Introduction: Part 2

Scientific Programming in Python

Installation instructions: Miniconda & Linux

- Download your version from https://docs.conda.io/en/latest/miniconda.html
- bash Miniconda3-latest-Linux-x86_64.sh (saying yes when it asks you to add it to the terminal)
 - (which python should now answer .../anaconda3/bin/python)
 - o (alternatively: conda update --all)
- If you don't have git already (try by running which git), install it using sudo apt-get install git

To have jupyterlab globally on your system:

- conda install jupyter
- conda install jupyterlab
- conda install conda-forge::nodejs
- jupyter labextension install @lckr/jupyterlab_variableinspector

To create the environment for the class:

- git clone https://github.com/scientificprogrammingUOS/lectures.git
- conda env create -f lectures/environment.yml
- conda activate scientific_programming
- jupyter labextension install @lckr/jupyterlab_variableinspector

Installation instructions: Miniconda & Windows

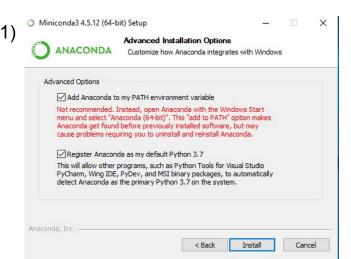
- Download your version from https://docs.conda.io/en/latest/miniconda.html
- Run the graphical installer.
 - Make sure to add conda to your PATH¹, such that you can use it from your standard terminal.
- Afterwards, open the command-prompt as Administrator (hit Win-Key, type "cmd", right-click "Command Prompt", select "as Admin")
 - Test if your installation was correct by running where python
 - → it should return a path containing .../Anaconda3/...
 - Update your Conda installation by running conda update conda
- Install git from https://git-scm.com/downloads
 - Make sure that git can be used from your command-line²
 - Make sure that you use one of the two options committing unix-style³
 - Leave everything else the way it is
- Afterwards you should have the commands python, conda and git as registered commands⁴

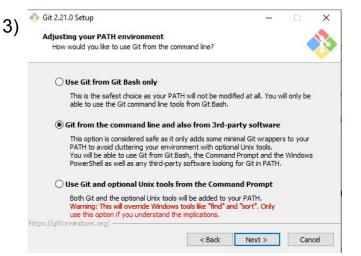
To have jupyterlab globally on your system:

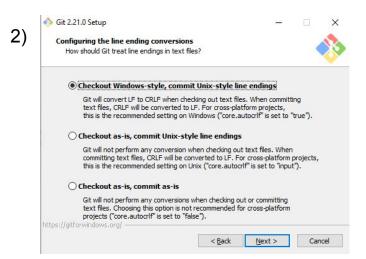
- conda install jupyter
- conda install jupyterlab
- conda install conda-forge::nodejs
- jupyter labextension install @lckr/jupyterlab_variableinspector⁵

To create the environment for the class:

- git clone https://github.com/scientificprogrammingUOS/lectures.git
- conda env create -f lectures/environment.yml
- conda activate scientific_programming
- jupyter labextension install @lckr/jupyterlab_variableinspector⁵







Microsoft Windows [Version 10.0.17763.348]
(c) 2018 Microsoft Corporation. All rights reserved.

C:\Users\User>where python
C:\Users\User\Miniconda3\python.exe

C:\Users\User\Where conda
C:\Users\User\Miniconda3\Library\bin\conda.bat
C:\Users\User\Miniconda3\Scripts\conda.exe

C:\Users\User\Where git
C:\Program Files\Git\cmd\git.exe

C:\Users\User>

Windows: If the previous didn't work

- Sorry for the huge mess that was today's lecture we know that for many of you, the previous installation process doesn't work like that.
- If you are sure you followed the previous steps as described, and you still get an error containing something along the lines of "qt linking failed", you can instead not install the complete environment all in once, but start with what's needed for the first few lectures and install the rest on demand

```
conda create -n scientific_programming python=3.7
conda activate scientific_programming
pip install jupyter
pip install jupyterlab
pip install pytest
conda install nodejs -y
jupyter labextension install @lckr/jupyterlab_variableinspector<sup>5</sup>
```

• Afterwards, you can enable this environment just as if you installed it using the environment.yml file.

After Installation

- Once you activate your environment using conda activate scientific_programming, your shell should indicate that you're inside this environment
- Note that you have to activate your this environment every time you work on the exercises!
- To test if all packages are installed successfully, run conda list and check if all demanded packages are indeed listed.
- To start working inside jupyter lab, navigate to the correct directory using *cd*, and then start jupyterlab by executing *jupyter lab*. (yes, including the dot)⁵

- 5) If the commands involving jupyter don't work on Windows, try using a hyphen instead of a space:
 - → jupyter-labextension install @lckr/jupyterlab_variableinspector
 - → jupyter-lab .

Intro: git

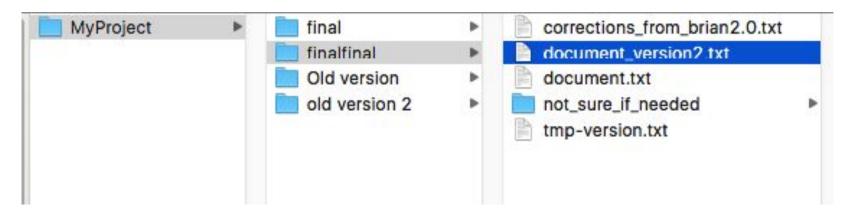
[These slides are basing on the ones created by Lukas Kalbertodt, all credits to him]

Getting started with git



- Git is a free and open source VCS (version control system)
- It allows you to track changes to files over time, compare new versions to old versions, have multiple versions in parallel, and work simultaneously on projects
- VCS are commonly used for programming projects, but can also be useful for any other project

Why version control?



Version control

Tracks & logs changes in your files with...

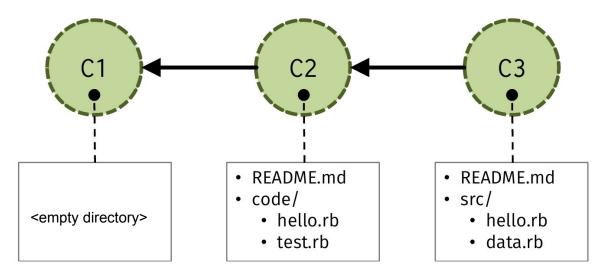
- Author
- Timestamp
- Description

Allows...

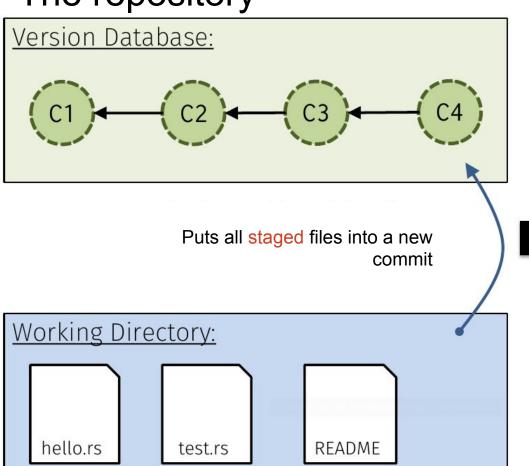
- Restoring old versions
- Having multiple parallel versions
- Analyzing your code
- Collaborating on code

A commit

- Snapshot of the whole project at certain time
- A commit saves...
 - Its predecessor
 - Changes in the files (delta from predecessor)
 - Author, time, commit message
- Identified by Hash (eg. C1, C2, ..)



The repository



- Contains all commits
- Saved in a hidden folder called .git

git commit



File status

Staged

File will be committed with the next commit

Modified

File is registered for git and was changed since the last commit

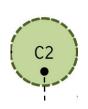
Unmodified

File is registered in git, but equal to the last commit

Untracked

Git knows the file exists, but won't do anything with it





Modified

Unmodified

Untracked

git status

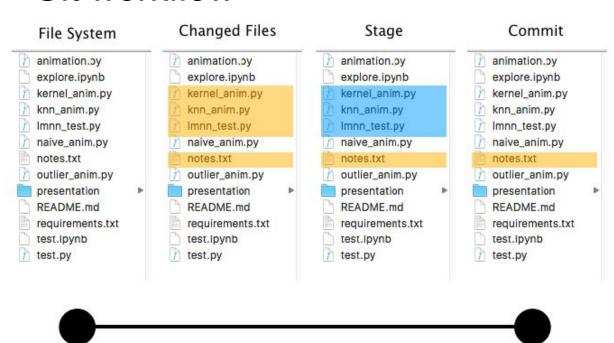
\$ git status Staged On branch dev Your branch is up-to-date with 'origin/dev'. Changes to be committed: Run git status before any (use "git reset HEAD <file>..." to unstage) other command to know what's going on! Modified new file: bye.rs new file: hello.rs Changes not staged for commit: (use "git add <file>..." to update what will be committed) (use "git checkout -- <file>..." to discard changes in working directory) Unmodified modified: Cargo.toml Untracked files: (use "git add <file>..." to include in what will be committed) Untracked test.rs

Git workflow

File System

- animation.py
 explore.ipynb
- kernel_anim.py
- knn_anim.py
- mnn_test.py
- naive_anim.py
- notes.txt
- noutlier_anim.py
- presentation
- README.md
- requirements.txt
- test.lpynb
- test.py

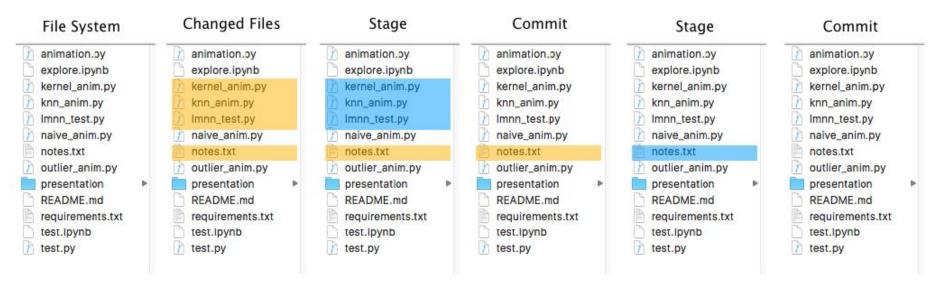
Git workflow



Initial Commit

2nd Commit (3 files changed)

Git workflow



Initial Commit

2nd Commit (3 files changed) 3rd Commit (1 file changed)

Getting started with GitHub

- Github is a website, providing a server to store your projects and also a web-interface to easily access them and to collaborate with others
- GitHub adds many additional features, like Pull-Requests with Code review, Issues, Wikis, ...

- Github is only an external storage (+UI) for git projects
- Git works perfectly fine locally, without GitHub
- Github allows for easy access from multiple computers
- You need to manually synchronize your local directory with GitHub!



Distributed VCS Computer B* (remote) Server **Computer A** git pull (C6) Computer C* C3 **←** Susi You

Demo: git

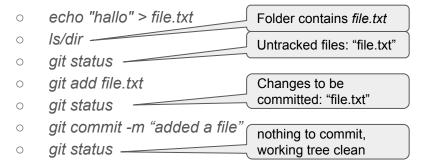
Demo: shells

What to do

- Clone with SSH ③ Use HTTPS
 Use an SSH key and passphrase from account.

 git@github.com:torvalds/linux.git

 Download ZIP
- 1. Create a new repository OR 1. Clone a repository
 - o *git init* PROJECT1
 - Creates a new folder PROJECT1
 - o cd PROJECT1
- Add some files



- git clone GIT URL
- Creates a local copy of the repository and adds URL as remote origin

- 3. Push local changes
 - o (Create repo: https://github.com/new
 - git remote add origin GIT_URL)
 - git push origin master

Git commands cheat-sheet

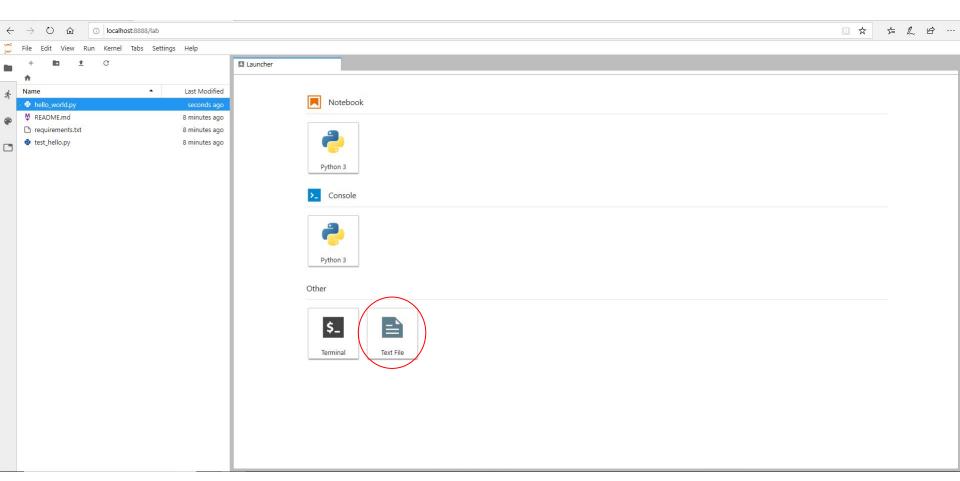
- git init to create a new project
- git clone <url>

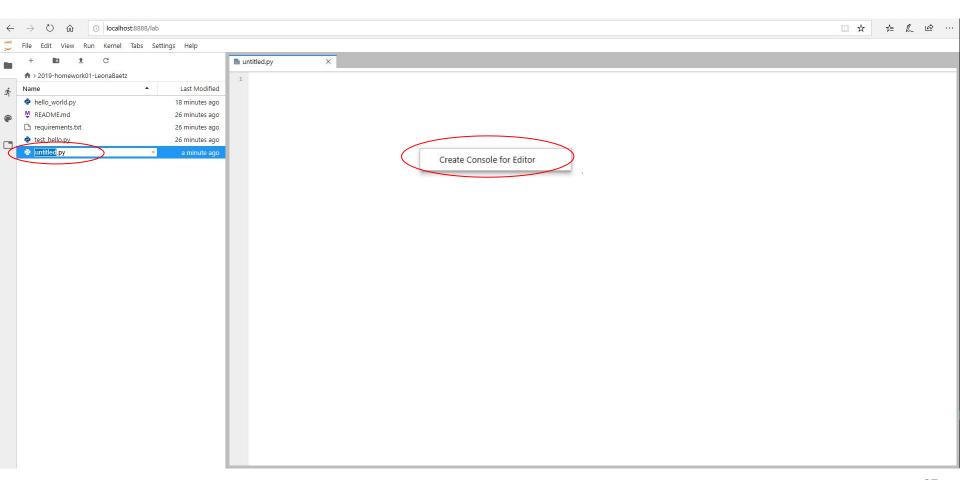
 to copy an existing project from eg. GitHub or BitBucket
- git status to view which files changed in status
- git diff to view each file's difference to the last commit (or also between commits)
- git checkout <file> to reset a file to the last commit
- git checkout -b
branch> <hash> to completely restore an older commit (to a branch)
- git checkout <branch> to switch branches (eg. back to master)
- git log to view your latest commits incl. messages
- git pull to update your local repository to the state of the one on GitHub/BitBucket
- git push to update the repository on GitHub/BitBucket to your local version
- git add <file> such that git will stage the file to be considered in the next commit
- git rm <file> to delete a file from filesystem and also stop tracking it
- git commit -m "<message>" to create a commit of the currently staged files

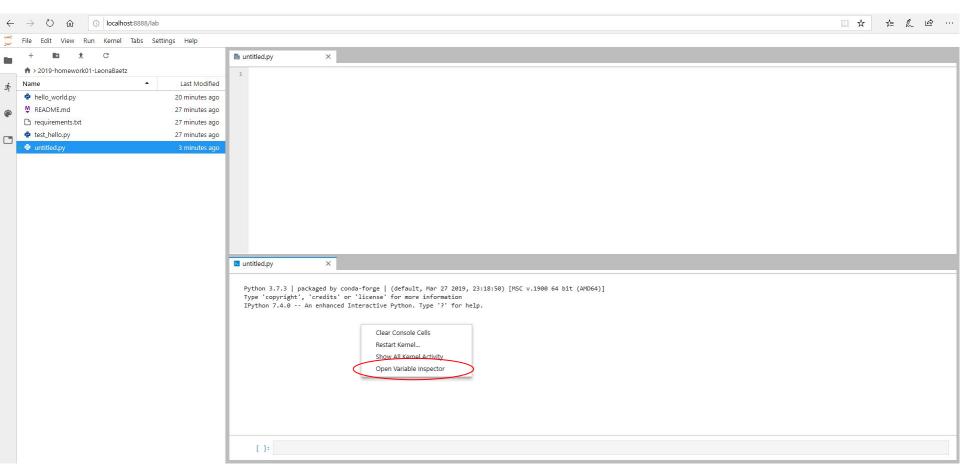
Final remarks on git

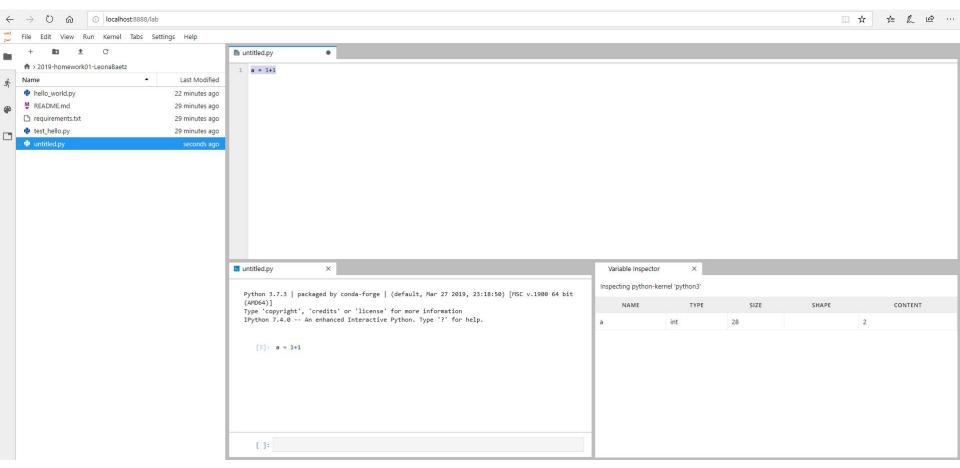
- Git is made for source-code and is no dropbox! → Add only text-based (diff'able) files
- Gitignores may help to not add unnecessary files. Add a ".gitignore" file to your repository and write filename-masks you want git to completely ignore into it. A useful start is https://github.com/github/gitignore/blob/master/Python.gitignore
- Modern editors all come with git integration, however we advise to not use it until you're really familiar with git! Learning the console always helps!
- If you are not familiar with git https://try.github.io/
- For deeper looks https://git-scm.com/book/en/v2

Howto: Interactive Kernel









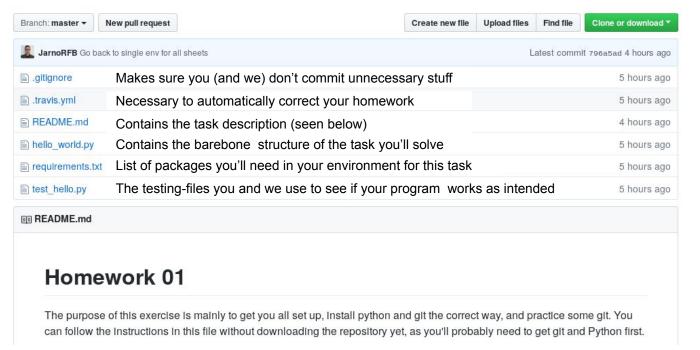
Getting used to Jupyter lab

- Jupyter Lab Cheat-sheet:
 https://www.cheatography.com/weidadeyue/cheat-sheets/jupyter-notebook/pdf_bw/
- Markdown-Commands Cheat-Sheet:
 https://github.com/adam-p/markdown-here/wiki/Markdown-Cheatsheet

Homework

Homework

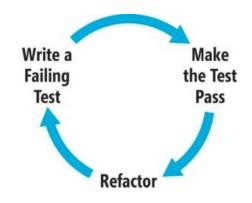
- Homework is distributed via Github classroom
- You need a github-account to submit the homework!
- If there are mistakes in the homework, we will announce that and update the repositories, so regularly pull!



Pytest and Test-Driven Development

- pytest is a testing library included with python
- It will grab all test -functions in all test -files, execute them, and check for errors
- To do so, it uses assertions: assert prime.find_prime(1) ==2

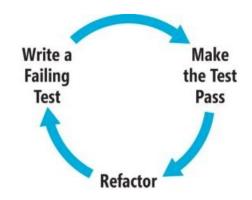
```
chris@debian:~/Documents/UNI/sem_10/Scientific_Programming_Python/homework/bonus01$_pytest
          platform linux -- Python 3.6.5rc1, pytest-3.5.0, py-1.5.3, pluggy-0.6.0
rootdir: /home/chris/Documents/UNI/sem 10/Scientific Programming Python/homework/bonus01, inifile:
collected 2 items
test_prime.py .F
                                                                                         [100%]
                                     ====== FAILURES ==========
                                     test find prime method
   def test find prime method():
      assert hasattr(prime, 'find_prime'), "Your Script must have a 'find_prime'-method!"
      assert prime.find prime(1) == 2
      assert prime.find_prime(8) == 19
       assert 11 == 19
       + where 11 = <function find prime at 0x7f8407982bf8>(8)
           where <function find_prime at 0x7f8407982bf8> = prime.find_prime
test_prime.py:19: AssertionError
               ========= 1 failed, 1 passed in 0.02 seconds =========
chris@debian:~/Documents/UNI/sem_10/Scientific_Programming_Python/homework/bonus01$
```



Pytest and Test-Driven Development

- pytest is a testing library included with python
- It will grab all test -functions in all test -files, execute them, and check for errors
- To do so, it uses assertions: assert prime.find prime(1) == 2

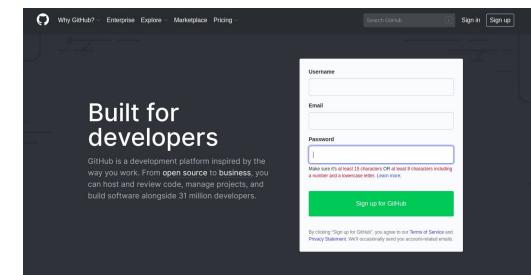
```
hris@debian:~/Documents/UNI/sem_10/Scientific_Programming_Python/homework/bonus01$ pytest:
                              ====== test session starts =======
platform linux -- Python 3.6.5rc1, pytest-3.5.0, py-1.5.3, pluggy-0.6.0
rootdir: /home/chris/Documents/UNI/sem 10/Scientific Programming Python/homework/bonus01, inifile:
collected 2 items
test_prime.py ...
                                                                                         100%
      ------ 2 passed in 0.03 seconds ------
chris@debian:~/Documents/UNI/sem_10/Scientific_Programming_Python/homework/bonus01$
```



Once this is the result of pytest, your homework will pass!

Create a GitHub account

- Go to https://github.com/
- Your GitHub account is like your portfolio for programming, so use something you can show to others instead of xXOmqItzPotatoXx

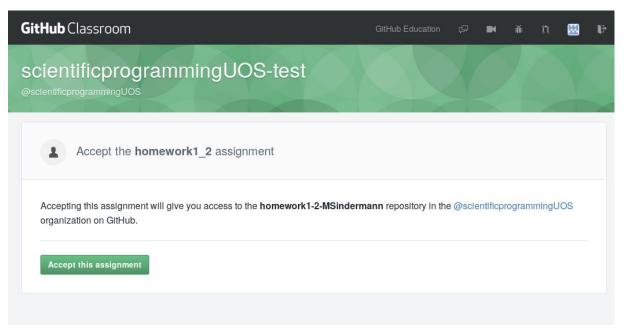


Your homework

- Homework-link:
 - https://classroom.github.com/a/2RXLdM_r

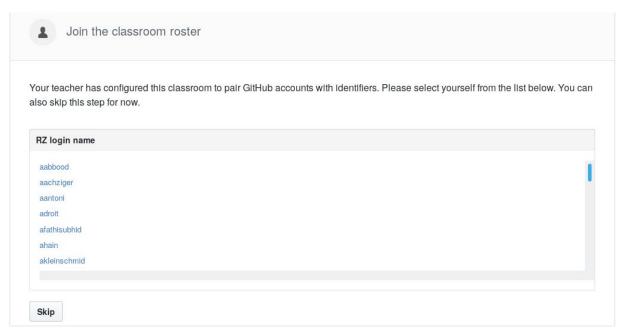
<demo: homework>

- Homework-link:
 - https://classroom.github.com/a/2RXLdM_r



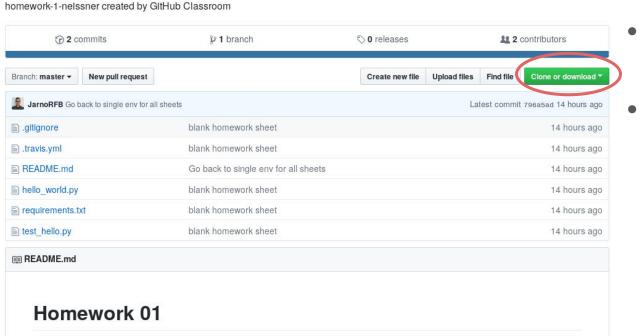
- You need to sign in to github
- Use your @uos-mail to get unlimited free repositories! https://education.github.com/pack
 /offers

- Homework-link:
 - https://classroom.github.com/a/2RXLdM_r



- If your RZ-login is not listed here or spelled incorrectly, please write us an email!
- When it says "preparing your new repository, there is no need to keep this window open, we'll email you when the import is done", just hit F5 after 5 seconds

- Homework-link:
 - https://classroom.github.com/a/2RXLdM_r



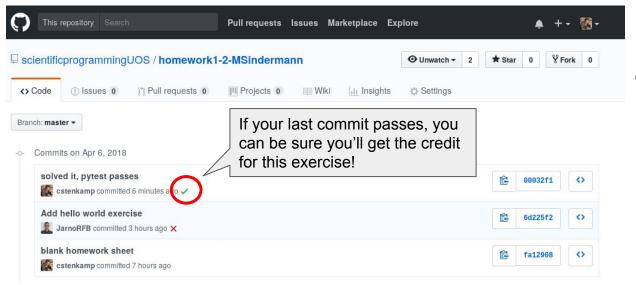
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- Homework-link:
 - https://classroom.github.com/a/2RXLdM_r

```
git clone REPOSITORY URL
cd YOUR REPOSITORY PATH
conda activate scientific programming
jupyter lab .
. . .
pytest
git status
git add CHANGED FILE
git commit -m "solved the exercise"
git push origin master
conda deactivate
```

- Homework-links:
 - https://classroom.github.com/a/2RXLdM_r

git config --get remote.origin.url tells you the domain of your remote repository



Note that the first check will be performed 5-15 minutes after accepting the exercise, from then on ASAP

- Homework-links:
 - https://classroom.github.com/a/2RXLdM_r

- Note that the first check will be performed 5-15 minutes after accepting the exercise, from then on ASAP
- First deadline is next Tuesday, 12:00 (hard)
- Clone the repository >15 minutes before the deadline passes, make the last commit before the deadline passes
- Yes, you get the test-scripts, but don't change them, we check for that!
- You'll get an email telling you if you passed or failed, including your overall pass/fail-count right after the next lecture!

<Screenshots of Presentation>

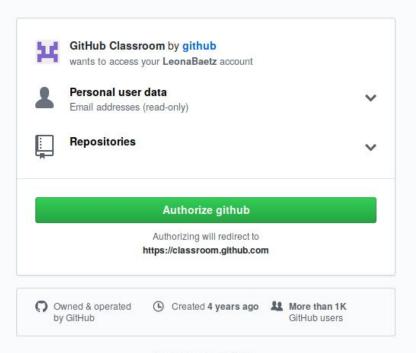


Sign in to GitHub	
Username or em	ail address
Password	Forgot password
E	Sign in

Terms Privacy Security Contact GitHub



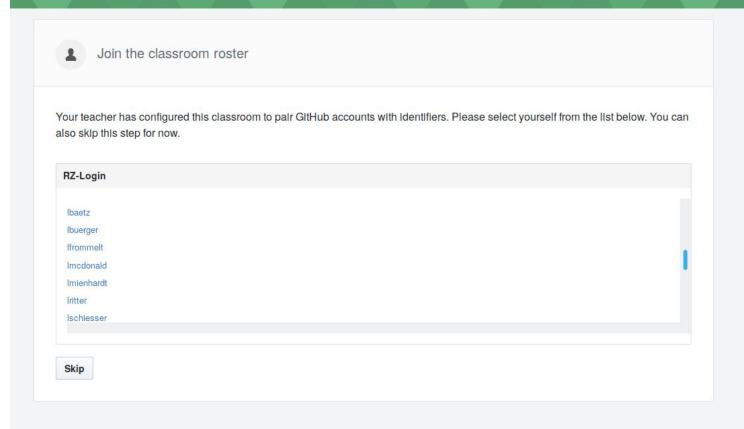
Authorize GitHub Classroom



Learn more about OAuth



@scientificprogrammingUOS













@scientificprogrammingUOS

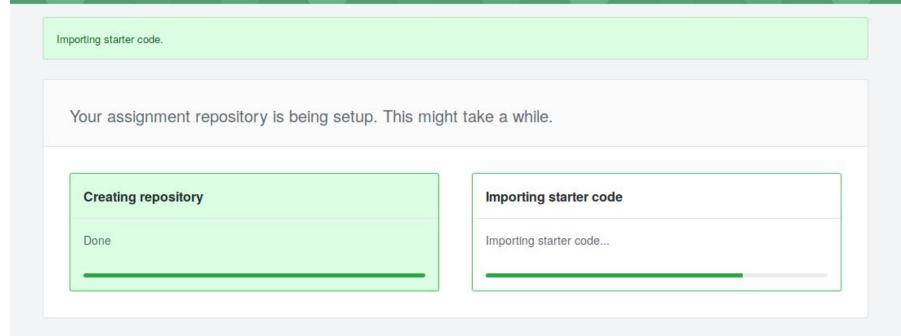


Accept the 2019-homework01 assignment

Accepting this assignment will give you access to the **2019-homework01-LeonaBaetz** repository in the @scientificprogrammingUOS organization on GitHub.

Accept this assignment

@scientificprogrammingUOS













@scientificprogrammingUOS

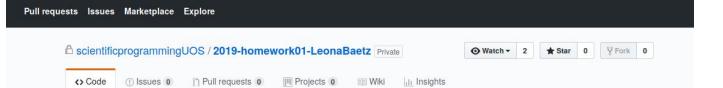


Accepted the 2019-homework01 assignment

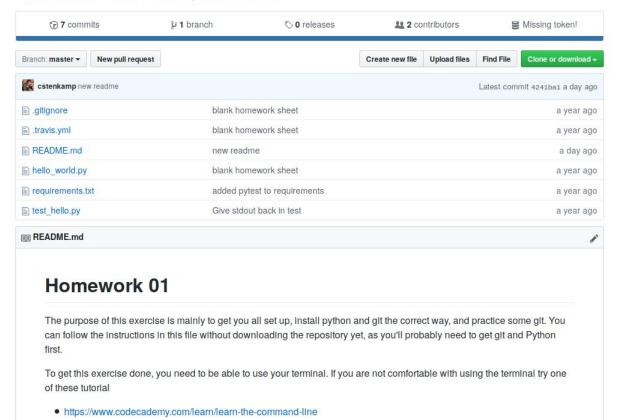
You are ready to go!

You may receive an invitation to join @scientificprogrammingUOS via email invitation on your behalf. No further action is necessary.

Your assignment has been created here: https://github.com/scientificprogrammingUOS/2019-homework01-LeonaBaetz

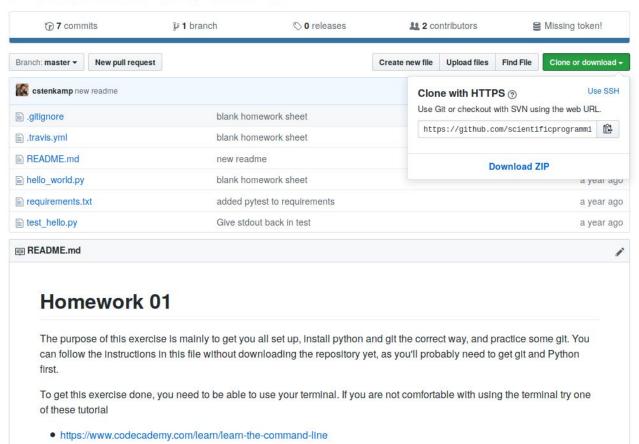


2019-homework01-LeonaBaetz created by GitHub Classroom





2019-homework01-LeonaBaetz created by GitHub Classroom



```
Microsoft Windows [Version 10.0.17763.348]
(c) 2018 Microsoft Corporation. All rights reserved.

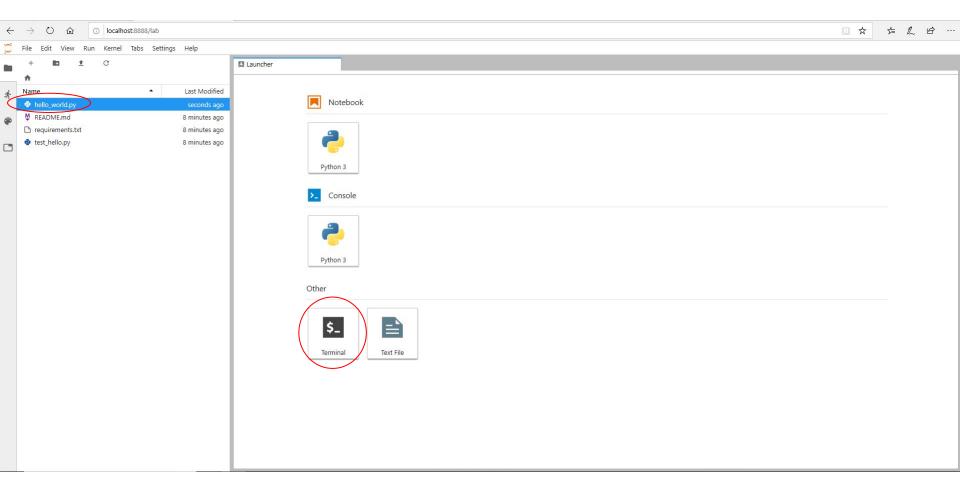
C:\Users\User\mkdir python_homework && cd python_homework

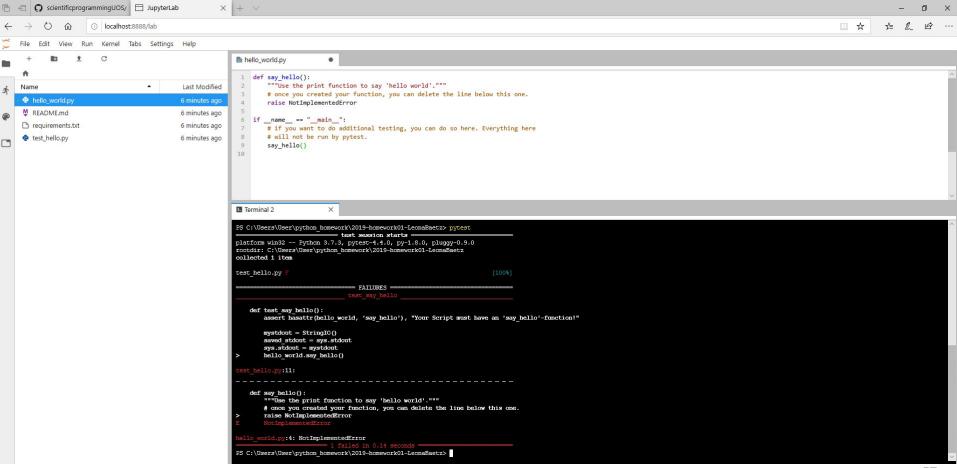
C:\Users\User\python_homework\git clone https://github.com/scientificprogrammingUOS/2019-homework01-LeonaBaetz.git
Cloning into '2019-homework01-LeonaBaetz'...
remote: Enumerating objects: 25, done.
remote: Counting objects: 100% (25/25), done.
remote: Compressing objects: 100% (13/13), done.
remote: Total 25 (delta 10), reused 25 (delta 10), pack-reused 0
Unpacking objects: 100% (25/25), done.

C:\Users\User\python_homework>cd 2019-homework01-LeonaBaetz
```

```
C:\Users\User\python homework\2019-homework01-LeonaBaetz>dir
Volume in drive C has no label.
Volume Serial Number is 045F-2CF3
Directory of C:\Users\User\python homework\2019-homework01-LeonaBaetz
04/03/2019 11:42 AM
04/03/2019 11:42 AM
                  <DIR>
04/03/2019 11:42 AM
                         1.339 .gitignore
                       138 .travis.yml
04/03/2019 11:42 AM
04/03/2019 11:42 AM
                         346 hello world.py
04/03/2019 11:42 AM
                         6.937 README.md
04/03/2019 11:42 AM
                          15 requirements.txt
          .:42 AM
6 File(s)
04/03/2019 11:42 AM
                          382 test hello.py
                          9,157 bytes
           2 Dir(s) 92,013,391,872 bytes free
C:\Users\User\python homework\2019-homework01-LeonaBaetz>conda activate scientific programming
(scientific_programming) C:\Users\User\python_homework\2019-homework01-LeonaBaetz>pytest
platform win32 -- Python 3.7.3, pytest-4.4.0, py-1.8.0, pluggy-0.9.0
rootdir: C:\Users\User\python homework\2019-homework01-LeonaBaetz
collected 1 item
test hello.py
                                                                                         [100%]
test say hello
  def test_say_hello():
      assert hasattr(hello world, 'say hello'), "Your Script must have an 'say hello'-function!"
      mystdout = StringIO()
      saved stdout = sys.stdout
      sys.stdout = mystdout
      hello world.say hello()
  def say hello():
      """Use the print function to say 'hello world'."""
      # once you created your function, you can delete the line below this one.
      raise NotImplementedError
ello world.py:4: NotImplementedError
  (scientific programming) C:\Users\User\python homework\2019-homework01-LeonaBaetz>
```

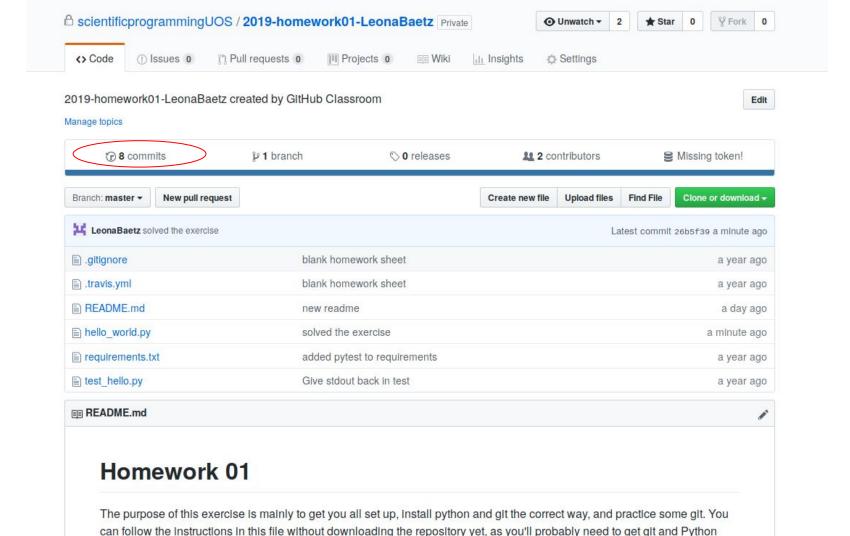
```
(scientific programming) C:\Users\User\python homework\2019-homework01-LeonaBaetz>jupyter lab .
[I 11:44:32.582 LabApp] Writing notebook server cookie secret to C:\Users\User\AppData\Roaming\jupyter\runtime\notebook
cookie secret
[I 11:44:35.474 LabApp] JupyterLab extension loaded from C:\Users\User\Miniconda3\envs\scientific programming\lib\site-p
ackages\jupyterlab
[I 11:44:35.474 LabApp] JupyterLab application directory is C:\Users\User\Miniconda3\envs\scientific programming\share\j
upyter\lab
[W 11:44:35.474 LabApp] JupyterLab server extension not enabled, manually loading...
[I 11:44:35.490 LabAppl JupyterLab extension loaded from C:\Users\User\Miniconda3\envs\scientific programming\lib\site-p
ackages\jupyterlab
[I 11:44:35.490 LabApp] JupyterLab application directory is C:\Users\User\Miniconda3\envs\scientific programming\share\
upyter\lab
[I 11:44:35.490 LabApp] Serving notebooks from local directory: C:\Users\User\python homework\2019-homework01-LeonaBaetz
[I 11:44:35.490 LabApp] The Jupyter Notebook is running at:
[I 11:44:35.490 LabApp] http://localhost:8888/?token=c087e9072427f4b2f2f3c0f57d9d1d8c7e5669c91a047813
[I 11:44:35.490 LabApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
[C 11:44:35.551 LabApp]
   To access the notebook, open this file in a browser:
       file:///C:/Users/User/AppData/Roaming/jupyter/runtime/nbserver-7196-open.html
   Or copy and paste one of these URLs:
        http://localhost:8888/?token=c087e9072427f4b2f2f3c0f57d9d1d8c7e5669c91a047813
[I 11:44:44.752 LabApp] Node v11.11.0
[I 11:44:45.755 LabApp] Build is up to date
[W 11:44:46.102 LabApp] 404 GET /lab/api/workspaces/lab?1554317083806 (::1): Workspace 'lab' ('lab-a511') not found
[W 11:44:46.117 LabApp] Workspace 'lab' ('lab-a511') not found
W 11:44:46.117 LabApp] 404 GET /lab/api/workspaces/lab?1554317083806 (::1) 157.66ms referer=http://localhost:8888/lab
```

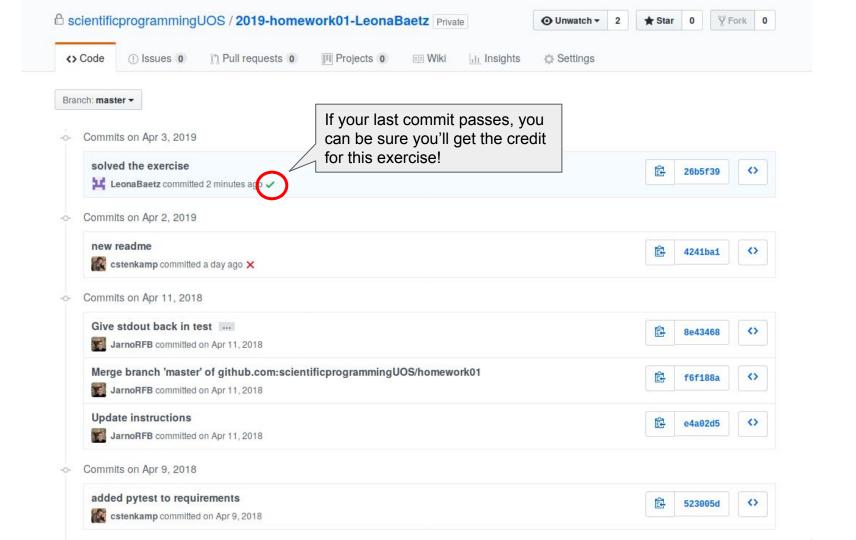




(in between here you should solve the given task)

```
(scientific_programming) C:\Users\User\python_homework\2019-homework01-LeonaBaetz>pytest
platform win32 -- Python 3.7.3, pytest-4.4.0, py-1.8.0, pluggy-0.9.0
rootdir: C:\Users\User\python_homework\2019-homework01-LeonaBaetz
collected 1 item
test_hello.py
                                                                                                      [100%]
             (scientific programming) C:\Users\User\python homework\2019-homework01-LeonaBaetz>git status
on branch master
Your branch is up to date with 'origin/master'.
changes not staged for commit:
 (use "git add <file>..." to update what will be committed)
 (use "git checkout -- <file>..." to discard changes in working directory)
no changes added to commit (use "git add" and/or "git commit -a")
scientific programming) C:\Users\User\python homework\2019-homework01-LeonaBaetz>git add hello world.py(
warning: LF will be replaced by CRLF in hello world.py.
The file will have its original line endings in your working directory
 scientific programming) C:\Users\User\python homework\2019-homework01-LeonaBaetz>git commit -m "solved the exercise"
*** Please tell me who you are.
Run
 git config --global user.email "you@example.com"
 git config --global user.name "Your Name"
to set your account's default identity.
Omit --global to set the identity only in this repository.
fatal: unable to auto-detect email address (got 'User@WinDev1903Eval.(none)')
(scientific programming) C:\Users\User\python homework\2019-homework01-LeonaBaetz>git config --global user.email "lbaetz
@uos.de"
(scientific programming) C:\Users\User\python homework\2019-homework01-LeonaBaetz>git config --global user.name "Leona B
ätz"
scientific programming) C:\Users\User\python homework\2019-homework01-LeonaBaetz>git commit -m "solved the exercise"
 master 26b5f39] solved the exercise
1 file changed, 1 insertion(+), 1 deletion(-)
 scientific programming) C:\Users\User\python homework\2019-homework01-LeonaBaetz>git push
Enumerating objects: 5, done.
```





Thanks for your attention!

- We will have have a feedback-questionnaire after 4-5 sessions
- Any questions and remarks please via email!
- Content-suggestions are always welcome!

Further reading

Review of scientific languages http://flow.byu.edu/posts/sci-prog-lang

Sources

- 1. https://commons.wikimedia.org/wiki/File:Python.svg
- 2. https://pixabay.com/vectors/swiss-army-knife-pocket-knife-blade-154314/
- 3. https://en.wikipedia.org/wiki/R (programming language)
- 4. https://commons.wikimedia.org/wiki/File:Matlab Logo.png
- 5. https://commons.wikimedia.org/wiki/File:Images 200px-ISO C%2B%2B Logo svg.png
- 6. https://pt.wikipedia.org/wiki/Julia (linguagem_de_programa%C3%A7%C3%A3o)
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- 8. https://farm2.staticflickr.com/1482/24588096069 59a0513790 z.jpg