

# CS6208 : Advanced Topics in Artificial Intelligence

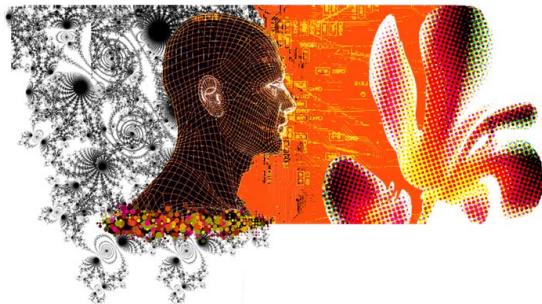
## Graph Machine Learning

Running Course Notebooks with  
GitHub, Google Colab & Local Installation

Semester 2 2022/23

Xavier Bresson

<https://twitter.com/xbresson>



Department of Computer Science  
National University of Singapore (NUS)



# Outline

- Running course demos & coding exercises
  - Google Colab
  - Local installation

# Outline

- Running demos & coding exercises
  - Google Colab
  - Local installation

# Google Colab

- Follow these instructions :
  - Go to the GitHub folder of the course :

<https://github.com/xbresson/GML2023>

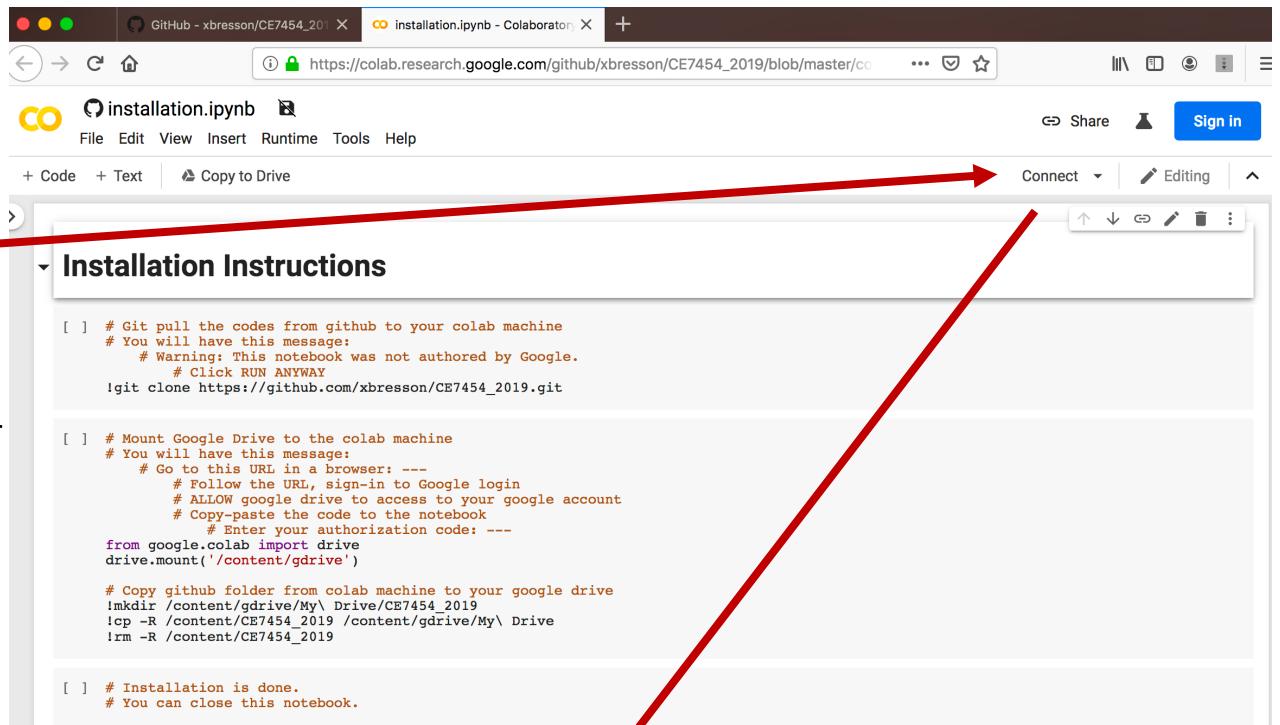
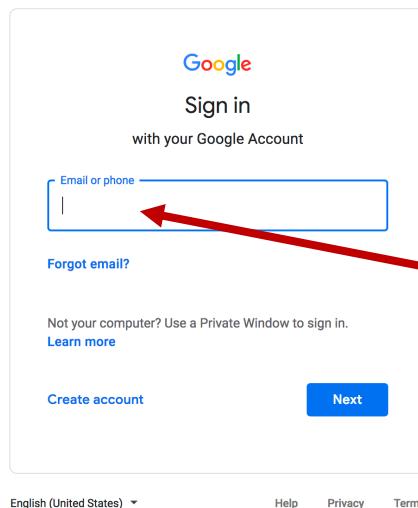
Click on this link.

The screenshot shows the GitHub repository page for 'GML2023'. The 'Code' button in the top navigation bar is highlighted with a red arrow. Below it, the 'installation.ipynb' file is listed in the code section. The page also includes sections for README, MIT license, Graph Machine Learning course, 2023, Xavier Bresson, Cloud Machine: Google Colab (Free GPU), and Suggested workflows.

The screenshot shows the Google Colab interface. It features a large yellow 'CO' logo at the top right. The main window displays the 'Welcome To Colaboratory' page, which includes sections for Introducing Colaboratory, Getting Started, More Resources, and Machine Learning Examples: Seedbank. On the right side, there is a video player titled 'Intro to Google Colab' featuring a smiling man and the text 'Coding TensorFlow'.

# Google Colab

- Click on CONNECT.
- It will ask you to sign-in with your Gmail account.



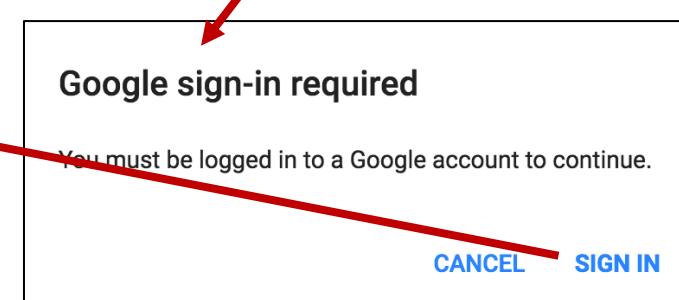
A screenshot of a Google Colab notebook titled 'installation.ipynb'. The notebook contains code for installing a GitHub repository and mounting Google Drive. A red arrow points from the 'CONNECT' button in the list above to the 'Connect' button in the top right corner of the Colab interface. Another red arrow points from the 'SIGN IN' button in the sign-in dialog below to the 'Sign in' button in the top right corner of the Colab interface.

```
[ ] # Git pull the codes from github to your colab machine
# You will have this message:
#   Warning: This notebook was not authored by Google.
#   # Click RUN ANYWAY
!git clone https://github.com/xbresson/CE7454_2019.git

[ ] # Mount Google Drive to the colab machine
# You will have this message:
# Go to this URL in a browser: ---
#   # Follow the URL, sign-in to Google login
#   # ALLOW google drive to access to your google account
#   # Copy-paste the code to the notebook
#   # Enter your authorization code: ---
from google.colab import drive
drive.mount('/content/gdrive')

# Copy github folder from colab machine to your google drive
!mkdir /content/gdrive/My\ Drive/CE7454_2019
!cp -R /content/CE7454_2019 /content/gdrive/My\ Drive
!rm -R /content/CE7454_2019

[ ] # Installation is done.
# You can close this notebook.
```



# Google Colab

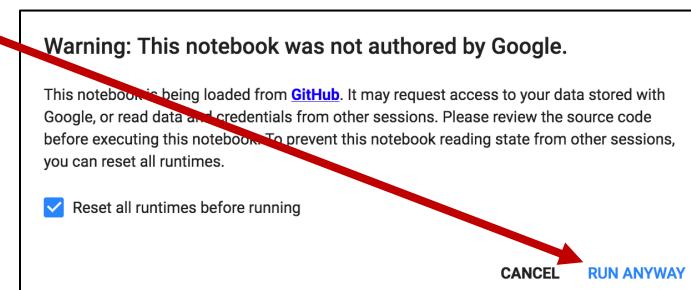
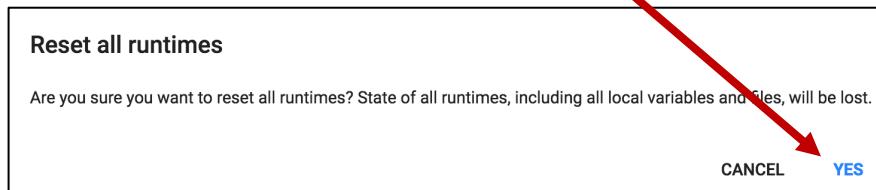
- Click on CONNECT again to start the Google Cloud machine.
- Run the first cell to clone the codes from GitHub to the Google Cloud machine.
  - It will give a warning, click on RUN ANYWAY.
  - Answer YES to the next question RESET ALL RUNTIMES.

```
# Git pull the codes from github to your colab machine
# You will have this message:
# Warning: This notebook was not authored by Google.
!git clone https://github.com/xbresson/CE7454_2019.git

# Mount Google Drive to the colab machine
# You will have this message:
# Go to this URL in a browser: ---
# Follow the URL, sign-in to Google login
# ALLOW google drive to access to your google account
# Copy-paste the code to the notebook
# Enter your authorization code: ---
from google.colab import drive
drive.mount('/content/gdrive')

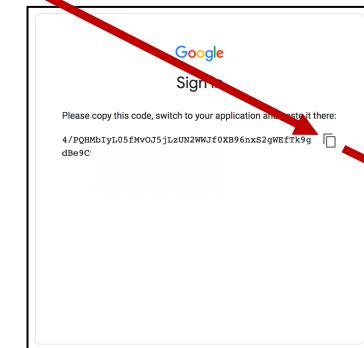
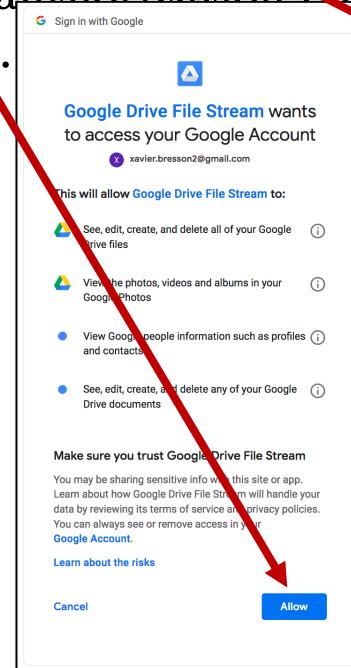
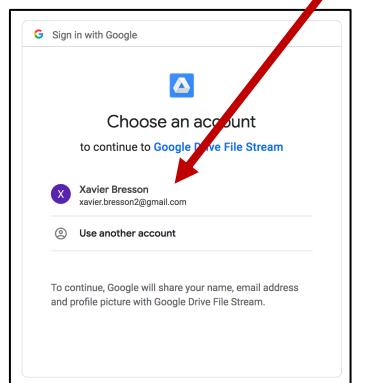
# Copy github folder from colab machine to your google drive
!mkdir /content/gdrive/My\ Drive/CE7454_2019
!cp -R /content/CE7454_2019 /content/gdrive/My\ Drive
!rm -R /content/CE7454_2019

# Installation is done.
# You can close this notebook.
```



# Google Colab

- Run the second cell to mount your Google Drive to the Google Cloud machine (all your codes will be saved in Google Drive).
  - Click on the provided URL.
  - Select your Gmail account.
  - ALLOW Google Drive File Stream.
  - Copy-paste the code to the notebook (Enter your authorization code) and press Return.



```
[1] # Git pull the codes from github to your colab machine
# You will have this message:
# Warning: This notebook was not authored by Google.
# Click RUN ANYWAY
!git clone https://github.com/xbresson/CE7454_2019.git

Cloning into 'CE7454_2019'...
remote: Enumerating objects: 223, done.
remote: Counting objects: 100% (223/223), done.
remote: Compressing objects: 100% (135/135), done.
remote: Total 223 (delta 100), reused 191 (delta 72), pack-reused 0
Receiving objects: 100% (223/223), 2.63 MiB | 6.68 MiB/s, done.
Resolving deltas: 100% (100/100), done.

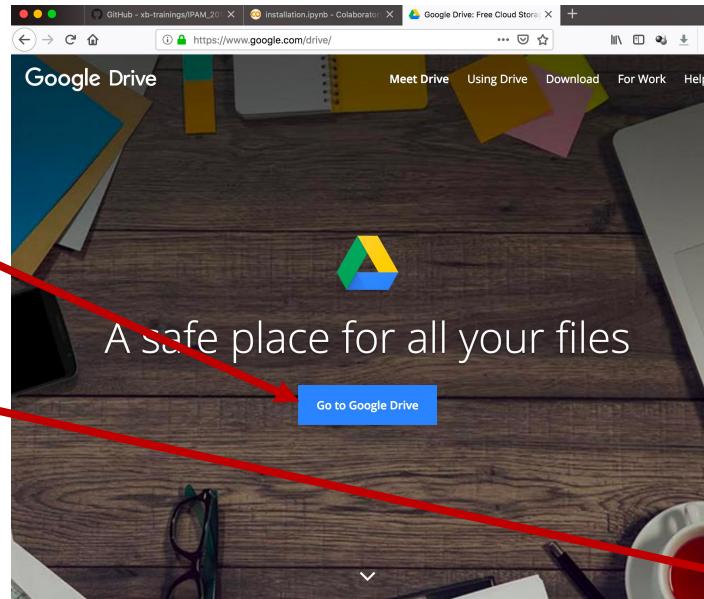
# Mount Google Drive to the colab machine
# You will have this message:
# Go to this URL in a browser: ---
# Follow the URL, sign-in to Google login
# ALLOW google drive to access to your google account
# Copy-pastes the code to the notebook
# Enter your authorization code: ---
from google.colab import drive
drive.mount('/content/gdrive')

# Copy github folder from colab machine to your google drive
mkdir /content/gdrive/My\ Drive/CE7454_2019
lcp -R /content/CE7454_2019 /content/gdrive/My\ Drive/CE7454_2019

...
... Go to this URL in a browser: https://accounts.google.com/o/oauth2/auth?client\_id=947318989803-6bn6qk8g
Enter your authorization code:
```

# Google Colab

- Open your Google Drive :  
<https://www.google.com/drive>
- Go folder GML2023\_codes/



My Drive > GML2023\_codes

| Name            | Owner | Last modified |
|-----------------|-------|---------------|
| .git            | me    | 10:16 AM me   |
| codes           | me    | 10:16 AM me   |
| .gitignore      | me    | 10:16 AM me   |
| environment.yml | me    | 10:16 AM me   |
| LICENSE         | me    | 10:16 AM me   |
| README.md       | me    | 10:16 AM me   |

Click here for List View

My Drive - Google Drive

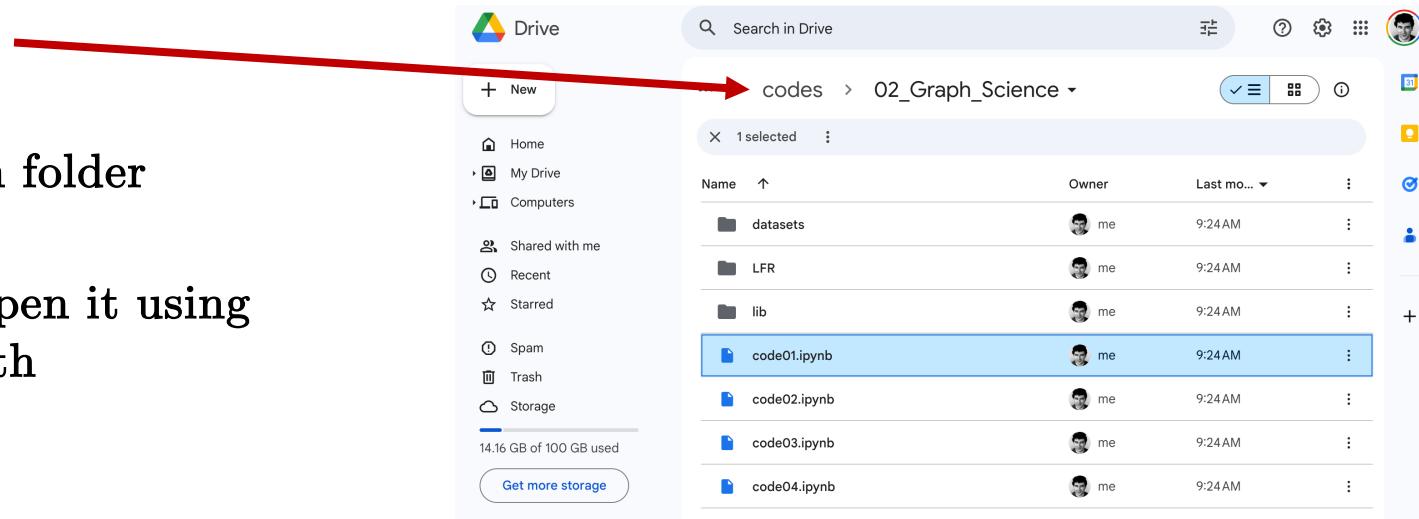
My Drive

Name ↑ Owner Last modified

|                       |    |             |
|-----------------------|----|-------------|
| GML2023_codes         | me | 10:16 AM me |
| Shared with me        |    |             |
| Recent                |    |             |
| Starred               |    |             |
| Trash                 |    |             |
| Backups               |    |             |
| Storage               |    |             |
| 50.2 MB of 15 GB used |    |             |
| UPGRADE STORAGE       |    |             |

# Google Colab

- Go folder GML2023\_codes/
- Open notebook code01.ipynb in folder codes/02\_Graph\_Science
  - Select the notebook and open it using Control Click + Open With Colaboratory



Google Drive interface showing the context menu for 'code01.ipynb'. The 'Open with' option is selected, and the 'Google Colaboratory' option is highlighted with a red arrow.

The right side of the image shows the Google Colab interface for the 'code01.ipynb' notebook. The code cell contains the following Python code:

```
# For Google Colaboratory
import sys, os
if 'google.colab' in sys.modules:
    # mount google drive
    from google.colab import drive
    drive.mount('/content/gdrive')
    path_to_file = '/content/gdrive/My Drive/GML2023_codes/codes/02_Graph_Science'
    print(path_to_file)
    # change Current path to the folder containing "path_to_file"
    os.chdir(path_to_file)
    !pwd

# Load libraries
# Math
import numpy as np

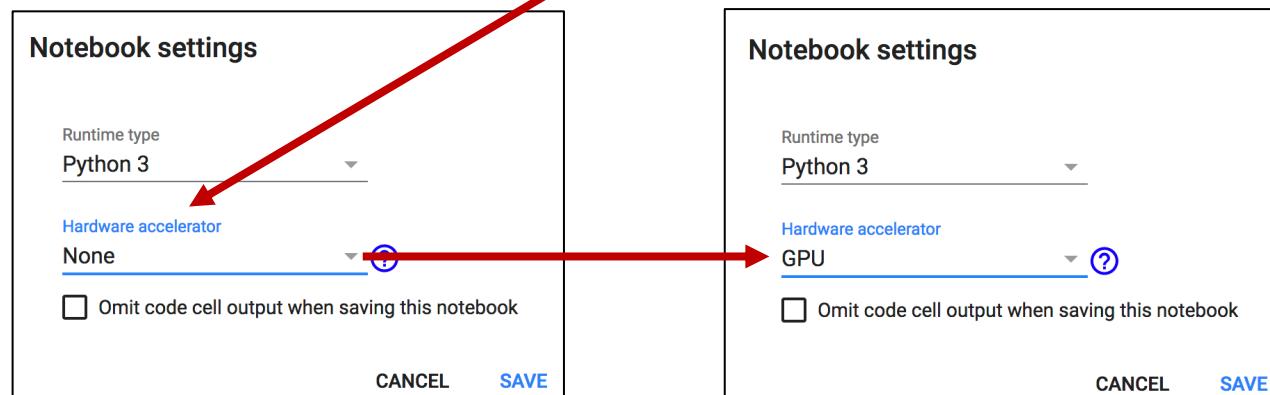
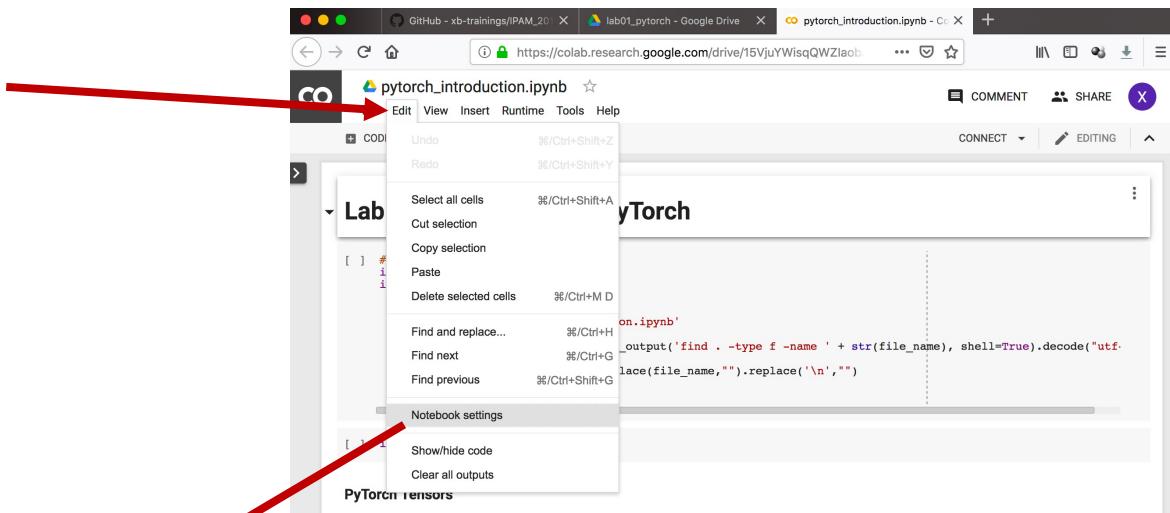
# Visualization
%matplotlib inline
#%matplotlib notebook
import matplotlib.pyplot as plt
plt.rcParams.update({'figure.max_open_warning': 0})
from mpl_toolkits.axes_grid1 import make_axes_locatable
from scipy import ndimage

# Print output of LFR code
import subprocess
```

# Google Colab

- GPU acceleration :

- Select Edit in the menu and Notebook settings.
- Select GPU in Hardware accelerator.



# Outline

- Running demos & coding exercises
  - Google Colab
  - Local installation

# Local Installation for OSX & Linux

- Install Python and run the notebooks on your OSX or Linux machine :

## Local Installation for OSX & Linux

- Open a Terminal and type

```
# Conda installation
curl https://repo.continuum.io/miniconda/Miniconda3-latest-Linux-x86_64.sh -o miniconda.sh
curl https://repo.continuum.io/miniconda/Miniconda3-latest-MacOSX-x86_64.sh -o miniconda.sh
chmod +x miniconda.sh
./miniconda.sh
source ~/.bashrc

# Clone GitHub repo
git clone https://github.com/xbresson/GML2023.git
cd GML2023

# Install python libraries
conda env create -f environment.yml
source activate gnn_course

# Run the notebooks in Chrome
jupyter notebook
```

<https://github.com/xbresson/GML2023#local-installation-for-osx--linux>

# Local Installation for OSX & Linux

```
Last login: Mon Aug  9 15:02:37 on ttys001
(base) xbresson@r-153-121-25-172 CS5242_2021 % curl https://repo.continuum.io/miniconda/Miniconda3-latest-MacOSX-x86_64.sh -o miniconda.sh -J -L -k
% Total    % Received % Xferd  Average Speed   Time   Time     Current
          Dload  Upload Total Spent   Left Speed
  0       0      0      0      0      0      0 --:--:-- --:--:-- --:--:--  0
100 42.3M  100 42.3M    0      0  23.2M      0  0:00:01  0:00:01 --:--:-- 30.5M
(base) xbresson@r-153-121-25-172 CS5242_2021 % chmod +x miniconda.sh
(base) xbresson@r-153-121-25-172 CS5242_2021 % ./miniconda.sh

Welcome to Miniconda3 py39_4.10.3

In order to continue the installation process, please review the license
agreement.
Please, press ENTER to continue
>>>
```

```
wheel      pkgs/main/noarch::wheel-0.36.2-pyhd3eb1b0_0
xz        pkgs/main/osx-64::xz-5.2.5-hide35cc_0
yaml      pkgs/main/osx-64::yaml-0.2.5-haf1e3a3_0
zlib      pkgs/main/osx-64::zlib-1.2.11-hide35cc_3

Preparing transaction: done
Executing transaction: \
done
installation finished.
Do you wish the installer to initialize Miniconda3
by running conda init? [yes|no]
[yes] >>>
no change  /Users/xbresson/miniconda3/condabin/conda
no change  /Users/xbresson/miniconda3/bin/conda
no Change  /Users/xbresson/miniconda3/bin/conda-env
no change  /Users/xbresson/miniconda3/bin/activate
no change  /Users/xbresson/miniconda3/bin/deactivate
no change  /Users/xbresson/miniconda3/etc/profile.d/conda.sh
no change  /Users/xbresson/miniconda3/etc/fish/conf.d/conda.fish
no change  /Users/xbresson/miniconda3/shell/condabin/Conda.psm1
no change  /Users/xbresson/miniconda3/shell/condabin/conda-hook.ps1
no change  /Users/xbresson/miniconda3/lib/python3.9/site-packages/xontrib/conda.xsh
no change  /Users/xbresson/miniconda3/etc/profile.d/conda.csh
no change  /Users/xbresson/.zshrc
No action taken.
If you'd prefer that conda's base environment not be activated on startup,
  set the auto_activate_base parameter to false:

conda config --set auto_activate_base false

Thank you for installing Miniconda3!
(base) xbresson@r-153-121-25-172 CS5242_2021 %
```

# Local Installation for OSX & Linux

```
(base) xbresson@r-153-121-25-172 CS5242_2021 % conda
usage: conda [-h] [-V] command ...

conda is a tool for managing and deploying applications, environments and packages.

Options:
  positional arguments:
    command
      clean      Remove unused packages and caches.
      compare   Compare packages between conda environments.
      config    Modify configuration values in .condarc. This is modeled after the git config command. Writes to the user .condarc file
                (/Users/xbresson/.condarc) by default.
      create     Create a new conda environment from a list of specified packages.
      help       Displays a list of available conda commands and their help strings.
      info       Display information about current conda install.
      init       Initialize conda for shell interaction. [Experimental]
      install   Installs a list of packages into a specified conda environment.
      list      List linked packages in a conda environment.
      package   Low-level conda package utility. (EXPERIMENTAL)
      remove   Remove a list of packages from a specified conda environment.
      uninstall Alias for conda remove.
      run       Run an executable in a conda environment. [Experimental]
      search   Search for packages and display associated information. The input is a MatchSpec, a query language for conda packages. See examples
                below.
      update   Updates conda packages to the latest compatible version.
      upgrade  Alias for conda update.

  optional arguments:
    -h, --help      Show this help message and exit.
    -V, --version   Show the conda version number and exit.

  conda commands available from other packages:
    env

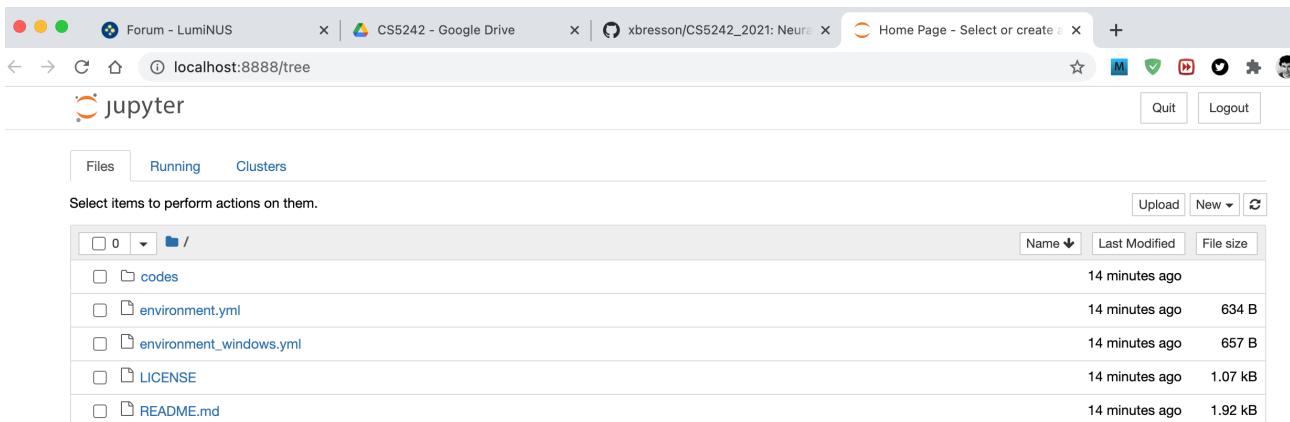
(base) xbresson@r-153-121-25-172 CS5242_2021 %
```

```
(base) xbresson@r-153-121-25-172 tmp % git clone https://github.com/xbresson/CS5242_2021.git
Cloning into 'CS5242_2021'...
remote: Enumerating objects: 201, done.
remote: Counting objects: 100% (201/201), done.
remote: Compressing objects: 100% (117/117), done.
remote: Total 201 (delta 82), reused 187 (delta 71), pack-reused 0
Receiving objects: 100% (201/201), 2.82 MiB | 6.62 MiB/s, done.
Resolving deltas: 100% (82/82), done.
(base) xbresson@r-153-121-25-172 tmp % cd CS5242_2021
(base) xbresson@r-153-121-25-172 CS5242_2021 % conda env create -f environment.yml
```

# Local Installation for OSX & Linux

```
Collecting protobuf>=3.8.0
  Using cached protobuf-3.17.3-cp37-cp37m-macosx_10_9_x86_64.whl (1.0 MB)
Requirement already satisfied: six>=1.9 in /Users/xbresson/miniconda3/envs/deeplearn_course/lib/python3.7/site-packages (from protobuf>=3.8.0->tensorboardx==2.2-->-r /Users/xbresson/Documents/Dropbox/10_NUS_2021_now/05_My_Teaching/06_CSS242_sem1_21:22/04_Github/tmp/CS5242_2021/condaenv.1o03j884.requirements.txt (line 2)) (1.16.0)
Collecting future
  Using cached future-0.18.2-py3-none-any.whl
Installing collected packages: future, pyglet, protobuf, cloudpickle, tensorboardx, gym, fastprogress
Successfully installed cloudpickle-1.6.0 fastprogress-1.0.0 future-0.18.2 gym-0.18.0 protobuf-3.17.3 pyglet-1.5.0 tensorboardx-2.2
done
#
# To activate this environment, use
#
#     $ conda activate deeplearn_course
#
# To deactivate an active environment, use
#
#     $ conda deactivate
(base) xbresson@r-153-121-25-172 CSS5242_2021 % conda activate deeplearn_course
[deeplearn_course] xbresson@r-153-121-25-172 CSS5242_2021 % jupyter notebook
[I 12:18:06.635 NotebookApp] Writing notebook server cookie secret to /Users/xbresson/Library/Jupyter/runtime/notebook_cookie_secret
[I 12:18:08.268 NotebookApp] Serving notebooks from local directory: /Users/xbresson/Documents/Dropbox/10_NUS_2021_now/05_My_Teaching/06_CSS5242_sem1_21:22/04_Github/tmp/CS5242_2021
[I 12:18:08.268 NotebookApp] Jupyter Notebook 6.4.2 is running at:
[I 12:18:08.268 NotebookApp] http://localhost:8888/?token=0e66862970f67d6ba62bcef6ffbe79d851bf26d95f292340
[I 12:18:08.268 NotebookApp] or http://127.0.0.1:8888/?token=0e66862970f67d6ba62bcef6ffbe79d851bf26d95f292340
[I 12:18:08.268 NotebookApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
[C 12:18:08.275 NotebookApp]

To access the notebook, open this file in a browser:
  file:///Users/xbresson/Library/Jupyter/runtime/nbserver-87552-open.html
Or copy and paste one of these URLs:
  http://localhost:8888/?token=0e66862970f67d6ba62bcef6ffbe79d851bf26d95f292340
  or http://127.0.0.1:8888/?token=0e66862970f67d6ba62bcef6ffbe79d851bf26d95f292340
```



# Local Installation for OSX & Linux

The image shows a local Jupyter environment running on a Mac OS X system. At the top, a browser window displays the Jupyter file browser at `localhost:8888/tree`. The browser title bar includes tabs for "xbresson/GML2023: Graph M" and "Home Page - Select or create". The file browser interface has tabs for "Files", "Running", and "Clusters". It lists several files and directories:

| Name            | Last Modified | File size |
|-----------------|---------------|-----------|
| codes           | 9 months ago  |           |
| pic             | 2 days ago    |           |
| environment.yml | 6 days ago    | 524 B     |
| LICENSE         | 9 months ago  | 1.07 kB   |
| README.md       | 2 days ago    | 1.85 kB   |

Below the file browser is a Jupyter notebook titled "code01". The notebook interface includes a toolbar with various icons for file operations, cell execution, and help. The notebook content is as follows:

## Introduction to Graph Science

### Lab 01 : Generate artificial LFR social networks

Xavier Bresson

```
In [1]: # For Google Colaboratory
import sys, os
if 'google.colab' in sys.modules:
    # mount google drive
    from google.colab import drive
    drive.mount('/content/gdrive')
    path_to_file = '/content/gdrive/My Drive/GML2023_codes/codes/02_Graph_Science'
    print(path_to_file)
    # change current path to the folder containing "path_to_file"
    os.chdir(path_to_file)
    !pwd

In [2]: # Load libraries
# Math
import numpy as np

# Visualization
%matplotlib inline
#%matplotlib notebook
import matplotlib.pyplot as plt
plt.rcParams.update({'figure.max_open_warning': 0})
from mpl_toolkits.axes_grid1 import make_axes_locatable
from scipy import ndimage
```

# Local Installation for Windows

- Install Anaconda and run the notebooks on your Windows machine :

## Local Installation for Windows

```
# Install Anaconda
https://repo.anaconda.com/miniconda/Miniconda3-latest-Windows-x86\_64.exe

# Open an Anaconda Terminal
Go to Application => Anaconda3 => Anaconda Prompt

# Install git : Type in terminal
conda install git

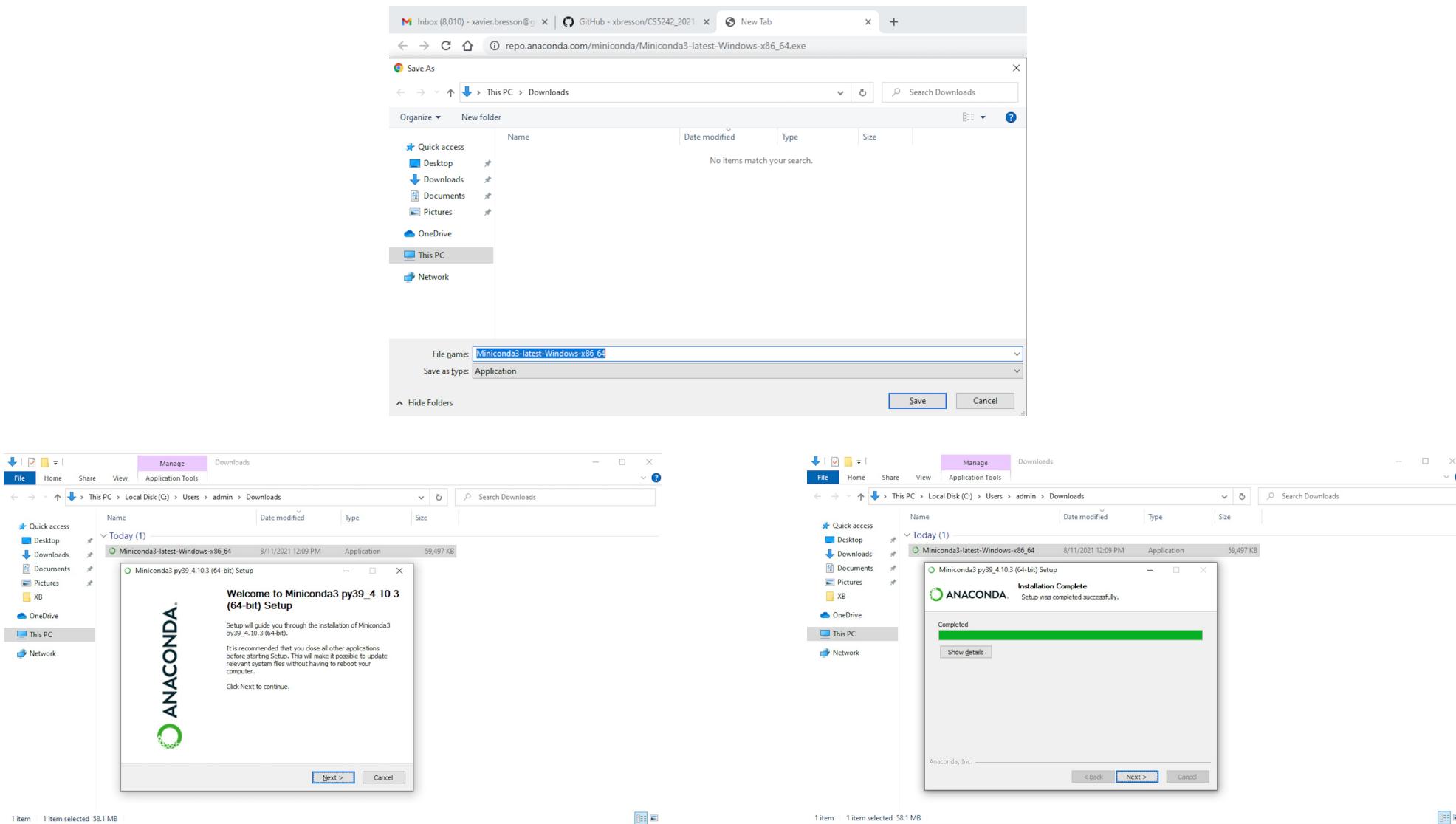
# Clone GitHub repo
git clone https://github.com/xbresson/GML2023.git
cd GML2023

# Install python libraries
conda env create -f environment.yml
conda activate gnn_course

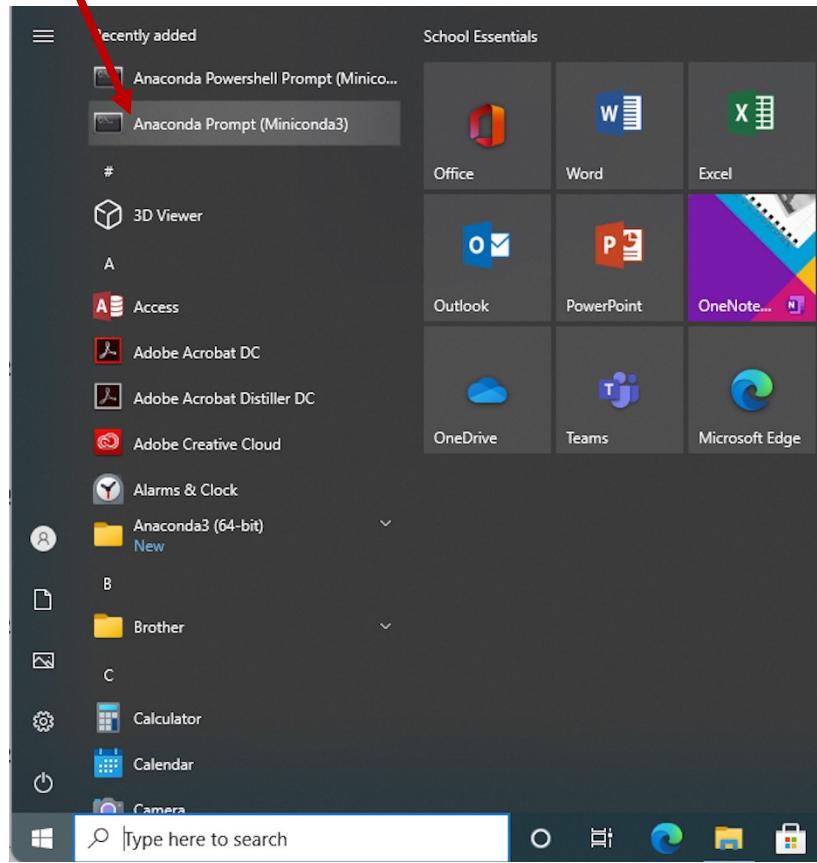
# Run the notebooks in Chrome
jupyter notebook
```

<https://github.com/xbresson/GML2023#local-installation-for-windows>

# Local Installation for Windows



# Local Installation for Windows



The image shows a terminal window titled 'Anaconda Prompt (Miniconda3)'. The command entered was 'conda install git'. The output shows the package being collected and solved, but then it fails with an 'EnvironmentNotWritableError' because the current user does not have write permissions to the target environment. The error message states: 'The current user does not have write permissions to the target environment. environment location: C:\ProgramData\Miniconda3'. A red arrow points from the text 'If you need admin rights to run Miniconda, then follow the next slide.' to this error message.

```
(base) C:\Users\admin>conda install git
Collecting package metadata (current_repotdata.json): done
Solving environment: done

## Package Plan ##

environment location: C:\ProgramData\Miniconda3

added / updated specs:
- git

The following NEW packages will be INSTALLED:

git          pkgs/main/win-64::git-2.23.0-h6bb4b03_0

Proceed ([y]/n)?
Preparing transaction: done
Verifying transaction: failed

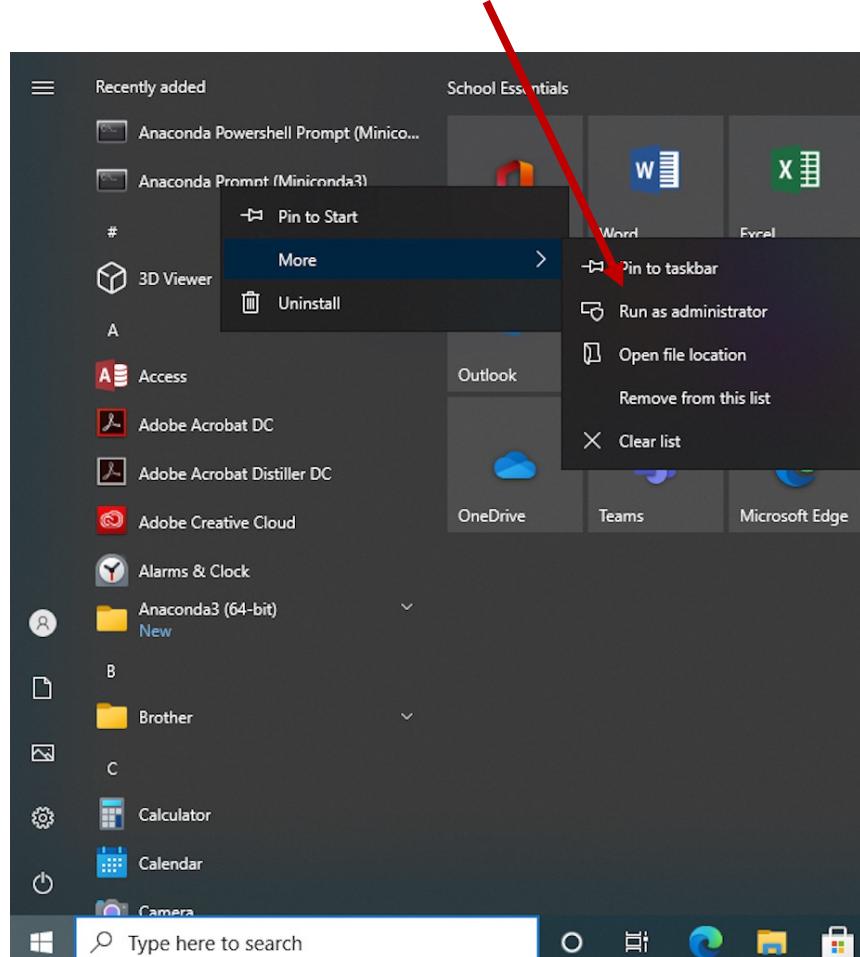
EnvironmentNotWritableError: The current user does not have write permissions to the target environment.
  environment location: C:\ProgramData\Miniconda3

(base) C:\Users\admin>
```

If you need admin rights to run Miniconda,  
then follow the next slide.

# Local Installation for Windows

Secondary click then select “Run as administrator”.



```
(base) C:\WINDOWS\system32>conda install git
Collecting package metadata (current_repodata.json): done
Solving environment: done

## Package Plan ##

environment location: C:\ProgramData\Miniconda3

added / updated specs:
- git

The following NEW packages will be INSTALLED:

git          pkgs/main/win-64::git-2.23.0-h6bb4b03_0

Proceed ([y]/n)?
Preparing transaction: done
Verifying transaction: done
Executing transaction: done

(base) C:\WINDOWS\system32>git clone https://github.com/xbresson/CS5242_2021.git
Cloning into 'CS5242_2021'...
remote: Enumerating objects: 201, done.
remote: Counting objects: 100% (201/201), done.
remote: Compressing objects: 100% (117/117), done.

Receiving objects: 100% (201/201), 2.82 MiB | 5.95 MiB/s, done.
Resolving deltas: 100% (82/82), done.

(base) C:\WINDOWS\system32>cd CS5242_2021
(base) C:\Windows\System32\CS5242_2021>conda env create -f environment_windows.yml
```

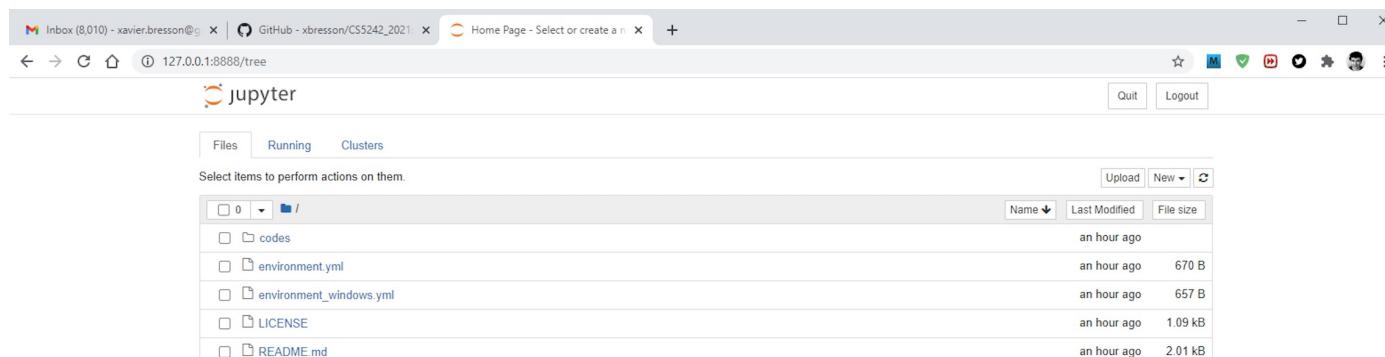
# Local Installation for Windows

```
■ Select Administrator: Anaconda Prompt (Miniconda3) - conda env create -f environment_windows.yml - jupyter notebook
Collecting package metadata (repodata.json): done
Solving environment: done
Preparing transaction: done
Verifying transaction: done
Executing transaction: \ "By downloading and using the CUDA Toolkit conda packages, you accept the terms and conditions
of the CUDA End User License Agreement (EULA): https://docs.nvidia.com/cuda/eula/index.html"
/ Enabling notebook extension jupyter-js-widgets/extension...
  - Validating: ok

done
#
# To activate this environment, use
#
#   $ conda activate deeplearn_course
#
# To deactivate an active environment, use
#
#   $ conda deactivate

(base) C:\Windows\System32\CS5242_2021> conda activate deeplearn_course
(deeplearn_course) C:\Windows\System32\CS5242_2021>jupyter notebook
[I 13:37:05.168 NotebookApp] Writing notebook server cookie secret to C:\Users\admin\AppData\Roaming\jupyter\runtime\notebook_cookie_secret
[I 13:37:05.921 NotebookApp] Serving notebooks from local directory: C:\Windows\System32\CS5242_2021
[I 13:37:05.922 NotebookApp] Jupyter Notebook 6.4.2 is running at:
[I 13:37:05.922 NotebookApp] http://localhost:8888/?token=522e83147822829171c9e979ad3deed8913ca2e55ad1c05e
[I 13:37:05.922 NotebookApp] or http://127.0.0.1:8888/?token=522e83147822829171c9e979ad3deed8913ca2e55ad1c05e
[I 13:37:05.922 NotebookApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
[C 13:37:06.002 NotebookApp]

To access the notebook, open this file in a browser:
  file:///C:/Users/admin/AppData/Roaming/jupyter/runtimes/nbserver-15624-open.html
Or copy and paste one of these URLs:
  http://localhost:8888/?token=522e83147822829171c9e979ad3deed8913ca2e55ad1c05e
  or http://127.0.0.1:8888/?token=522e83147822829171c9e979ad3deed8913ca2e55ad1c05e
```



# Local Installation for Windows

The image shows a local installation of Jupyter Notebook on a Windows system. At the top, a browser window displays the Jupyter interface with tabs for 'Files', 'Running', and 'Clusters'. Below the browser is a detailed file listing of files in the current directory, including 'codes', 'pic', 'environment.yml', 'LICENSE', and 'README.md'. The main area of the interface is a Jupyter Notebook cell containing Python code for generating artificial LFR social networks. The code includes imports for sys, os, and matplotlib, and sets up the environment for Google Colab. The notebook also includes a section for loading libraries like numpy and plt.

```
In [1]: # For Google Colaboratory
import sys, os
if 'google.colab' in sys.modules:
    # mount google drive
    from google.colab import drive
    drive.mount('/content/gdrive')
    path_to_file = '/content/gdrive/My Drive/GML2023_codes/codes/02_Graph_Science'
    print(path_to_file)
    # change current path to the folder containing "path_to_file"
    os.chdir(path_to_file)
!pwd

In [2]: # Load libraries
# Math
import numpy as np

# Visualization
%matplotlib inline
#%matplotlib notebook
import matplotlib.pyplot as plt
plt.rcParams.update({'figure.max_open_warning': 0})
from mpl_toolkits.axes_grid1 import make_axes_locatable
from scipy import ndimage
```



Questions?