

Lecture 01:

Introduction to Python and Command Line Basics



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Python for Molecular Sciences

MSSE 272, 3 Units



Outline

- What is an “environment”?

- installing **WSL** [instructions here](#)

- installing **miniconda**

- guide through **Jupyter**

- installing **Spyder**

- guide through **Spyder**



Outline

- **What is an “environment”?**
- installing **WSL**
- installing *miniconda*
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before we can start coding...we need an **environment**

your computer

Operational System (OS)

interface between the computer and all programs,
usually, Windows or Linux



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- in Computer Science, Software Engineering, Physics etc:
some version of Linux/Unix
- for Windows:

Windows Subsystem for Linux (WSL), see later





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Linux/WSL

Text Editor

- for actual coding
- in principle: any editor is fine

- but: code needs to be **compiled** and **ran!**



before we can start coding...we need an **environment**

your computer

Operational System (OS)

Linux/WSL

Coding platform

- **ANACONDA** (editor + compiler: **Jupyter**, **Spyder** + many other tools)
- **miniconda** (like **ANACONDA** but only basics, editor + compiler: **Jupyter**)
- **VS Code** (editor + compiler)

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before we can start coding...we need an **environment**

VS Code (see
lecture No 9)

The screenshot shows the VS Code editor interface. The Explorer panel on the left shows the file structure of a 'create-react-app' project, with 'src/serviceWorker.js' selected. The main editor area displays the code for 'serviceWorker.js'. The code includes comments about the service worker's origin and a function to register the service worker. A dropdown menu is visible over the code, showing various JavaScript methods and objects. The Terminal panel at the bottom shows the output of a command, indicating a successful compilation and providing the local and network URLs for the application.

```
src > JS serviceWorker.js
28 // Our service worker won't work if PUBLIC_URL is on a different origin
29 // from what our page is served on. This might happen if a CDN is used
30 // to serve assets; see https://github.com/facebook/create-react-app/issues/
31 // 5012
32 return;
33
34 window.addEventListener('load', () => {
35   const { addEventListener } = window;
36   if (isApplicationCache) {
37     // Try to register the service worker
38     // (should not be called if applicationCache is present)
39     checkForServiceWorker().then(() => {
40       // If successful, then the service worker has been
41       // successfully registered and is working. If
42       // that fails, then we might as well ignore
43       // the warning
44       navigator.serviceWorker.addEventListener('statechange', () => {
45         // The service worker is now in the state where
46         // it can be installed
47       });
48     });
49   } else {
50     // Is not localhost. Just register service worker
51     registerValidSW(swUrl, config);
52   }
53 });
```

PROBLEMS OUTPUT **TERMINAL** DEBUG CONSOLE

node

Compiled successfully!

You can now view create-react-app in the browser.

Local: http://localhost:3000/
On Your Network: http://192.168.86.138:3000/

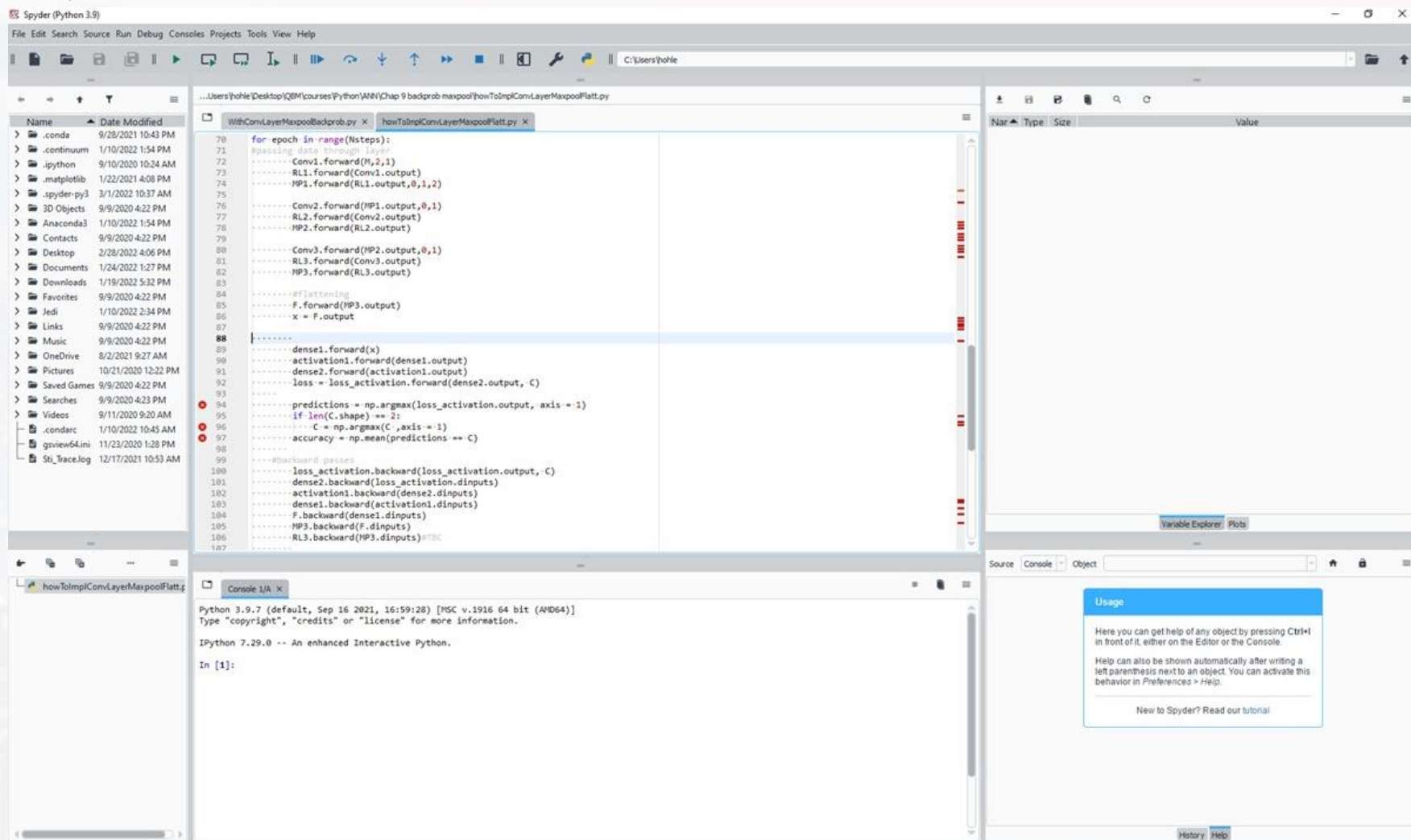
Note that the development build is not optimized.
To create a production build, use `yarn build`.

Ln 34, Col 13 Spaces: 2 UTF-8 LF JavaScript



Environment


Spyder (see later)






before we can start coding...we need an **environment**

Jupyter (see later)

 **jupyter** ANNIII Last Checkpoint: 3 months ago

File Edit View Run Kernel Settings Help



1) Defining all the Parts we need for an ANN

We start with defining the dense layer, including backpropagation:

```
[7]: class Layer_Dense():  
  
    def __init__(self, n_inputs, n_neurons):  
        self.weights = np.random.randn(n_inputs, n_neurons)  
        self.biases = np.zeros((1, n_neurons))  
  
    def forward(self, inputs):  
        self.output = np.dot(inputs, self.weights) + self.biases  
        self.inputs = inputs  
  
    def backward(self, dvalues):  
        #gradients  
        self.dweights = np.dot(self.inputs.T, dvalues)  
        self.dbiases = np.sum(dvalues, axis = 0, keepdims = True)  
        self.dinputs = np.dot(dvalues, self.weights.T)
```

and as well as for the activation layer.

```
[11]: class Activation_ReLU():
```



before we can start coding...we need an **environment**

your computer

Operational System (OS)

Linux/WSL

Coding platform

finetuning settings (ANACONDA or miniconda **environment**)

- **ANACONDA** (editor + compiler: **Jupyter**, **Spyder** + many other tools)
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- **VS Code** (editor + compiler)

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Windows Subsystem for Linux (WSL)



follow the instructions [here](#)

The screenshot shows the Microsoft Learn website interface. At the top, there's a navigation bar with 'Learn' and various dropdown menus. Below that, a breadcrumb trail reads 'Learn / Windows / WSL /'. The main heading is 'How to install Linux on Windows with WSL', dated 11/19/2024, with 10 contributors. A left sidebar contains a 'Filter by title' search box and a list of links: 'WSL Documentation', 'Overview', 'Install' (with 'Install WSL' highlighted), 'Manual install steps for older versions', 'Install on Windows Server', 'Tutorials', 'Concepts', 'How-to', and 'Download PDF'. To the right of the article title, there are icons for expand, edit, and share, followed by a 'Feedback' link. On the far right, an 'Additional resources' section includes a 'Training' module titled 'Developing in the Windows Subsystem for Linux with Visual Studio Code - Training' and a 'Certification' section for 'Microsoft Certified: Windows Server Hybrid Administrator Associate - Certifications'.

check out the video **01a_Installing_WSL** in bcourses



Linux commands

list your files and folders

`ls`

check out the video [*01b_Quick_Guide_Unix_Commands*](#) on bcourses

```
(base) mmh_user@DESKTOP-PPSA666:~$ ls
Anaconda3-2023.09-0-Linux-x86_64.sh  AppAcademy  Untitled.ipynb  snap
Anaconda3-2024.06-1-Linux-x86_64.sh Downloads  anaconda3
```

files

folder

shell scripts
→ like executables



Linux commands

check out the video [01b_Quick_Guide_Unix_Commands](#) on bcourses

list your files and folders

ls

-lrt

called *flags*

- **l** stands for *long*: shows a file with all permissions and properties, each per line
- **r** stands for *reverse* (oldest first)
- **t** stands for the *time* flag (as criterium for r)

```
(base) mmh_user@DESKTOP-PPSA666:~$ ls -lrt
total 2158464
drwx----- 2 mmh_user mmh_user      4096 Apr  8 20:03 Downloads
drwx----- 3 mmh_user mmh_user      4096 Apr 10 19:16 snap
drwxr-xr-x  5 mmh_user mmh_user      4096 Apr 24 18:29 AppAcademy
-rwxr-xr-x  1 mmh_user mmh_user 1153404010 Jul 24 12:36 Anaconda3-2023.09-0-Linux-x86_64.sh
-rwxr-xr-x  1 mmh_user mmh_user 1056829859 Aug  5 18:53 Anaconda3-2024.06-1-Linux-x86_64.sh
drwxr-xr-x 31 mmh_user mmh_user      4096 Aug  5 19:22 anaconda3
-rw-r--r--  1 mmh_user mmh_user      616 Aug  5 19:30 Untitled.ipynb
```



Linux commands

check out the video [01b_Quick_Guide_Unix_Commands](#) on bcourses

but these are only those files you see.

try:

```
ls -la
```

will be
important
(see later)

pointer/
links/aliases

```
(base) mmh_user@DESKTOP-PPSA666:~$ ls -la
total 2158640
drwxr-x--- 23 mmh_user mmh_user      4096 Aug  5 19:41 .
drwxr-xr-x  3 root      root          4096 Apr  2 21:35 ..
drwxr-xr-x  4 mmh_user mmh_user      4096 Apr  3 04:49 .aa-setup-checker
drwxr-xr-x  3 mmh_user mmh_user      4096 Aug  4 13:14 .anaconda
lrwxrwxrwx  1 mmh_user mmh_user         21 Apr  3 04:31 .aws -> /mnt/c/Users/MMH/.aws
lrwxrwxrwx  1 mmh_user mmh_user         23 Apr  3 04:31 .azure -> /mnt/c/Users/MMH/.azure
-rw-----  1 mmh_user mmh_user    26898 Aug  5 23:07 .bash_history
-rw-r--r--  1 mmh_user mmh_user     220 Apr  2 21:35 .bash_logout
-rw-r--r--  1 mmh_user mmh_user     4582 Jul 24 12:40 .bashrc
drwx----- 11 mmh_user mmh_user      4096 Aug  5 19:42 .cache
drwxr-xr-x  2 mmh_user mmh_user      4096 Jul 24 12:42 .conda
-rw-r--r--  1 mmh_user mmh_user         25 Aug  5 19:03 .condarc
drwx-----  6 mmh_user mmh_user      4096 Aug  5 19:45 .config
drwxr-xr-x  5 mmh_user mmh_user      4096 Apr  3 04:31 .docker
drwxr-xr-x  3 mmh_user mmh_user      4096 Apr  2 22:52 .dotnet
```



Linux commands

check out the video [01b_Quick_Guide_Unix_Commands](#) on bcourses

You can search for files/folders with particular substrings using a “wildcard”

```
ls *.py
ls *py*
```

```
(base) mmh_user@DESKTOP-PPSA666:~$ ls -lrt *A*
-rwxr-xr-x 1 mmh_user mmh_user 1153404010 Jul 24 12:36 Anaconda3-2023.09-0-Linux-x86_64.sh
-rwxr-xr-x 1 mmh_user mmh_user 1056829859 Aug 5 18:53 Anaconda3-2024.06-1-Linux-x86_64.sh
```

```
AppAcademy:
total 12
drwxr-xr-x 13 mmh_user mmh_user 4096 Apr 17 18:34 HTMLExercises
drwxr-xr-x 4 mmh_user mmh_user 4096 Apr 23 21:13 GitExercises
drwxr-xr-x 7 mmh_user mmh_user 4096 May 3 23:36 JavaExercises
```




Linux commands

check out the video [*01b_Quick_Guide_Unix_Commands*](#) on bcourses

changing your directory

`cd`

always leads back to the home directory

`cd ../`

one level up

`cd ../my_dir`

one level up, down to my_dir

`cd another/dir`

one level down to dir

`mkdir test`

creating the new directory *test*

`rm -r test`

removing the directory using the flag *r* (here: recursively)

`rm any_file`

when removing a file, no flag is needed



Linux commands

check out the video ***01b_Quick_Guide_Unix_Commands*** on bcourses

copying files and folders

```
cp my_file ../somewhere/else
```

```
cp my_file_original my_file_copy
```

```
cp my_file ../somewhere/else/my_file_copy
```

```
cp -r entireDirectory somewhere/else/to/new_destination
```

note: there are way more commands and flags we will be learning soon :)



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- What is an “environment”?
- installing WSL
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- installing **Spyder**
- guide through **Spyder**



open your **WSL** shell and run the following commands:

```
mmh_user@DESKTOP-PPSA666: ~  
(base) mmh_user@DESKTOP-PPSA666:~$ wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
```

1) download installer: `wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh`

2) run installer: `bash Miniconda3-latest-Linux-x86_64.sh`

confirm - license agreement,
- folder location and
- settings

3) close and reopen **WSL**

4) activate conda: `conda activate`

for windows

see the video **01c_Installing_Miniconda**
on bcourses

for mac

see the video
01cd_Installing_Miniconda_and_Jupyter_Mac
on bcourses



5) create environment: `conda create --name <My_Environment>`

6) check environment: `conda env list`

7) activate environment: `conda activate <My_Environment>`

<My_Environment>

8) check python:

```
mmh_user@DESKTOP-PPSA666: ~  
(base) mmh_user@DESKTOP-PPSA666:~$ conda activate MSSE_Python  
(MSSE_Python) mmh_user@DESKTOP-PPSA666:~$ python  
Python 3.9.4 (default, Apr 2 2024, 23:27:39)  
[GCC 11.4.0] on linux  
Type "help", "copyright", "credits" or "license" for more information.  
>>>
```



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1) install Jupyter:

`conda install jupyter`

```
(MSSE_Python) mmh_user@DESKTOP-PPSA666:~$ conda install jupyter
```

confirm settings

2) open Jupyter:

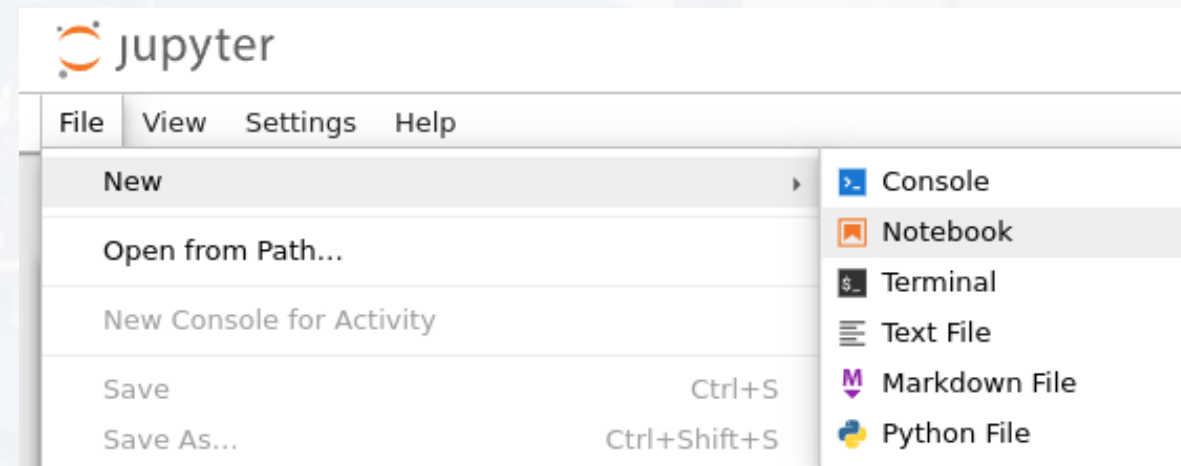
`jupyter notebook &`

a browser will open

go to → File
 → New
 → Notebook
 → confirm kernel

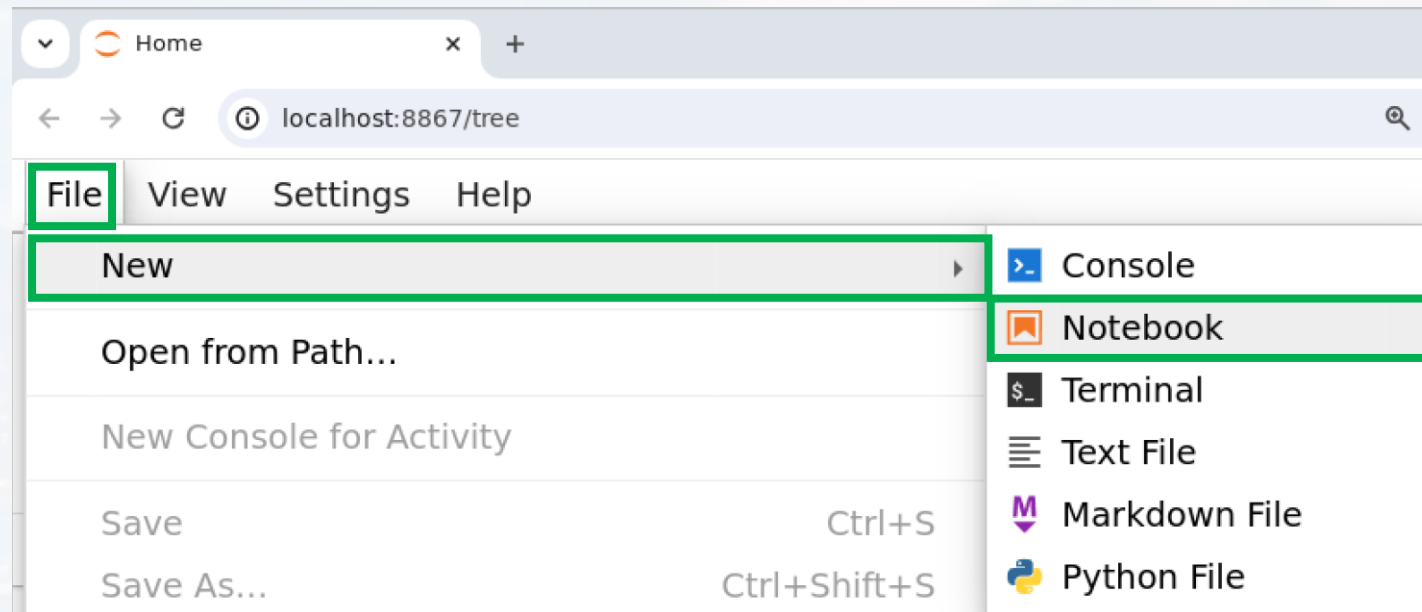
the notebook will open

check out the video **01d_Installing_Jupyter** on bcourses



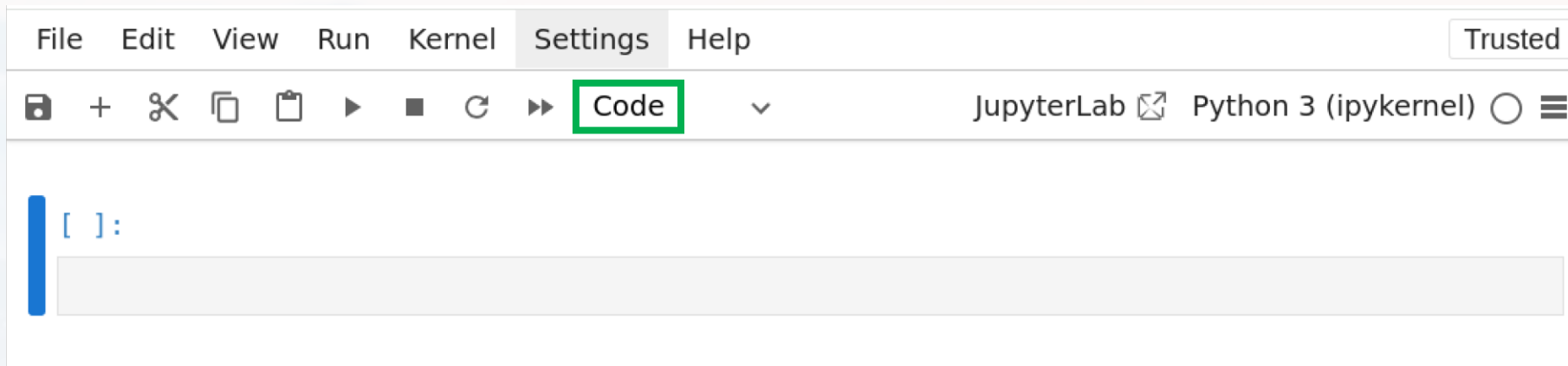


open new notebook





an empty cell will show up



markdown
code

→ text
→ actual code

check out the video *01e_Quick_Guide_Jupyter* in bcourses



saving notebook as pdf

note: you might get an error message

fix:

in your **conda** environment, run:

`conda install pandoc`

500 : Internal Server Error

The error was:

nbconvert failed: Pandoc wasn't found.
Please check that pandoc is installed:
<https://pandoc.org/installing.html>

```
(MSSE_Python) mmh_user@DESKTOP-PPSA666:~$ conda install pandoc
Channels:
- defaults
Platform: linux-64
Collecting package metadata (repodata.json): done
Solving environment: done

## Package Plan ##

  environment location: /home/mmh_user/miniconda3/envs/MSSE_Python

added / updated specs:
- pandoc

The following packages will be downloaded:



| package     | build      |         |
|-------------|------------|---------|
| pandoc-2.12 | h06a4308_3 | 10.5 MB |
| Total:      |            | 10.5 MB |



The following NEW packages will be INSTALLED:

pandoc                pkgs/main/linux-64::pandoc-2.12-h06a4308_3

Proceed ([y]/n)? y
```




saving notebook as pdf

note: you might get an error message

500 : Internal Server Error

The error was:

nbconvert failed: Pandoc wasn't found.
Please check that pandoc is installed:
<https://pandoc.org/installing.html>

fix:

in your **shell**, run:

```
sudo apt-get install texlive-xetex
```

& confirm your password

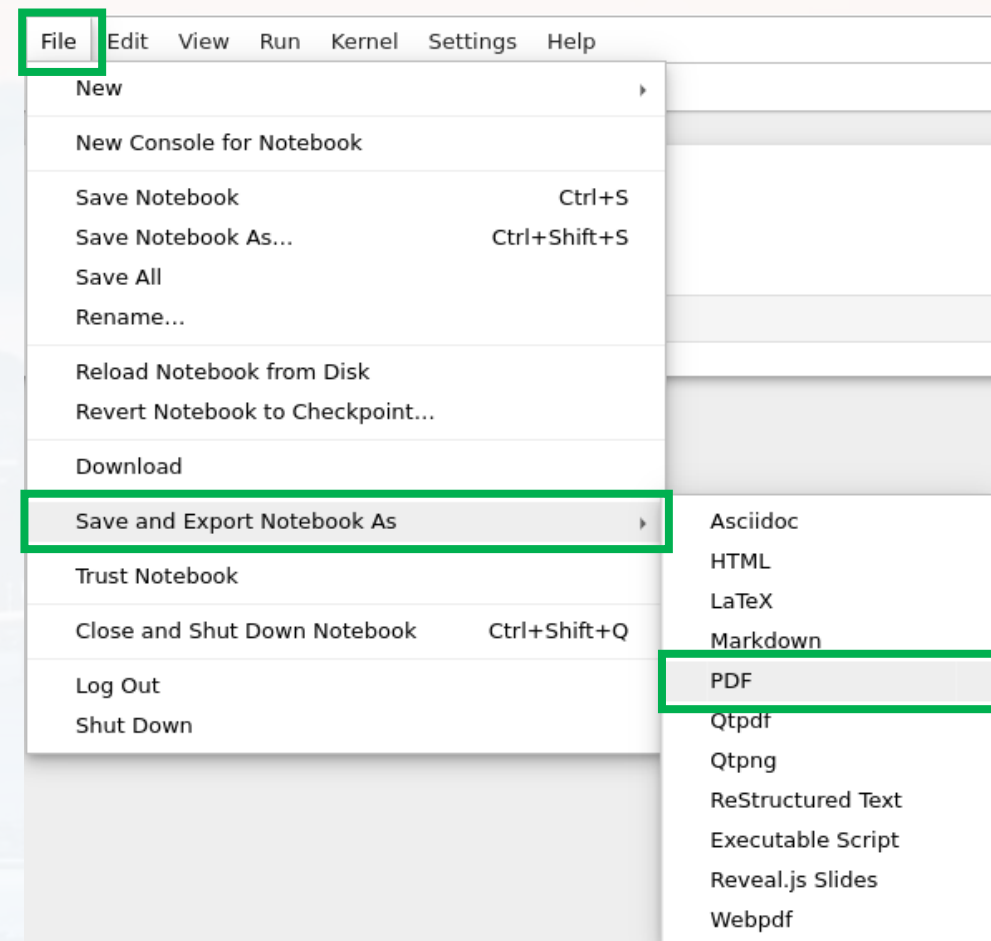


saving notebook as pdf

Now it works!

alternatively, the notebook can be converted via command line:

```
jupyter nbconvert My1stNB.ipynb --to pdf
```





My1stJNB

January 15, 2025

1 My First Notebook

1.1 Font Sizes and Styles

bold *italic*

here is a line break next line

1.2 Jupyter knows LaTeX

$\sigma_{i,j,k}^{\mu}$ $\Sigma_{i,j,k}^{\mu}$

1.3 Code

```
[2]: print('Hello')
```

Hello

```
[ ]:
```



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- guide through *Spyder*



check out the video *01f_Installing_Spyder* on bcourses

or follow instructions [here](#):

1) creating spyder environment

```
conda create -c conda-forge -n spyder-env spyder numpy scipy pandas matplotlib sympy cython
```

command for
creating the
environment

important for
installations/updates

name of the
environment

installing spyder alongside with
different libraries:

- numpy
- scipy
- pandas
- matplotlib
- Sympy
- cython



check out the video ***01f_Installing_Spyder*** on bcourses

or follow instructions [here](#):

1) creating spyder environment

```
conda create -c conda-forge -n spyder-env spyder numpy scipy pandas matplotlib sympy cython
```

2) activating and configure environment

```
conda activate spyder-env
```

```
conda config --env --add channels conda-forge
```

```
conda config --env --set channel_priority strict
```

3) open spyder

```
spyder &
```



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- **guide through *Spyder***



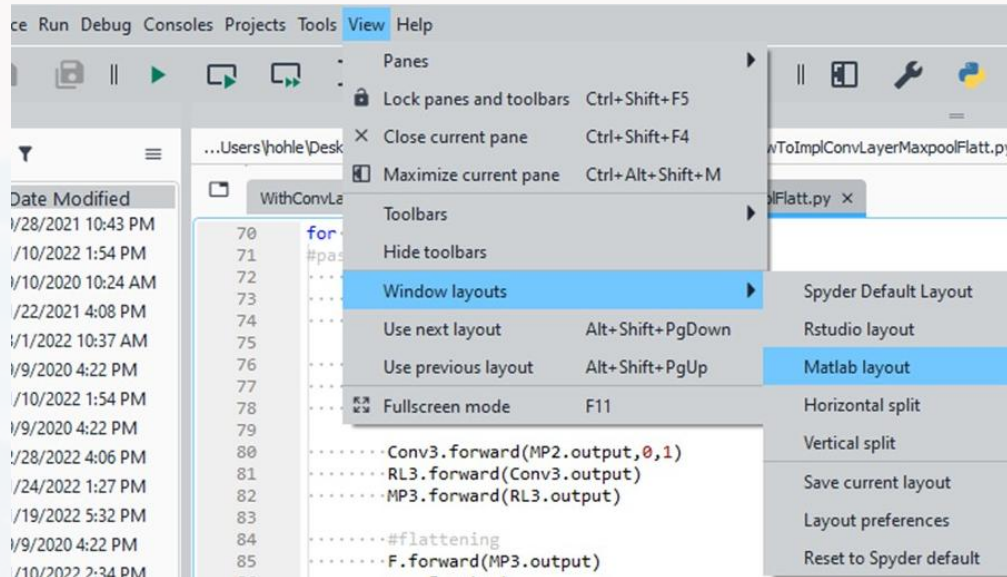
check out the video **01g_Quick_Guide_Spyder** on bcourses

The screenshot shows the Spyder Python IDE interface with several components and annotations:

- folder navigator**: A green box highlights the top-right pane, which displays the file explorer for the current project.
- py script: for coding**: A green box highlights the central editor pane, which contains a Python script for a neural network.
- workspace: displays current plots or variables**: A green box highlights the bottom-right pane, which displays the current workspace and plots.
- content of current folder**: A green box highlights the left pane, which displays the file explorer for the current project.
- console: typing commands & executing scripts**: A green box highlights the bottom-left pane, which displays the IPython console.

The Python script in the editor pane is as follows:

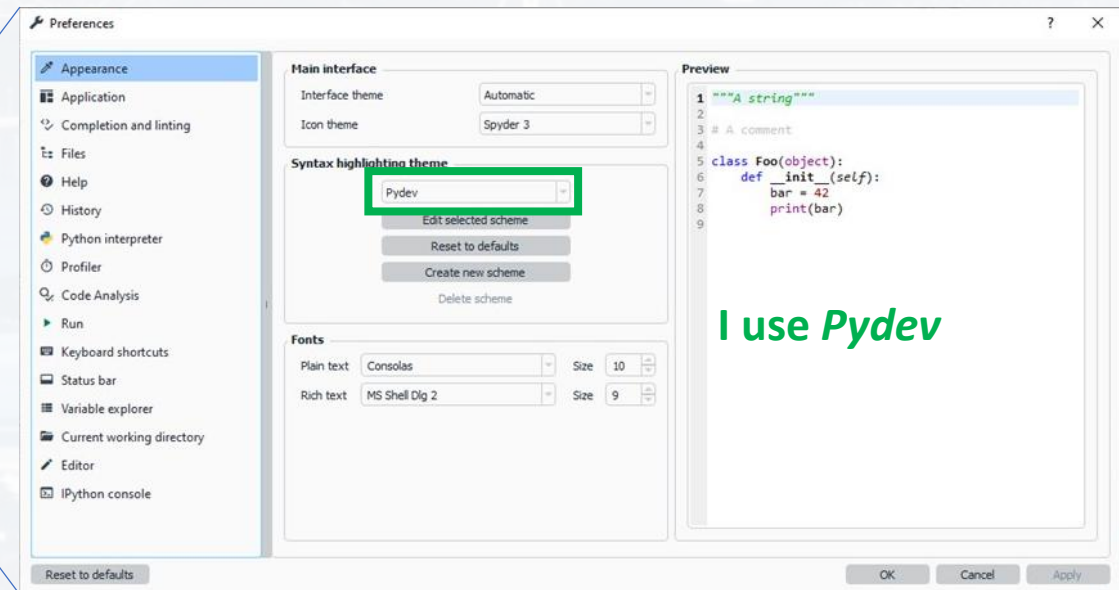
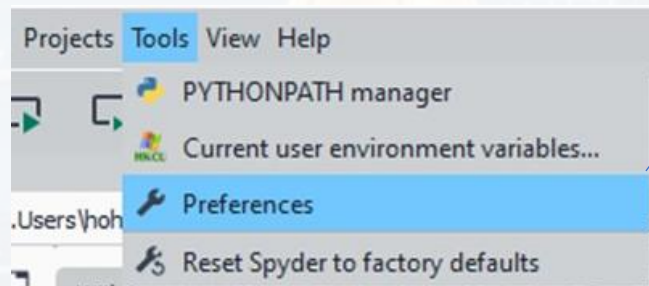
```
70 for epoch in range(Nsteps):
71     #passing data through layer
72     Conv1.forward(M,2,1)
73     RL1.forward(Conv1.output)
74     MP1.forward(RL1.output,0,1,2)
75
76     Conv2.forward(MP1.output,0,1)
77     RL2.forward(Conv2.output)
78     MP2.forward(RL2.output)
79
80     Conv3.forward(MP2.output,0,1)
81     RL3.forward(Conv3.output)
82     MP3.forward(RL3.output)
83
84     #flattening
85     F.forward(MP3.output)
86     x = F.output
87
88
89     dense1.forward(x)
90     activation1.forward(dense1.output)
91     dense2.forward(activation1.output)
92     loss = loss_activation.forward(dense2.output, C)
93
94     predictions = np.argmax(loss_activation.output, axis = 1)
95     if len(C.shape) == 2:
96         C = np.argmax(C, axis = 1)
97     accuracy = np.mean(predictions == C)
98
99     #backward passes
100     loss_activation.backward(loss_activation.output, C)
101     dense2.backward(loss_activation.dinputs)
102     activation1.backward(dense2.dinputs)
103     dense1.backward(activation1.dinputs)
104     F.backward(dense1.dinputs)
105     MP3.backward(F.dinputs)
106     RL3.backward(MP3.dinputs)
107
```

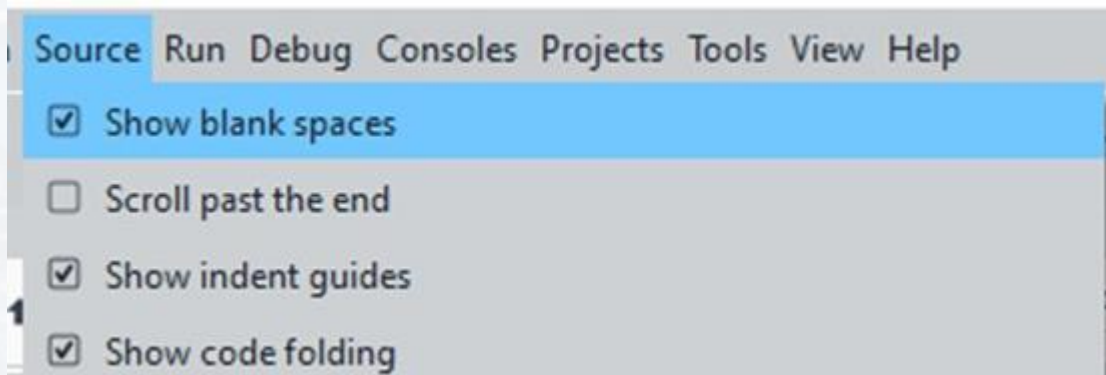
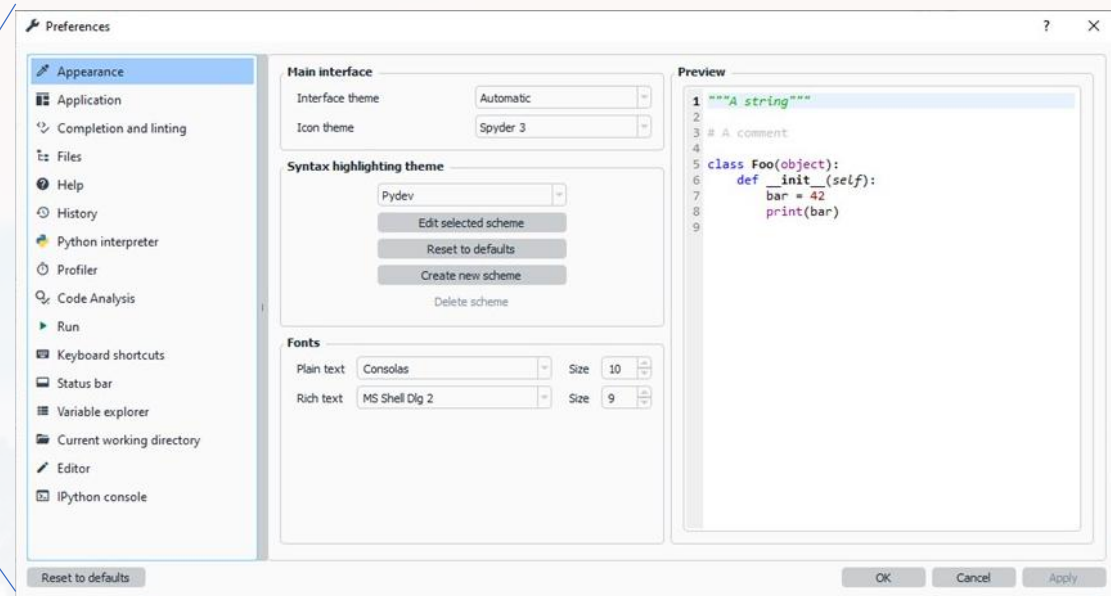
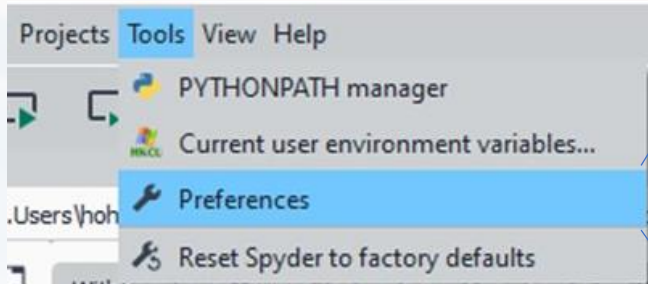



settings:

toolbar: *View* → *Window layouts*

e. g. Matlab





spaces are relevant for syntax!



Thank you very much for your attention

