Lecture 12:

Git and GitHub

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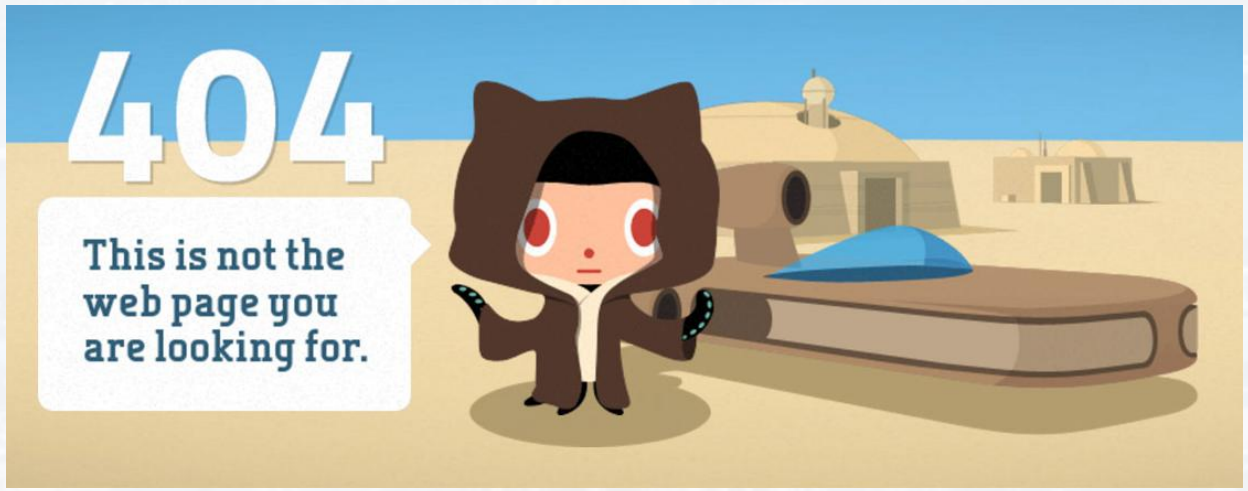
Python for Molecular Sciences

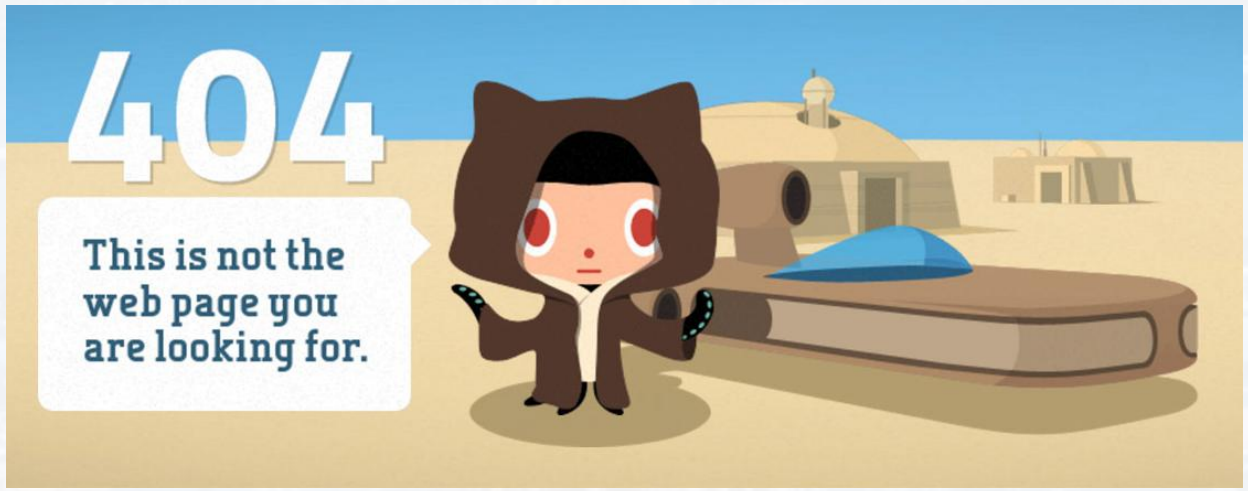
MSSE 272, 3 Units

Berkeley MSSE
MOLECULAR SCIENCE & SOFTWARE ENGINEERING



Outline

- **Motivation**
- **Git**
  - installation and VS Code
  - status, add and commit
  - compare differences
  - restoring from index, stage and commit
- **Git Hub**
  - create your repo
  - invite a co worker
  - push
  - fetch, merge, pull



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When working on a project: → many different versions

version 1

```
#################################
def DistToPotential(x, y, a, b,
    #takes locations of all part
    .......
    X     = np.tile(x, (L, 1))
    Y     = np.tile(y, (L, 1))
    
    Dx    = X - X.transpose()
    Dy    = Y - Y.transpose()
```

version 1a

```
#################################
def DistToPotential(x, y, a, b,
    #takes locations of all part
    .......
    X     = np.tile(x, (L, 1))
    Y     = np.tile(y, (L, 1))
    
    Dx    = X - X.transpose()
    Dy    = Y - Y.transpose()
```

version 2

```
#################################
def DistToPotential(x, y, a, b,
    #takes locations of all part
    .......
    X     = np.tile(x, (L, 1))
    Y     = np.tile(y, (L, 1))
    
    Dx    = X - X.transpose()
    Dy    = Y - Y.transpose()
```

version 2a

```
#################################
def DistToPotential(x, y, a, b,
    #takes locations of all part
    .......
    X     = np.tile(x, (L, 1))
    Y     = np.tile(y, (L, 1))
    
    Dx    = X - X.transpose()
    Dy    = Y - Y.transpose()
```

version 3

```
#################################
def DistToPotential(x, y, a, b,
    #takes locations of all part
    .......
    X     = np.tile(x, (L, 1))
    Y     = np.tile(y, (L, 1))
    
    Dx    = X - X.transpose()
    Dy    = Y - Y.transpose()
```

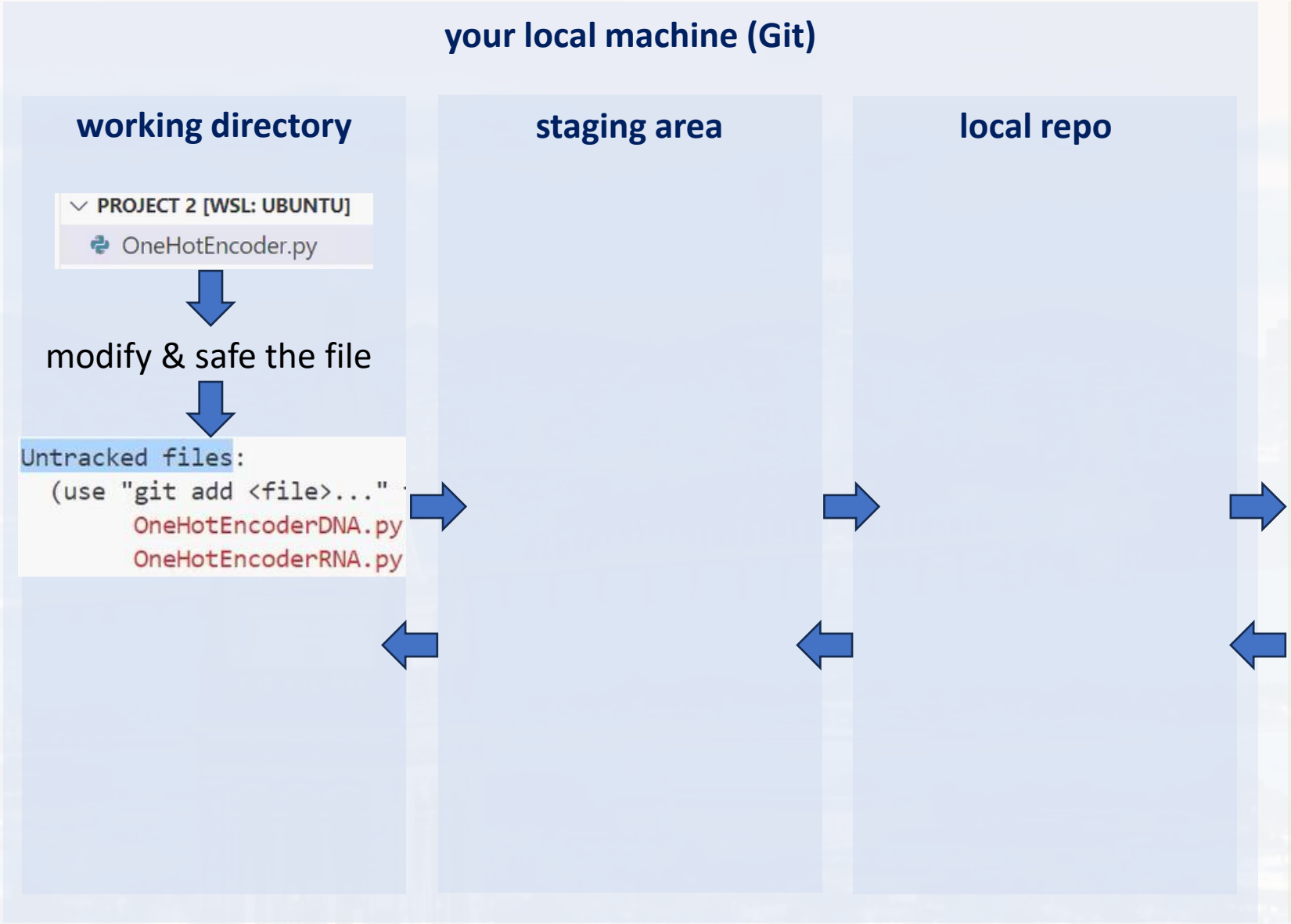
- easy to get **lost**
- What are the **differences between** the different **versions**?
- What if it turned out that **version 3c** was actually **better than 1f**?
- Sharing & exchanging with **co-workers**?

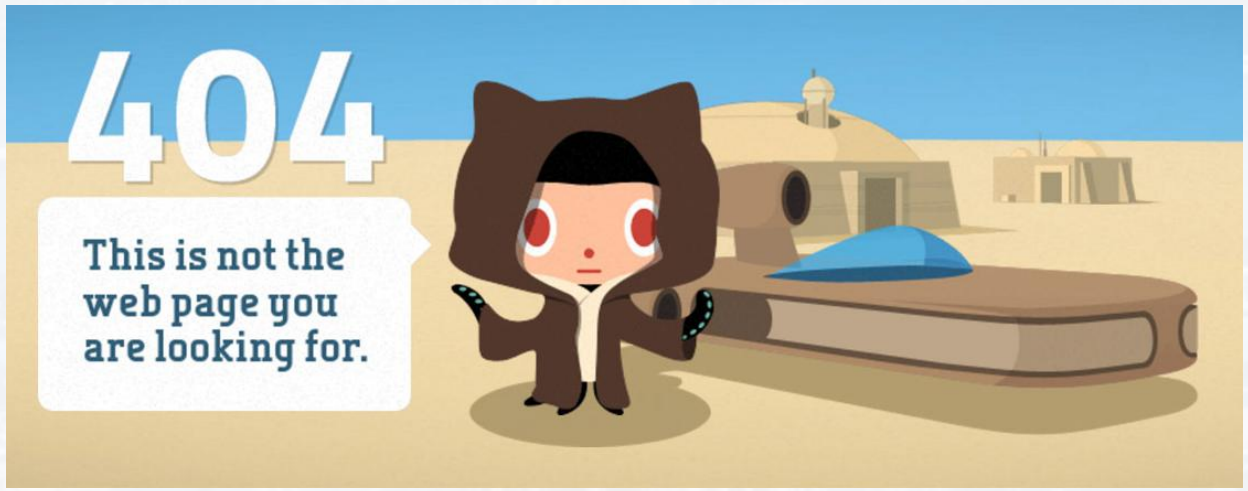
When working on a project: → many different versions

Version control system

- keeps track of **different** versions
- keeps track of **changes**
- **coordinates** work with co-workers
- **stores** data efficiently

structure


your local machine (Git)
remote repo (GitHub)
working directory
staging area
local repo
PROJECT 2 [WSL: UBUNTU]
OneHotEncoder.py
modify & safe the file
Untracked files:
(use "git add <file>..."
OneHotEncoderDNA.py
OneHotEncoderRNA.py



Outline

- Motivation
- **Git**
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1) open WSL terminal

note: Git should be installed already, nevertheless, let's run the following line:

2) install Git

```
mmh_user@DESKTOP-PPSA666:~$ sudo apt-get install git
```

3) confirm your password

```
Reading package lists... Done
Building dependency tree... Done
Reading state information... Done
git is already the newest version (1:2.34.1-1ubuntu1.12).
git set to manually installed.
0 upgraded, 0 newly installed, 0 to remove and 78 not upgraded.
```

4) check version:

```
(base) mmh_user@DESKTOP-PPSA666:~$ git --version
git version 2.34.1
```

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(base) mmh_user@DESKTOP-PPSA666:~$ git --version
git version 2.34.1
```

5) configure git: set your email address and user name

```
:~$ git config --global user.name MarkusMSSE_Chem272
:~$ git config --global user.email markus.hohle@berkeley.edu
```

4) check version:

```
(base) mmh_user@DESKTOP-PPSA666:~$ git --version
git version 2.34.1
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5) configure git: set your email address and user name

```
:~$ git config --global user.name MarkusMSSE_Chem272
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```

Git has three levels of access:

1 **Local**: only for a **specific repo**
2 **Global**: across all repos for **currently logged-in user** (here: *mmh_user*)
3 **System**: **all users** and repos **on your machine**
(for example if you are admin or group leader etc)

4) check version:

```
(base) mmh_user@DESKTOP-PPSA666:~$ git --version
git version 2.34.1
```

5) configure git: set your email address and user name

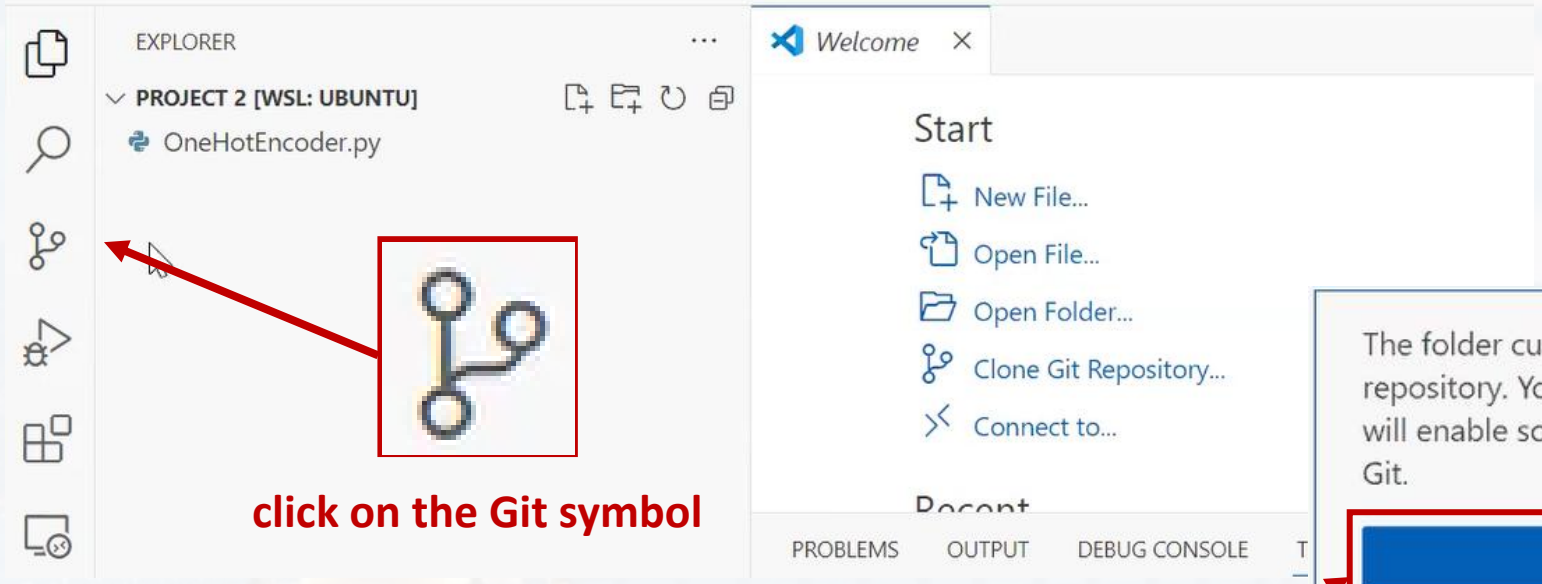
```
:~$ git config --global user.name MarkusMSSE_Chem272
:~$ git config --global user.email markus.hohle@berkeley.edu
```

6) check config: make sure everything is correct

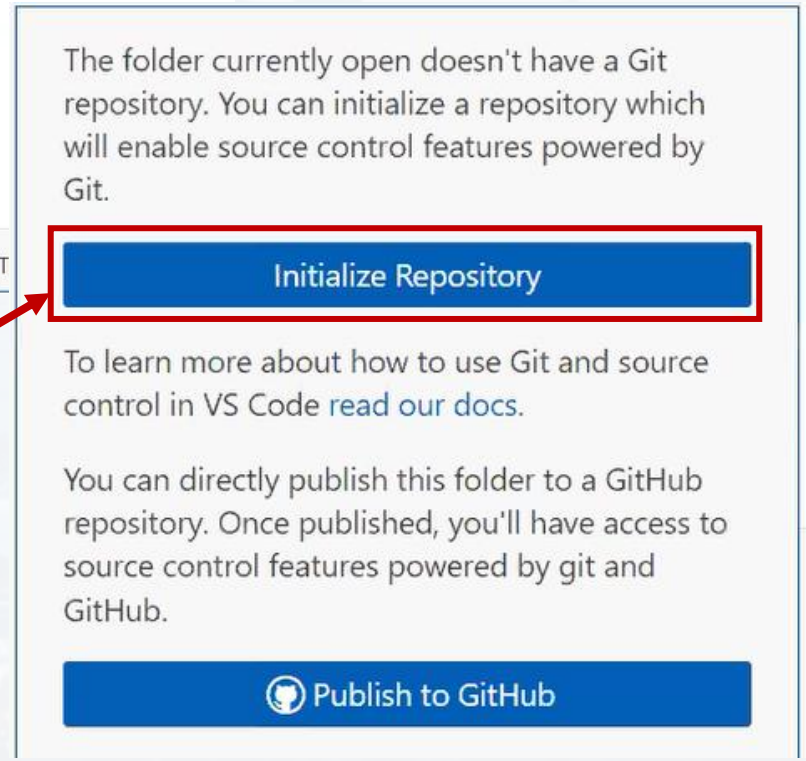
```
file:/home/mmh_user/.gitconfig  user.name=MarkusMSSE_Chem272
file:/home/mmh_user/.gitconfig  user.email=markus.hohle@berkeley.edu
file:/home/mmh_user/.gitconfig  init.defaultbranch=main
```

7) Git and VS Code:

- open VS code
- navigate to the folder which you want to use for your project



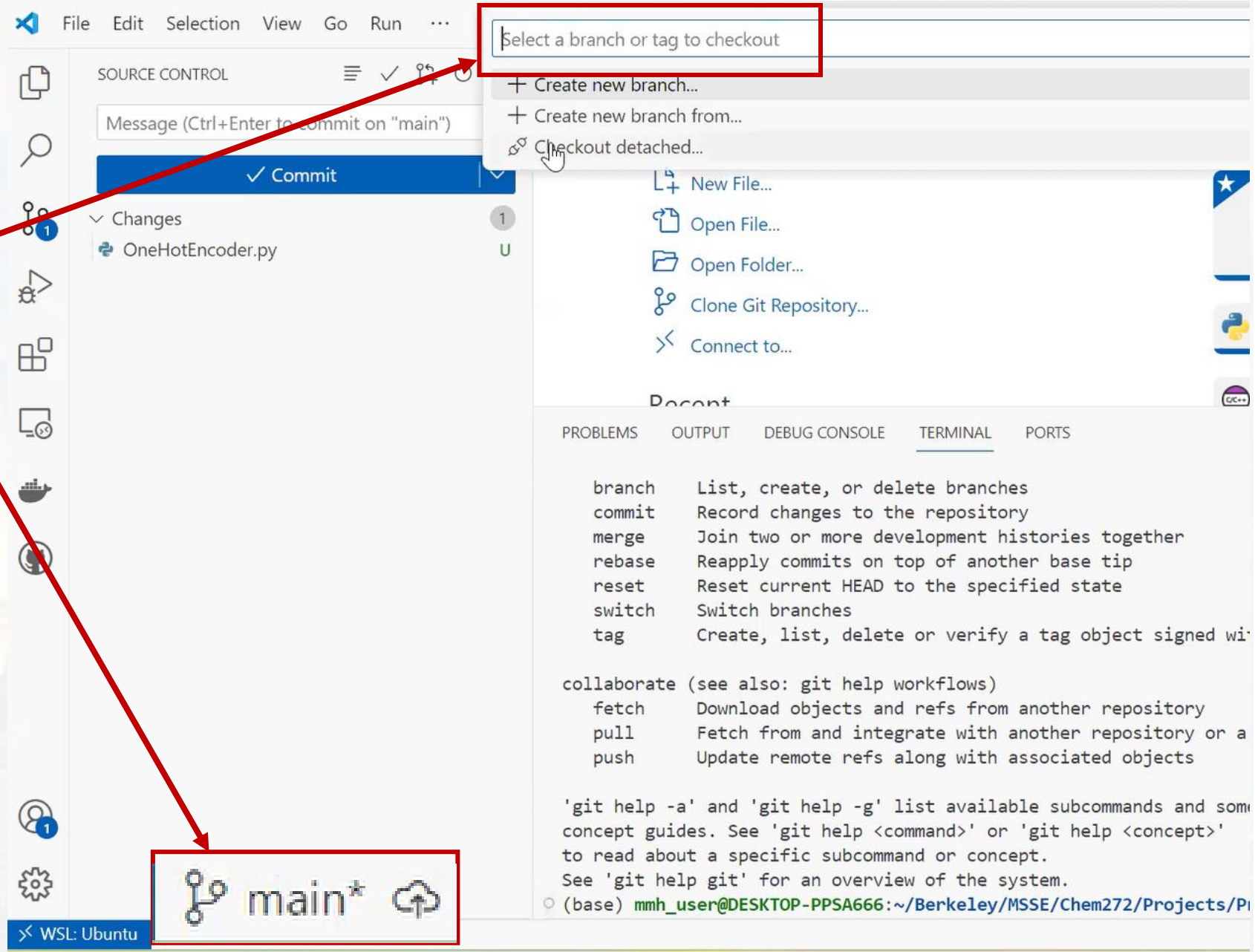
click on the Git symbol



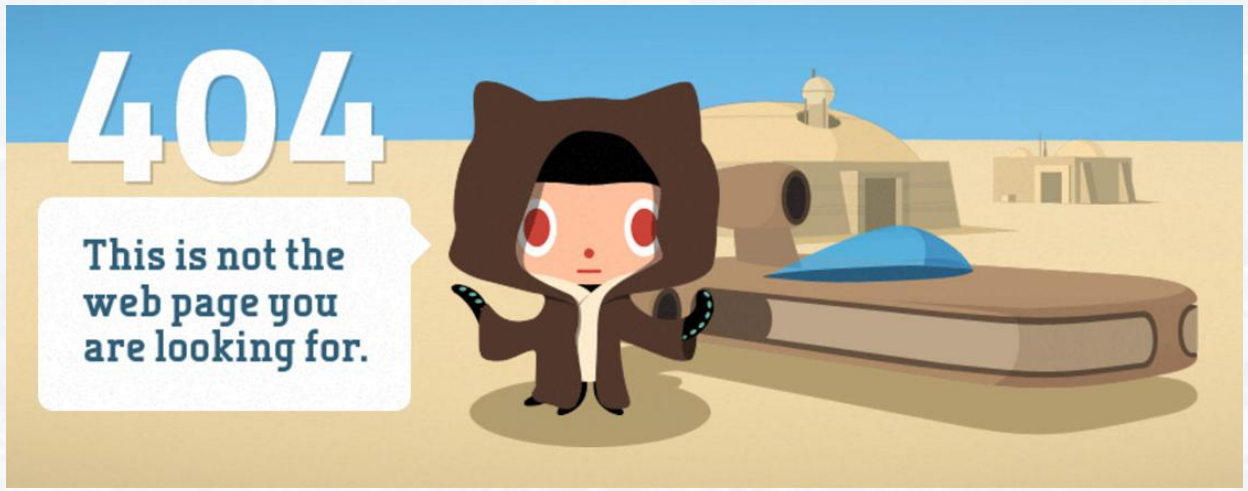
click on *Initialize Repository*

7) Git and VS Code:

default branch name is *"main"*, which can be renamed



watch:
12a_Installing_Git
12b_Git_and_VS_Code_in_WSL



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  - compare differences
  - restoring from index, stage and commit
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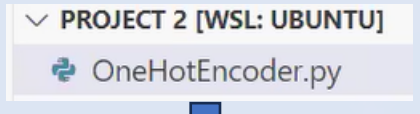
  - push
  - fetch, merge, pull

structure

your local machine (Git)

working directory	staging area	local repo

remote repo (GitHub)



modify & safe the file

Git notices the change!

`git status`

always check Git status
→ which files have been modified
→ which files are in the staging area

```
Untracked files:
  (use "git add <file>..." 
        OneHotEncoderDNA.py
        OneHotEncoderRNA.py
```

structure

your local machine (Git)

working directory	staging area	local repo

PROJECT 2 [WSL: UBUNTU]

OneHotEncoder.py

↓

modify & safe the file

↓

`git status`

```
Untracked files:
  (use "git add <file>..." 
        OneHotEncoderDNA.py
        OneHotEncoderRNA.py
```

adds files to staging area
→ file is ready for review

`git add`

`git add OneHotEncoderDNA.py`

remote repo (GitHub)

structure

your local machine (Git)

working directory

PROJECT 2 [WSL: UBUNTU]

OneHotEncoder.py

modify & safe the file

git status

```
Untracked files:
  (use "git add <file>..." 
        OneHotEncoderDNA.py
        OneHotEncoderRNA.py
```

git add

```
git add OneHotEncoderDNA.py
git add OneHotEncoderRNA.py
```

staging area

git status

```
On branch main
Changes to be committed:
  (use "git restore --staged <file>..." to unstage)
        new file:   OneHotEncoderDNA.py
        new file:   OneHotEncoderRNA.py
```

tells you how to move version of staged file back to working directory!

local repo

remote repo (GitHub)

structure

your local machine (Git)

working directory

PROJECT 2 [WSL: UBUNTU]

OneHotEncoder.py

modify & safe the file

git status

```
Untracked files:
  (use "git add <file>..."
        OneHotEncoderDNA.py
        OneHotEncoderRNA.py
```

git add

git restore --staged

staging area

```
h main
to be committed:
git restore --staged <file>..."
new file:   OneHotEncoderDNA.py
new file:   OneHotEncoderRNA.py
```

git commit

```
[main 6a080cc] Added RNA and DNA Version of Encoder
 2 files changed, 84 insertions(+)
 create mode 100644 OneHotEncoderDNA.py
 create mode 100644 OneHotEncoderRNA.py
```

files are now moved from staging area to the local repository

git status

```
On branch main
nothing to commit, working tree clean
```

local repo

remote repo (GitHub)

structure

your local machine (Git)

working directory

PROJECT 2 [WSL: UBUNTU]

OneHotEncoder.py

modify & safe the file

```
Untracked files:
  (use "git add <file>..." 
        OneHotEncoderDNA.py
        OneHotEncoderRNA.py
```

staging area

```
h main
to be committed:
git restore --staged <file>..."
new file:   OneHotEncoderDNA.py
new file:   OneHotEncoderRNA.py
```

local repo

`git add`

`git restore --staged`

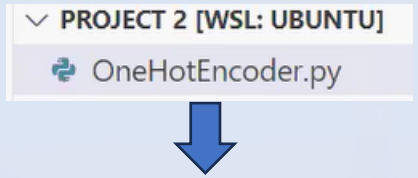
remote repo (GitHub)

structure

your local machine (Git)

working directory	staging area	local repo

remote repo (GitHub)



modify & safe the file

```
Untracked files:
  (use "git add <file>..." 
        OneHotEncoderDNA.py
        OneHotEncoderRNA.py
```

`git add`

`git restore --staged`

structure

your local machine (Git)

working directory

PROJECT 2 [WSL: UBUNTU]

OneHotEncoder.py

modify & safe the file

```
Untracked files:
  (use "git add <file>..." 
        OneHotEncoderDNA.py
        OneHotEncoderRNA.py
```

git add

staging area

```
h main
to be committed:
git restore --staged <file>..."
new file:   OneHotEncoderDNA.py
new file:   OneHotEncoderRNA.py
```

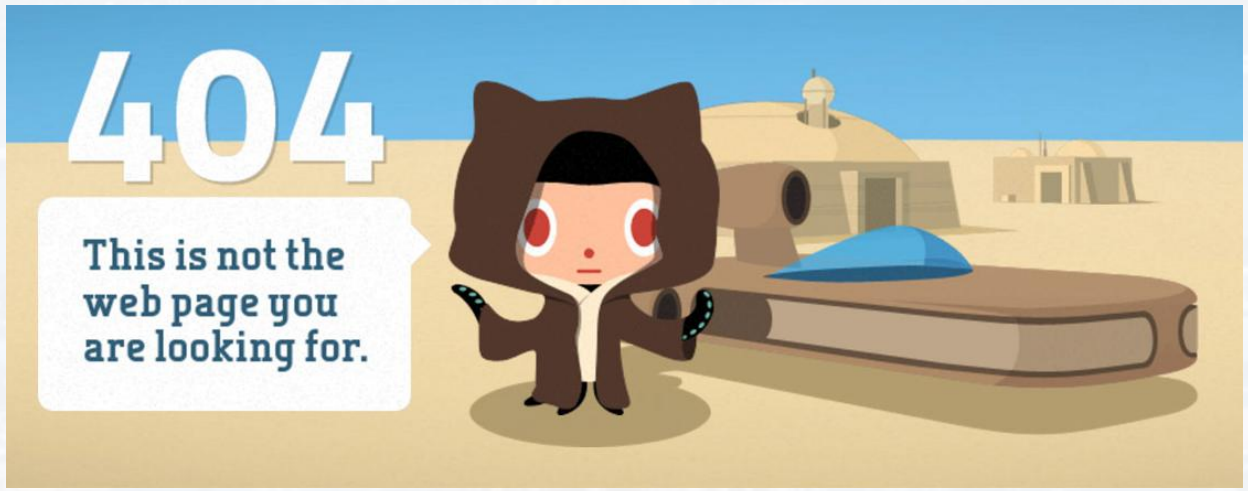
git commit

local repo

```
[main 6a080cc] Added RNA and DNA Version of Encoder
 2 files changed, 84 insertions(+)
 create mode 100644 OneHotEncoderDNA.py
 create mode 100644 OneHotEncoderRNA.py
```

remote repo (GitHub)

watch:
12c_Git_commit



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1) A new file (`OneHotEncoder.py`) in the working directory

`git status`

```
On branch main
Changes not staged for commit:
  (use "git add <file>..." to update what will be committed)
  (use "git restore <file>..." to discard changes in working directory)
        modified:   OneHotEncoder.py
```

`git add` `git add OneHotEncoder.py`

`git status`

```
On branch main
Changes to be committed:
  (use "git restore --staged <file>..." to unstage)
        modified:   OneHotEncoder.py
```

2) We kept working on the file and have two versions now!

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```
git status
```

```
On branch main
Changes to be committed:
  (use "git restore --staged <file>..." to unstage)
        modified:   OneHotEncoder.py

Changes not staged for commit:
  (use "git add <file>..." to update what will be committed)
  (use "git restore <file>..." to discard changes in working directory)
        modified:   OneHotEncoder.py
```

the **previous** version which is located at the **stage area**

the **current** version which is located at the **work folder**

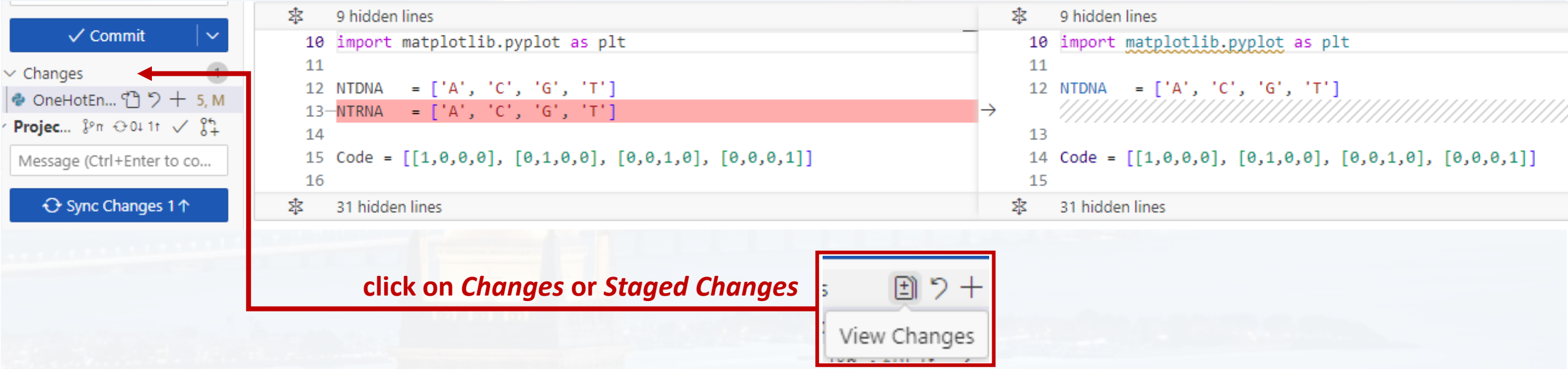
before adding or committing to the repo
→ review changes!

2) We kept working on the file and have two versions now!

before adding or committing to the repo
→ review changes!

staged version has one more line
(which got removed, hence highlighted in red)

folder version has one fewer line



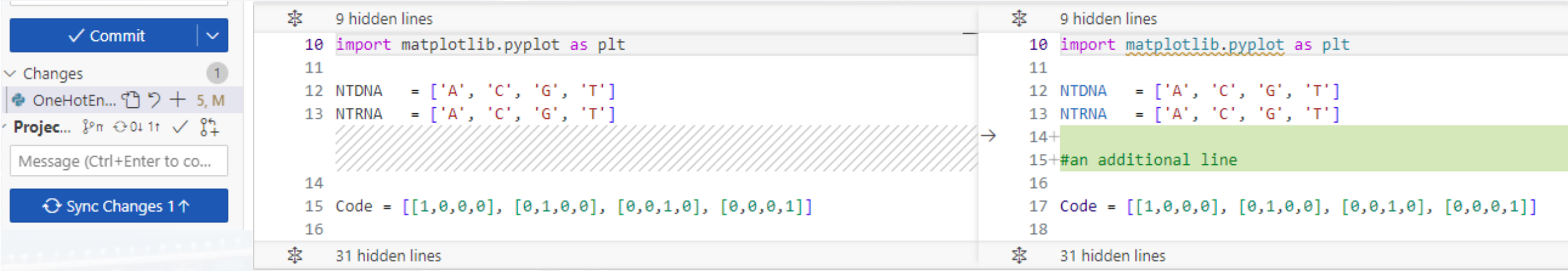
click on *Changes* or *Staged Changes*

2) We kept working on the file and have two versions now!

before adding or committing to the repo
→ review changes!

staged version

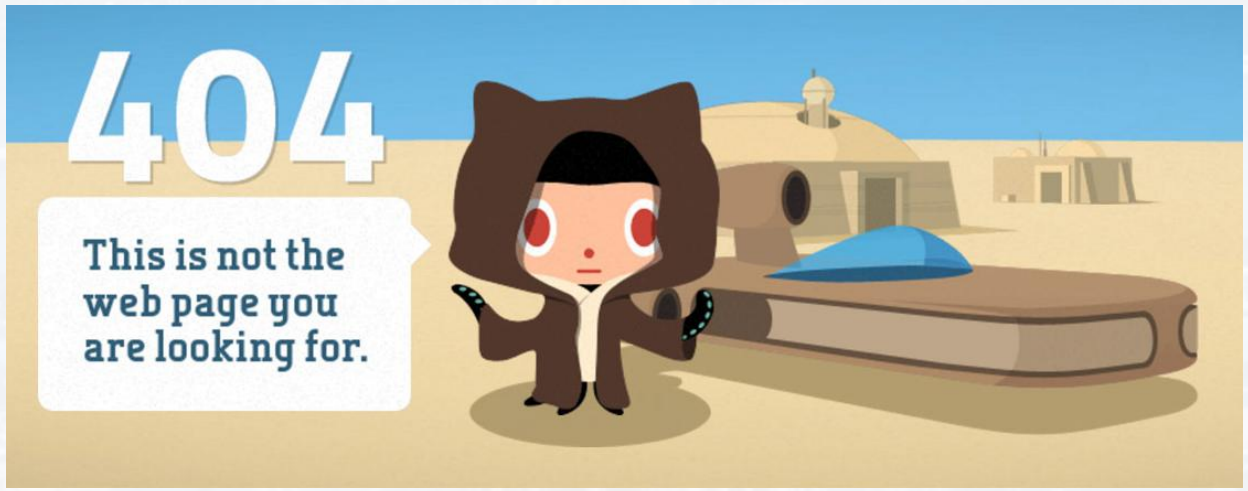
folder version has one more line
(hence highlighted in green)



once we add or commit, Git tells us the changes:

```
[main b4d5c49] RNA and DNA Encoder added
 1 file changed, 1 insertion(+), 1 deletion(-)
```

watch:
12d_Git_CompareDifferences



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  - compare differences
  - **restoring from index, stage and commit**
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  - push
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We can always rescue any file from any state of our project!

1) changing file in working directory

undo: `git restore`

2) `git add` file from working directory to stage area

undo: `git restore --staged`

watch:
12e_Git_RestoreFromIndexAndStage

What if we have committed many different versions to the repo but need to restore one particular version??

structure

your local machine (Git)

working directory

staging area

local repo

`git log`

```
commit b4d5c498d4d5db1d7a6cffa614ead30c1902aca2 (HEAD -> main)
Author: MarkusMSSE_Chem272 <markus.hohle@berkeley.edu>
Date:   Thu Jul 10 23:51:55 2025 +0200

    RNA and DNA Encoder added

commit 124f919fcfbfd72c3df0de1180c1e450d8dd2be5
Author: MarkusMSSE_Chem272 <markus.hohle@berkeley.edu>
Date:   Thu Jul 10 23:45:21 2025 +0200

    Test

commit 6a080ccee9b3ba8bde5151b810fcf0223e482f9e
Author: MarkusMSSE_Chem272 <markus.hohle@berkeley.edu>
Date:   Thu Jul 10 22:16:51 2025 +0200

    Added RNA and DNA Version of Encoder

commit 542391b0a769e142f4ef029c722abbecb3cdddf8
Author: MarkusMSSE_Chem272 <markus.hohle@berkeley.edu>
Date:   Thu Jul 10 22:00:58 2025 +0200

    message
```

remote repo (GitHub)

The last commit (HEAD)

`git log`

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    message
```

each commit has an **individual ID**

git log

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Date:   Thu Jul 10 22:00:58 2025 +0200

    message
```

each commit has a **date**

git log

```
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    message
```

the **messages** you added are also stored

git log

```
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    message
```

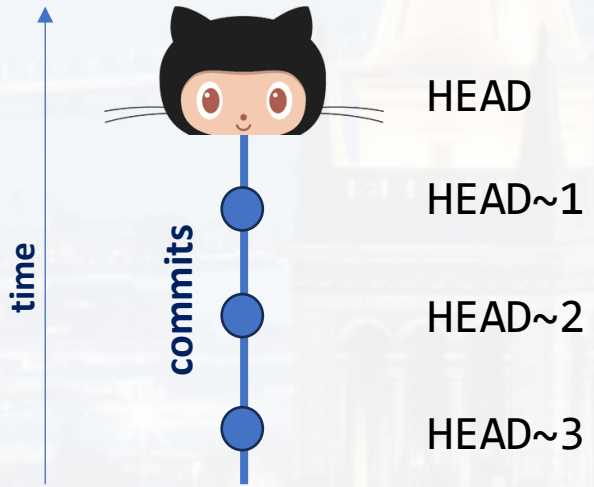
if we want to move a file from a given **commit back to the staging area**:

→ either referring to the **ID**

→ or to the **head**

```
git restore --source=HEAD~2 OneHotEncoder.py
```

two commits before the current one




```
git log
```

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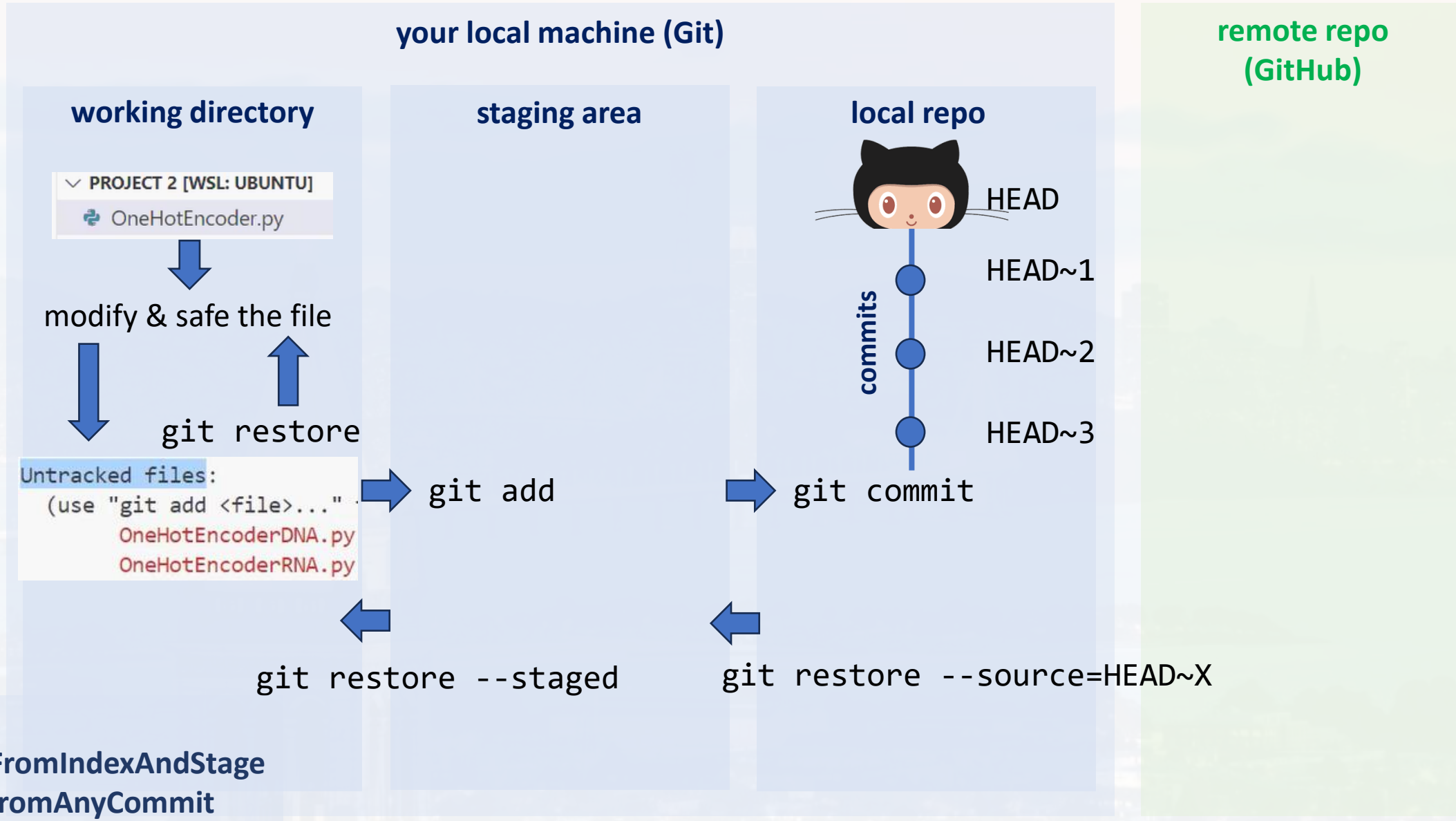
    message
```

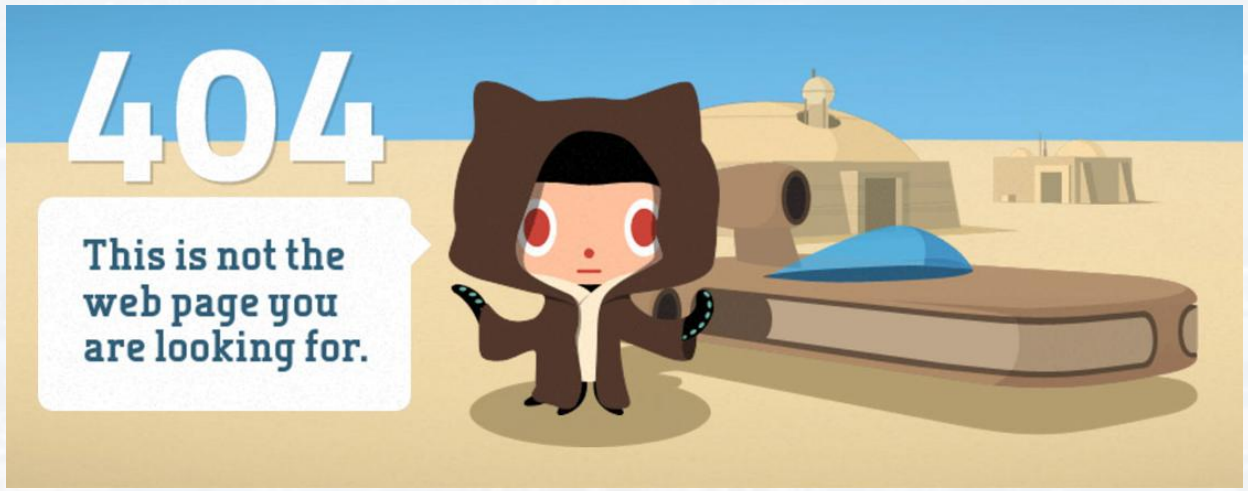
structure



watch:

12e_Git_RestoreFromIndexAndStage

12f_Git_RestoreFromAnyCommit



Outline

- Motivation
- Git
  - installation and VS Code
  - status, add and commit
  - compare differences
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  - **create your repo**
  - invite a co worker
  - push
  - fetch, merge, pull

structure

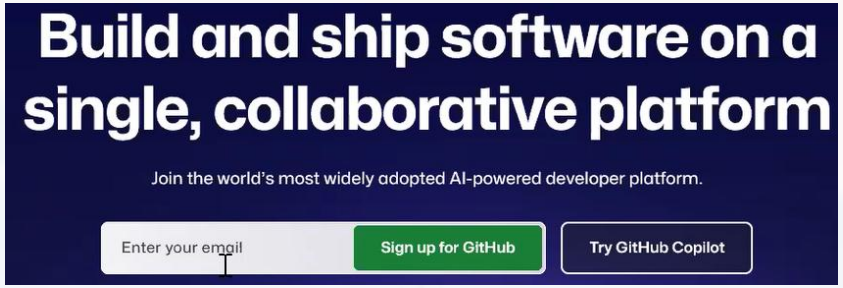
your local machine (Git)

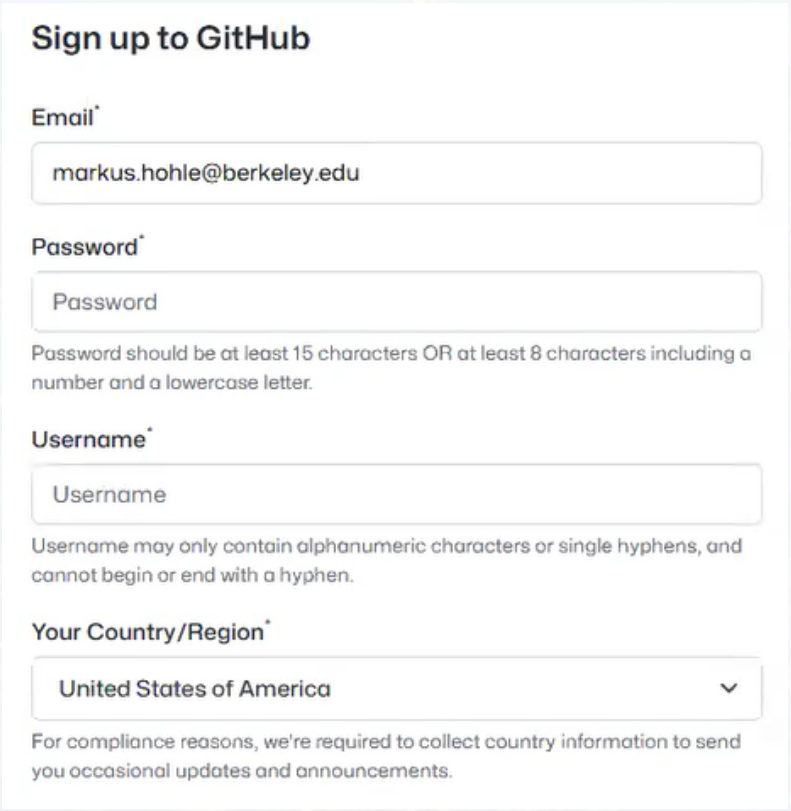
working directory	staging area	local repo

remote repo (GitHub)

Git & GitHub

got to **github.com**

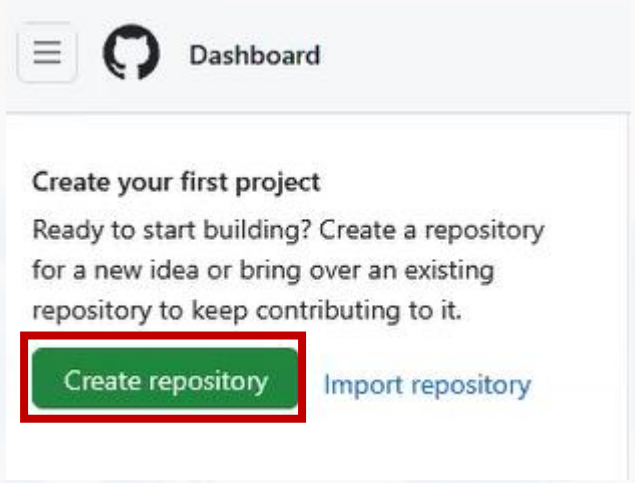




register and confirm email address

remote repo (GitHub)

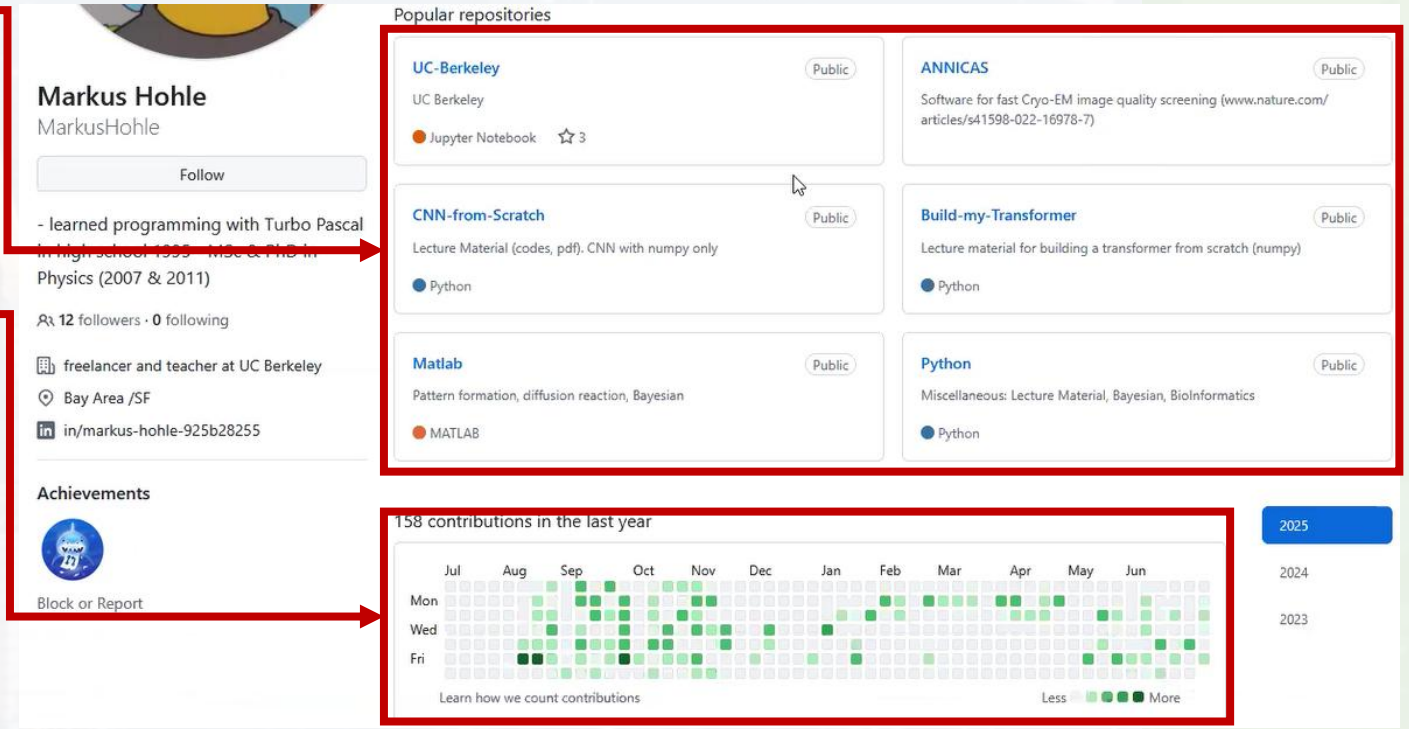
create new repository



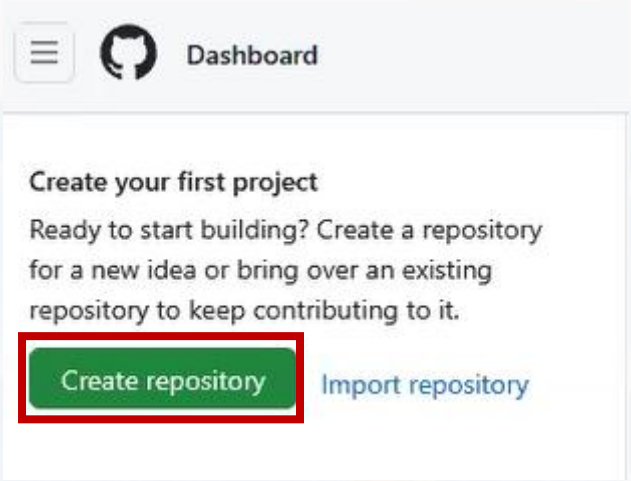
remote repo (GitHub)

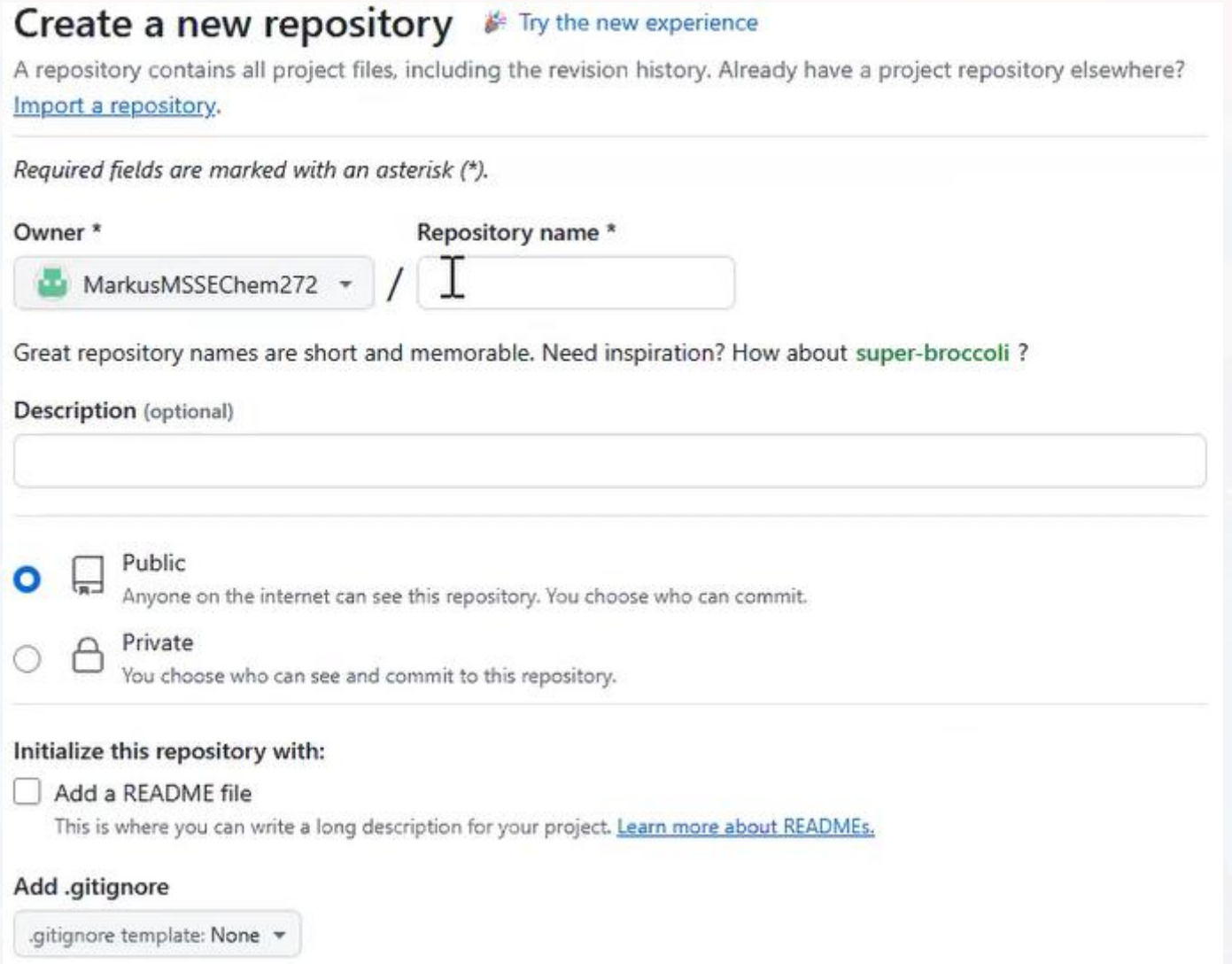
list of repos

your **garden** shows your activity: **keep it green!**



create new repository





create new repository

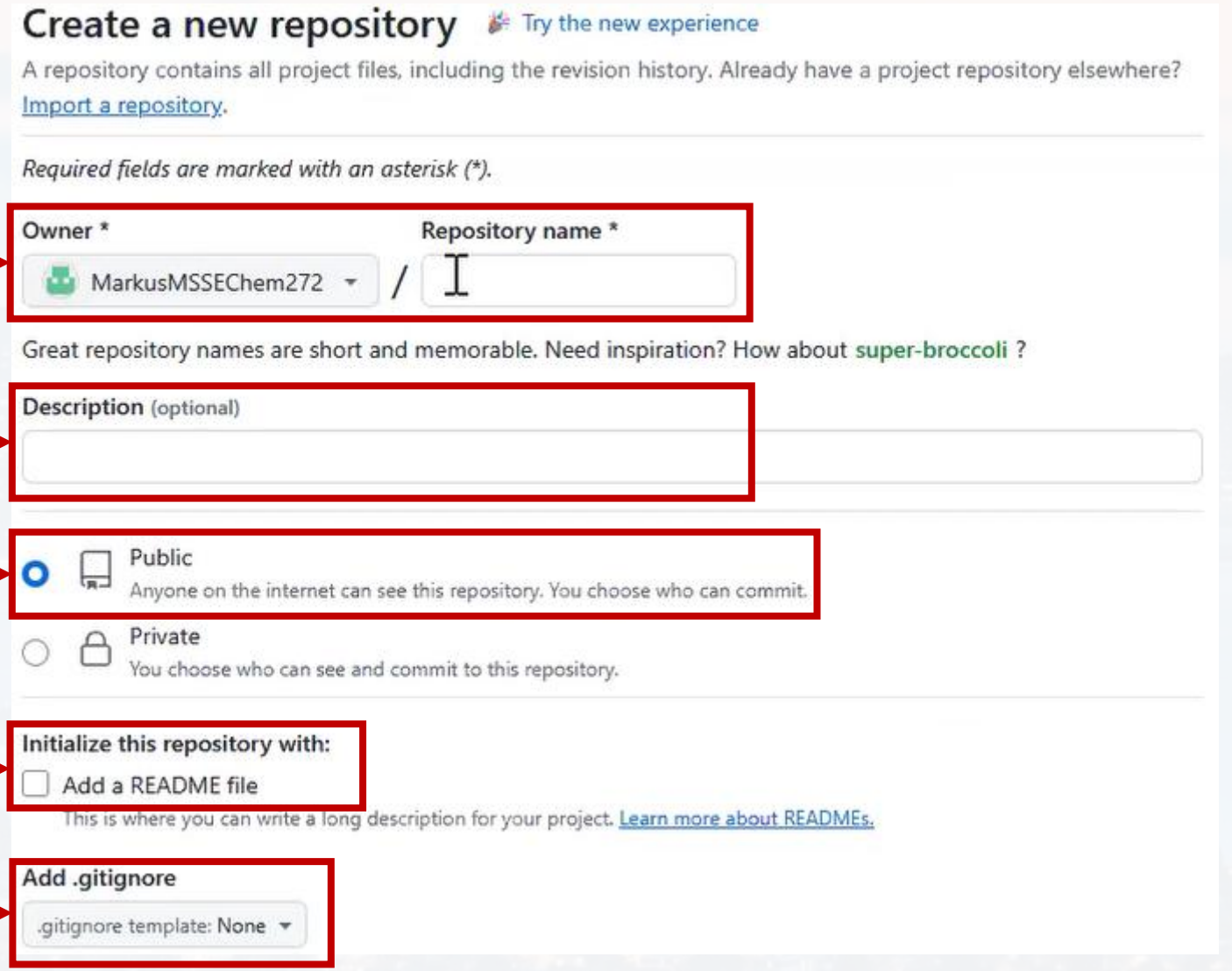
add a meaningful name…

…and discription…

public means **anyone** can see your repo

you can add more info in a ReadMe file

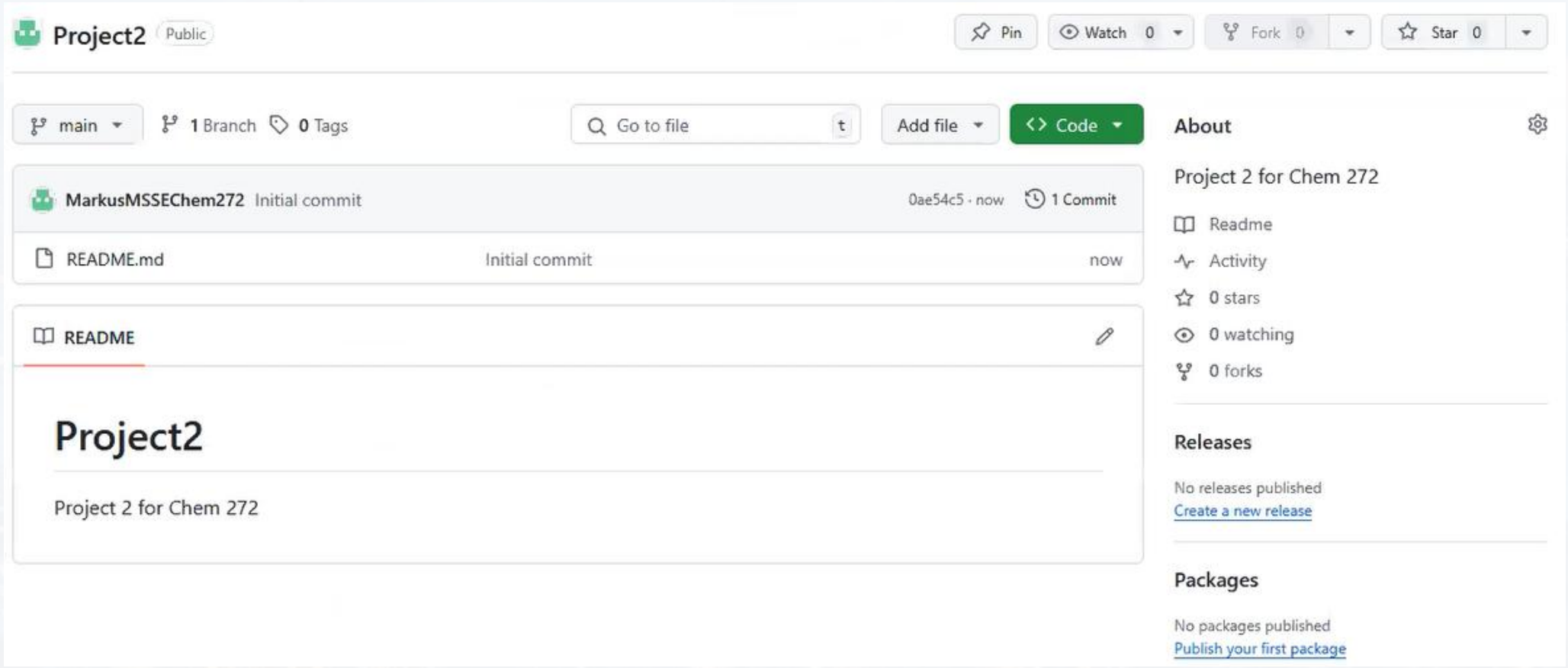
gitignore lists files and directories that will not be committed if you use the option -a



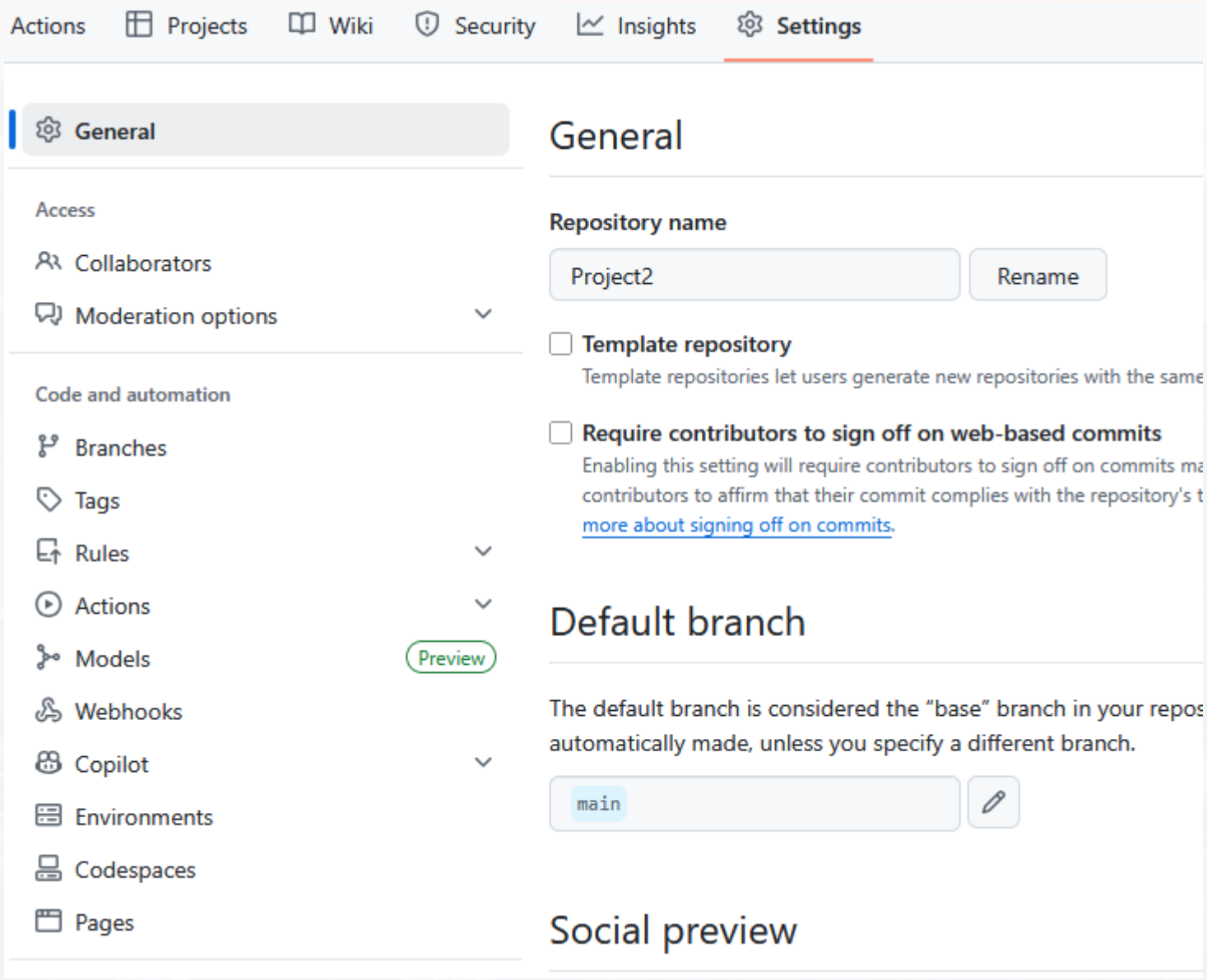
create new repository

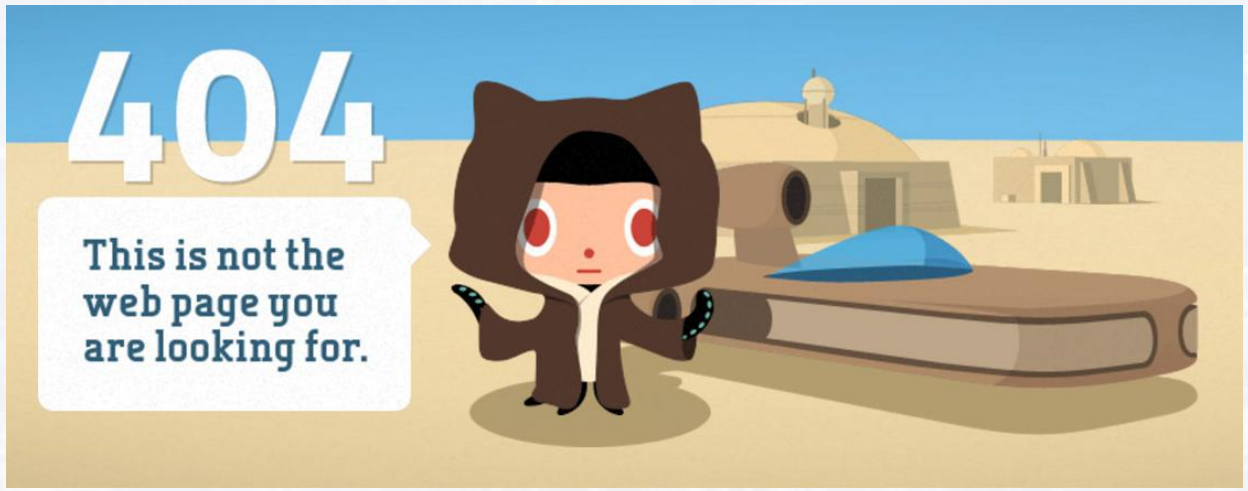
Create repository

Congratulations! You have created your first repository!



Note there are way more settings you can adjust





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- Git
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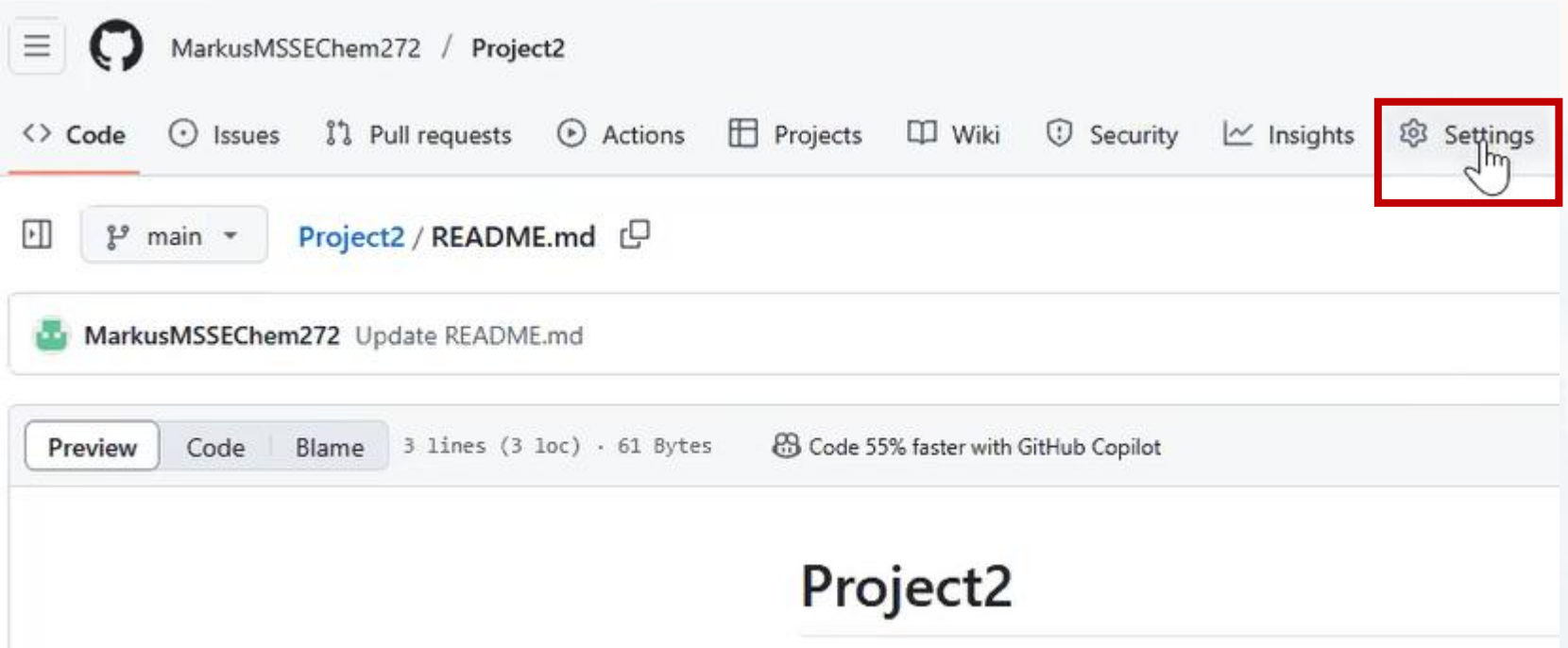
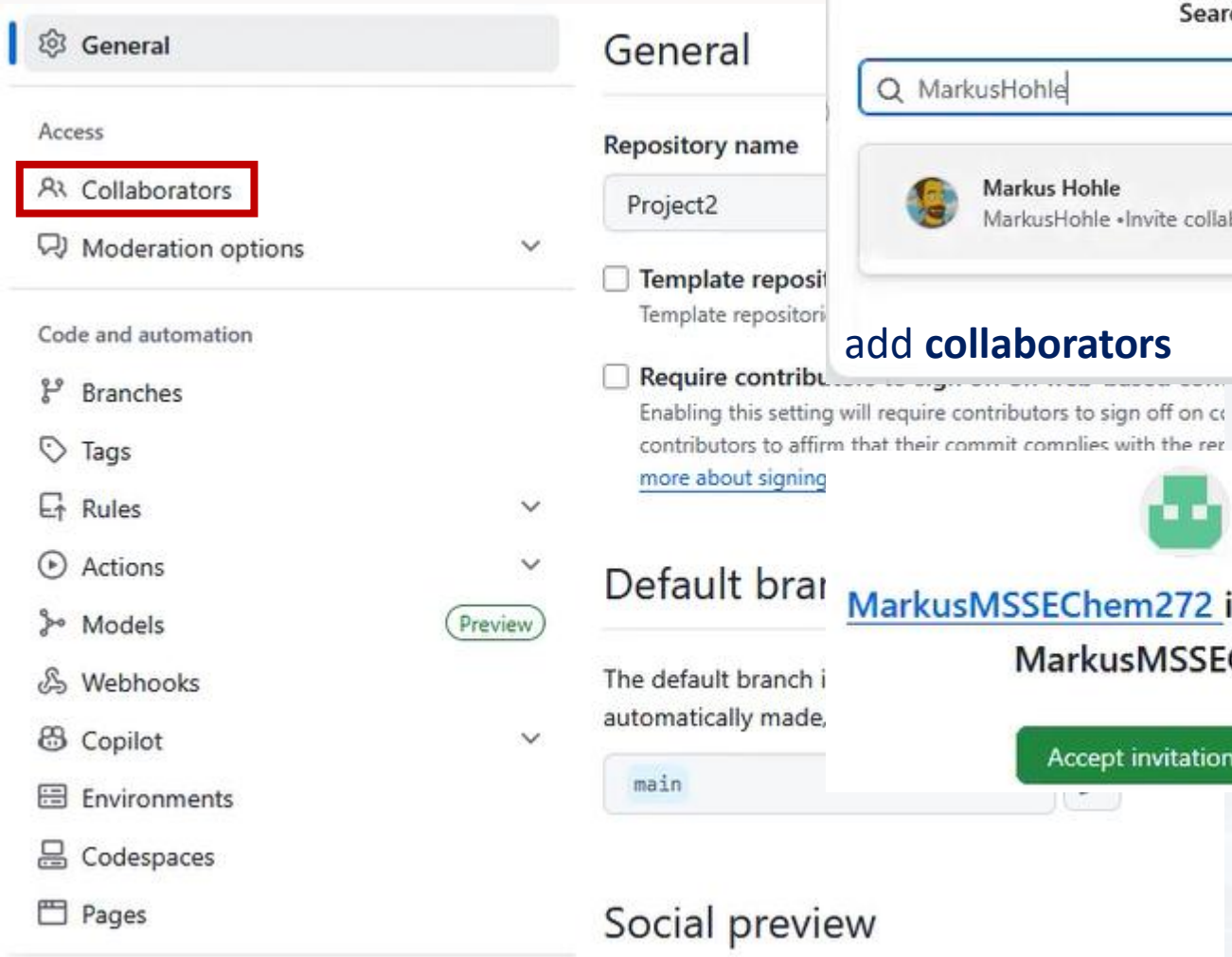
  - **invite a co worker**
  - push
  - fetch, merge, pull

go to **settings**

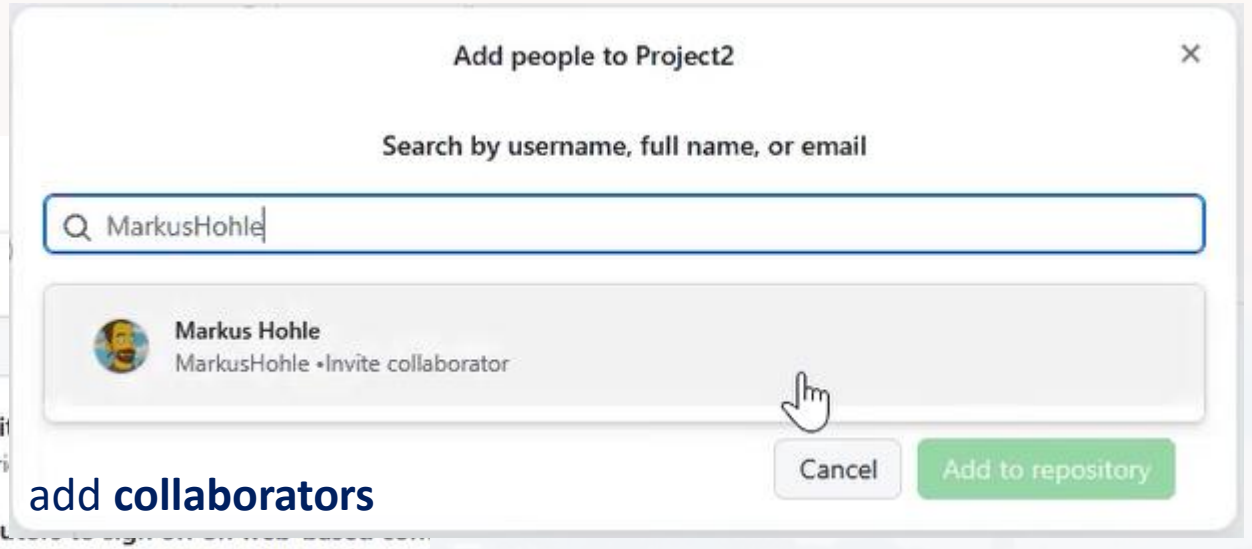


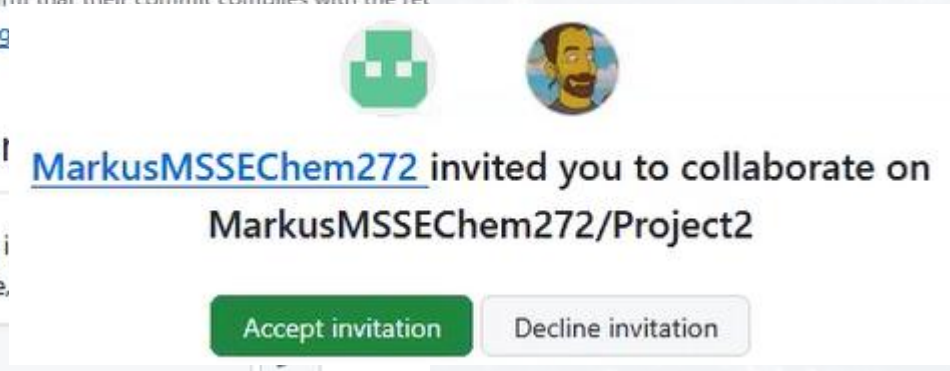
invite a co-worker

go to **collaborators**



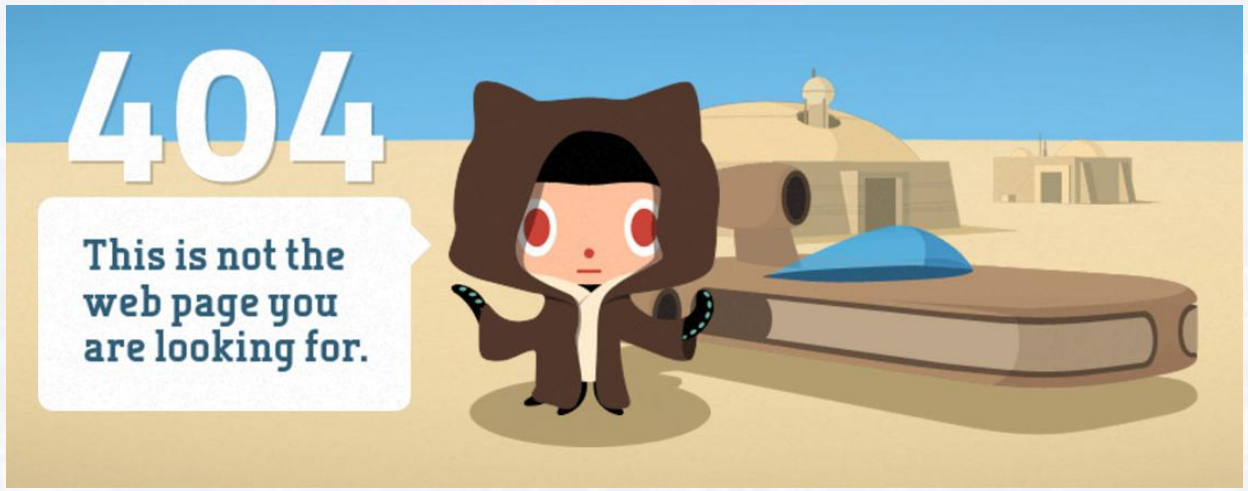
add **collaborators**





your **collaborator** will get an invitation and needs to confirm it

watch:
12h_GitHub_InviteCoWorker



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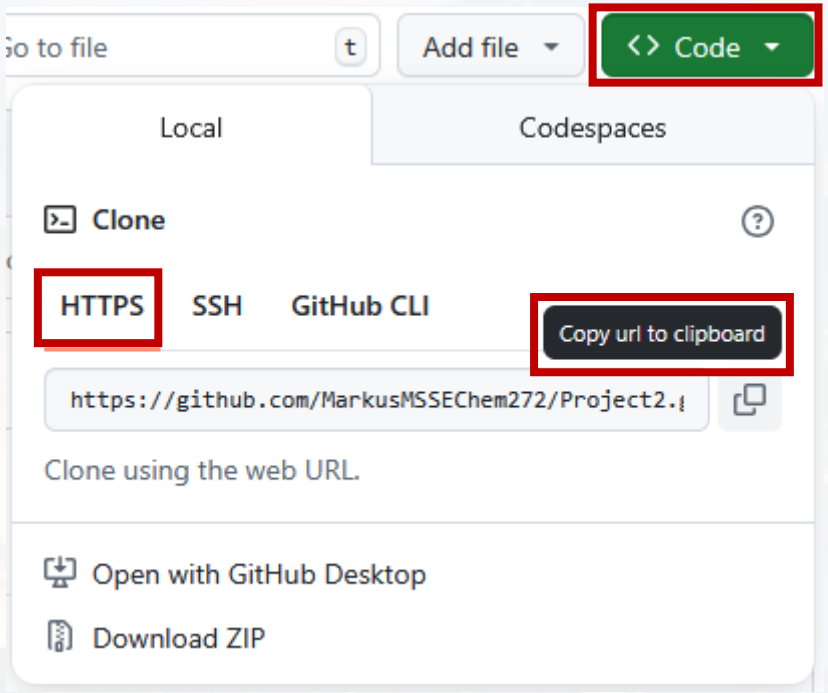
  - **push**
  - fetch, merge, pull

1) copying the remote repo to your local machine (`git clone`)

- copy the **url** of your repo



a) go to your repo and click *code*

b) select an option (e. g. HTTPS)

c) copy the url

next: open VS Code and navigate to the directory in which you want to copy the repo

next: open VS Code and navigate to the directory in which you want to copy the repo

```
:~/Berkeley/MSSE/Chem272/Projects/Project 2$
```

clone the repo:

the url we copied earlier

```
git clone https://github.com/MarkusMSSEChem272/Project2.git
```

```
Cloning into 'Project2'...
remote: Enumerating objects: 6, done.
remote: Counting objects: 100% (6/6), done.
remote: Compressing objects: 100% (3/3), done.
remote: Total 6 (delta 0), reused 0 (delta 0), pack-reused 0 (from 0)
Receiving objects: 100% (6/6), done.
```

the entire repo is being copied to your local machine now!

```
(base) mmh_user@DESKTOP-PPSA666:~/Berkeley/MSSE/Chem272/Projects/Project 2$ ls
OneHotEncoder.py  Project2
```

```
(base) mmh_user@DESKTOP-PPSA666:~/Berkeley/MSSE/Chem272/Projects/Project 2/Project2$ ls
README.md
```

2) workflow

a) navigate to your project folder

```
(base) mmh_user@DESKTOP-PPSA666:~/Berkeley/MSSE/Chem272/Projects/Project 2/Project2$ ls
README.md
```

b) check `git status`

either Git tells you that to local repo is up to date, or

it tells you that the **remote repo is X commits ahead**

→ run `git fetch` to update your local repo (**see later!**)!

c) you work on your code and want to add it to the remote repo now

```
git add
git commit -m "my message"
```

```
git push https://github.com/MarkusMSSEChem272/Project2.git main
```

pushes the new code to the remote repo

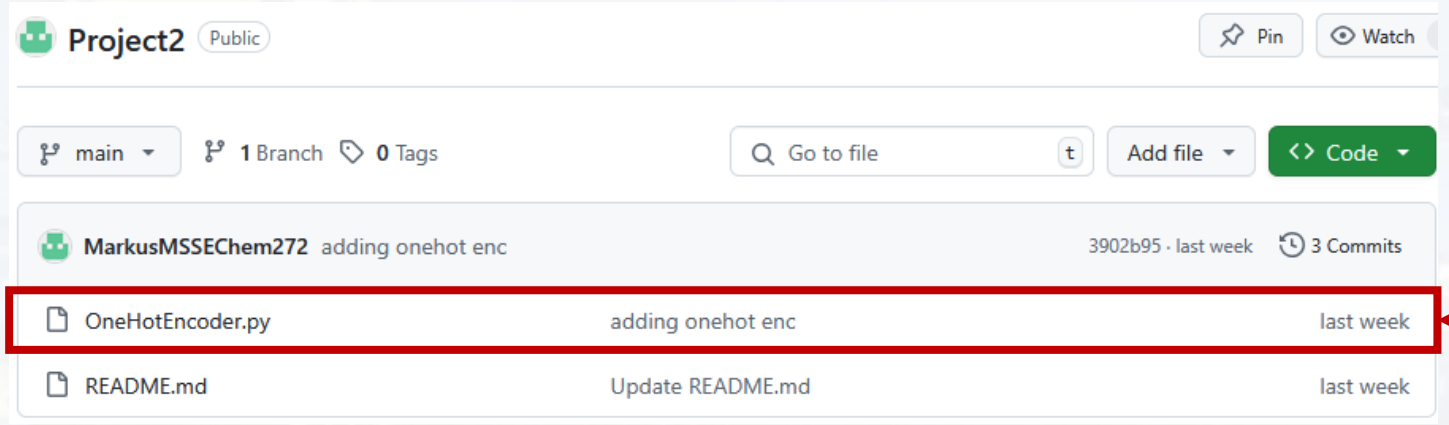
2) workflow

```
git add
git commit –m “my message”
```

pushes the new code to the remote repo

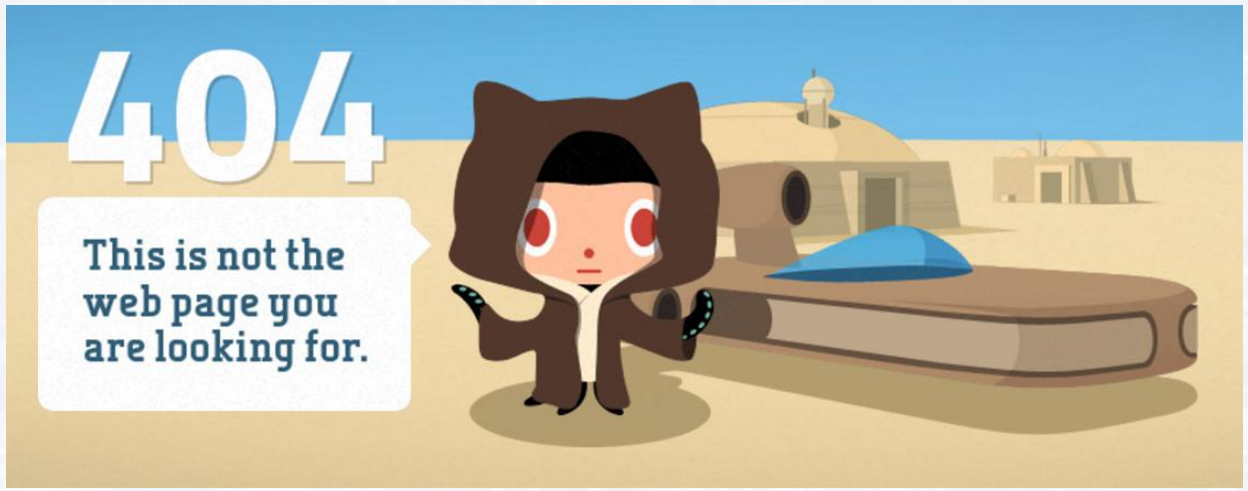
```
git push https://github.com/MarkusMSSEChem272/Project2.git main
```

```
(base) mmh_user@DESKTOP-PPSA666:~/Berkeley/MSSE/Chem272/Projects/Project 2/Project2$ git push https://github.com/MarkusMSSEChem272/P
roject2.git main
/mnt/c/Program\ Files/Git/mingw64/bin/git-credential-manager-core.exe get: 1: /mnt/c/Program Files/Git/mingw64/bin/git-credential-ma
nager-core.exe: not found
/mnt/c/Program\ Files/Git/mingw64/bin/git-credential-manager-core.exe store: 1: /mnt/c/Program Files/Git/mingw64/bin/git-credential-
manager-core.exe: not found
Enumerating objects: 4, done.
Counting objects: 100% (4/4), done.
Delta compression using up to 8 threads
Compressing objects: 100% (3/3), done.
Writing objects: 100% (3/3), 807 bytes | 807.00 KiB/s, done.
Total 3 (delta 0), reused 0 (delta 0), pack-reused 0
To https://github.com/MarkusMSSEChem272/Project2.git
   97d088a..3902b95  main -> main
```



code is online!

watch:
12i_GitHub_CloneRepo
12j_GitHub_Push



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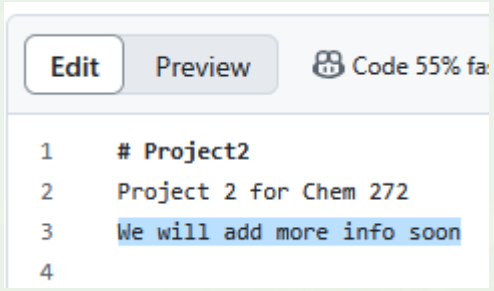
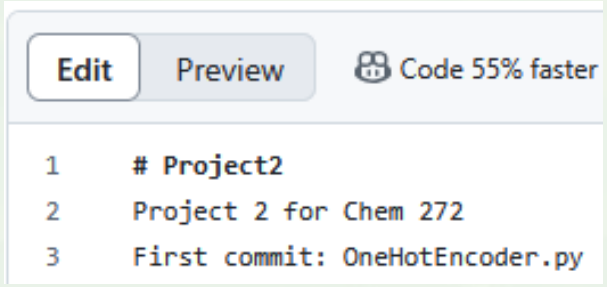
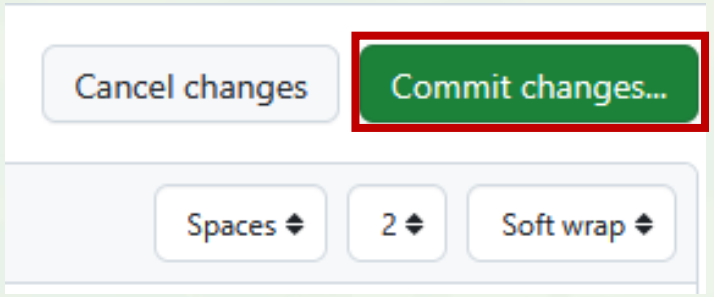
if your co-workers have pushed new code to the **remote repo**
→ update your **local repo/directory** accordingly

remote repo (GitHub)







local repo

`git status`

```
(base) mmh_user@DESKTOP-PPSA666:~/Berkeley/MSSE/Chem272/Projects/Project 2/Project2$ git status
On branch main
Your branch is ahead of 'origin/main' by 1 commit.
  (use "git push" to publish your local commits)
```

if your co-workers have pushed new code to the **remote repo**
→ update your **local repo/directory** accordingly

local repo

`git status`

```
(base) mmh_user@DESKTOP-PPSA666:~/Berkeley/MSSE/Chem272/Projects/Project 2/Project2$ git status
On branch main
Your branch is ahead of 'origin/main' by 1 commit.
  (use "git push" to publish your local commits)
```

`git fetch`

```
(base) mmh_user@DESKTOP-PPSA666:~/Berkeley/MSSE/Chem272/Projects/Project 2/Project2$ git fetch
remote: Enumerating objects: 5, done.
remote: Counting objects: 100% (5/5), done.
remote: Compressing objects: 100% (3/3), done.
remote: Total 3 (delta 0), reused 0 (delta 0), pack-reused 0 (from 0)
Unpacking objects: 100% (3/3), 1000 bytes | 142.00 KiB/s, done.
From https://github.com/MarkusMSSEChem272/Project2
   efeafe4..d82475c  main       -> origin/main
```

`git fetch`

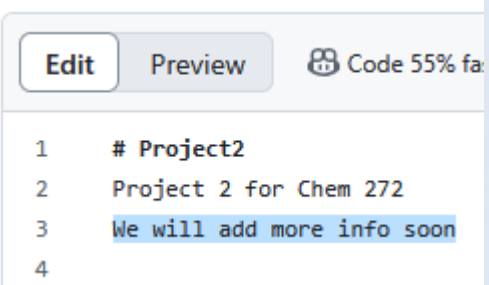
- **does not** update your working directory
- updates only commits, tags etc → **safe to inspect changes**

if your co-workers have pushed new code to the **remote repo**
→ update your **local repo/directory** accordingly

local repo

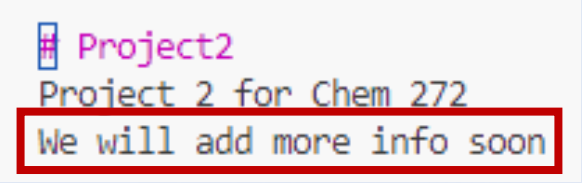
```
git fetch
```

- **does not** update your working directory
- updates only commits, tags etc → **safe to inspect changes**



old version is still stored in working directory

working directory




```
git merge
```

- **does** update your working directory

```
(base) mmh_user@DESKTOP-PPSA666:~/Berkeley/MSSE/Chem272/Projects/Project 2/Project2$ git merge
Updating 92d4c09..d82475c
Fast-forward
 README.md | 2 +-
 1 file changed, 1 insertion(+), 1 deletion(-)
```

if your co-workers have pushed new code to the **remote repo**
→ update your **local repo/directory** accordingly

working directory

```
# Project2
Project 2 for Chem 272
We will add more info soon
```

`git merge`

- **does** update your working directory

```
(base) mmh_user@DESKTOP-PPSA666:~/Berkeley/MSSE/Chem272/Projects/Project 2/Project2$  git merge
Updating 92d4c09..d82475c
Fast-forward
 README.md | 2 +-
 1 file changed, 1 insertion(+), 1 deletion(-)
```

```
# Project2
Project 2 for Chem 272
First commit: OneHotEncoder.py
```

Now, also the **working directory** has been updated

alternatively: `git pull`

runs `git fetch` **and** `git merge`

```
(base) mmh_user@DESKTOP-PPSA666:~/Berkeley/MSSE/Chem272/Projects/Project 2/Project2$ git pull
remote: Enumerating objects: 5, done.
remote: Counting objects: 100% (5/5), done.
remote: Compressing objects: 100% (3/3), done.
remote: Total 3 (delta 0), reused 0 (delta 0), pack-reused 0 (from 0)
Unpacking objects: 100% (3/3), 1011 bytes | 337.00 KiB/s, done.
From https://github.com/MarkusMSSEChem272/Project2
   d82475c..bce999b  main       -> origin/main
Updating d82475c..bce999b
Fast-forward
 README.md | 1 +
 1 file changed, 1 insertion(+)
```

watch:
12k_Git_Fetch_Merge_Pull

summary

`git add <my_file>`	adds a file to staging area
`git commit –m “my_message”`	commits files from staging area to local repo
`git push <remote_repo_name> <branch_name>`	updates remote repo
`git restore <my_file>`	undoes changes in indexed file
`git restore --staged <my_file>`	moves file from staged area to index
`git restore --source=HEAD~X`	moves commit (X commits before current one) back to staged area
`git fetch`	updates local commit from remote repo
`git merge`	updates local directory after `fetch`
`git pull`	runs `fetch` **and** `merge`
`git clone`	clones entire remote repo (has to be done only **once**!)

summary

`git add <my_file>`	adds a file to staging area
`git commit –m “my_message”`	commits files from staging area to local repo
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`git merge`	updates local directory after `fetch`
`git pull`	runs `fetch` **and** `merge`
`git clone`	clones entire remote repo (has to be done only **once**!)

note, there is way more you could do

check out different **branches**
moving **head**

We hope you have enjoyed the course!