that require many lines of code.

Import Statements

There are 3 different ways to import modules:

1)

```
import math
x = math.sqrt(10)
y = math.cos(10)
z = math.sin(10)
```

2)

```
from math import cos, sin, sqrt
x = sqrt(10)
y = cos(10)
z = sin(10)
```

3)

```
from math import *
x = sqrt(10)
y = cos(10)
z = sin(10)
```

There are also shortcuts for importing modules but be sure to use them appropriately!

Other Useful Modules in Python's Default Libraries

- argparse – library for command line arguments and argument parsing.
- copy, shutil – useful for creating copies of objects.
- os – useful for interfacing with your operating system.
- pickle – convert objects to smaller data types (object compression).
- sys – library for accessing specific system parameters and functions.
- time – useful for functions related to time (benchmarking).
- tkinter – useful for making programs with GUIs.
- itertools – useful functions and data types for efficient looping.

All of them can be found here: https://docs.python.org/3/py-modindex.html

NumPy and SciPy

- Useful for data science and scientific computing (written in C, so it works fast) – these are basically a better version of the default math module.

- NumPy:
  - Access to array objects (a good alternative to lists).
  - Has many useful functions related to linear algebra, random numbers, and vector/matrix operations.

- SciPy:
  - Has many useful functions related to numerical methods and analysis (integration, optimization, interpolation, statistics, signal processing).
  - Has a lot of overlap with NumPy.

- Documentation for both packages can be found here: https://docs.scipy.org/doc/

Creating Our Own Modules

- We can create our own modules to use in Python.

- We must first write the code that makes up the module, add the directory where the code is located to our PYTHONPATH, and then source the proper resource file.

- More details on this can be found in the "Python Modules" handout.