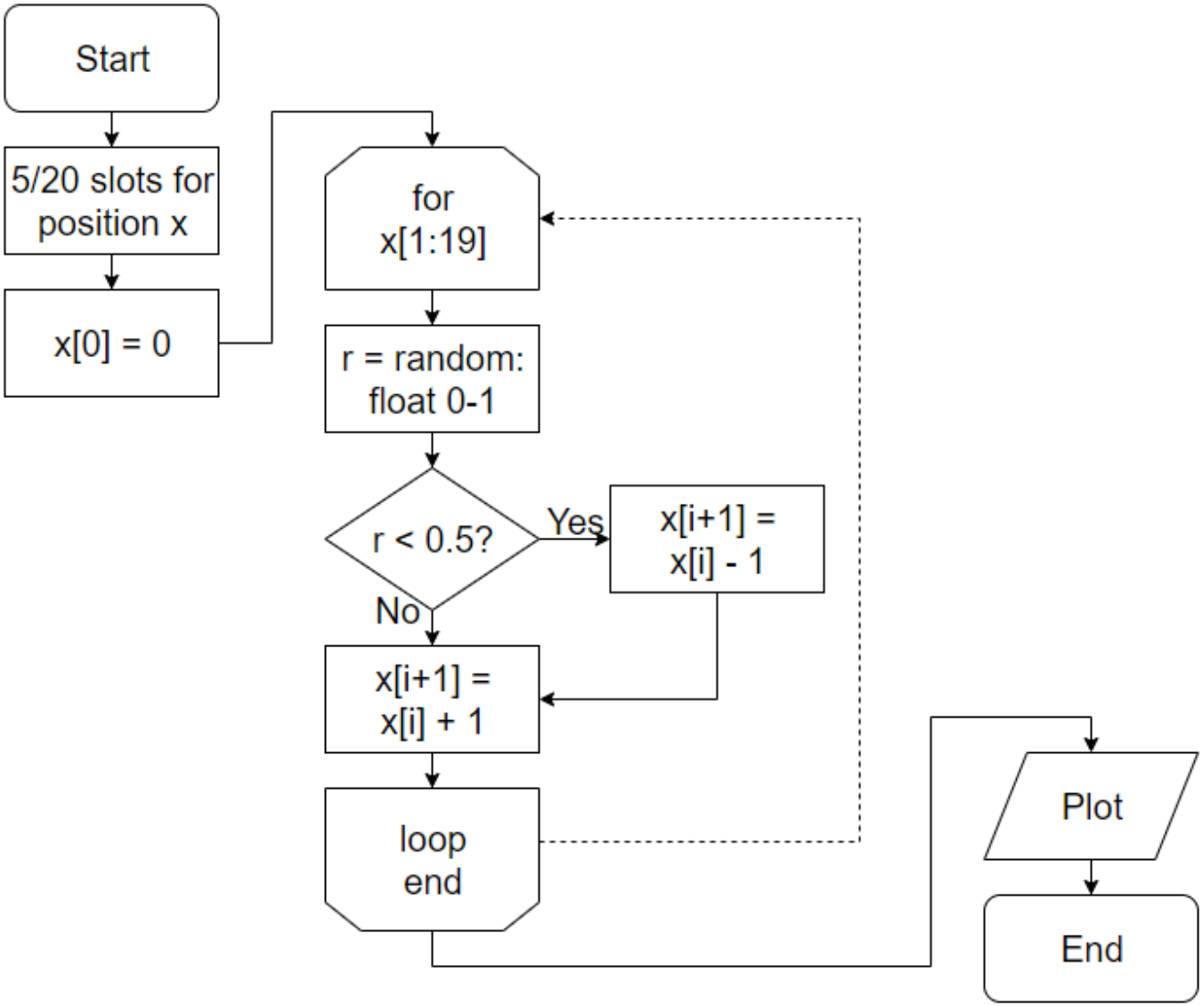
Coding seminar

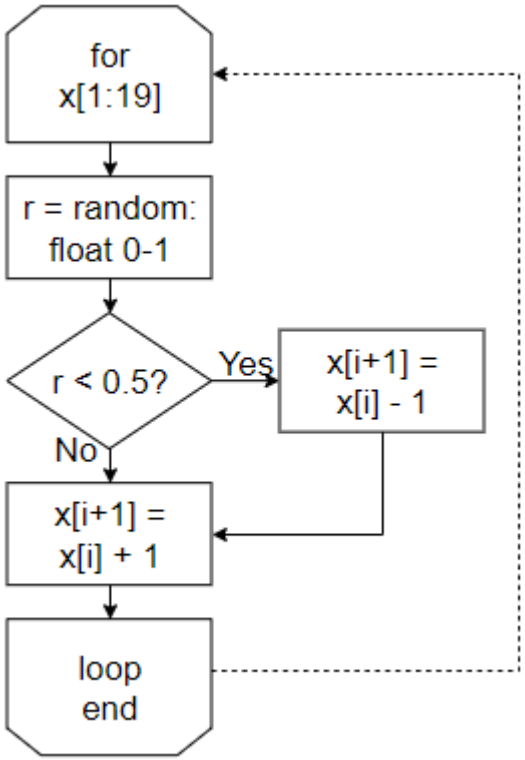
Lesson 3: Handling real-world data

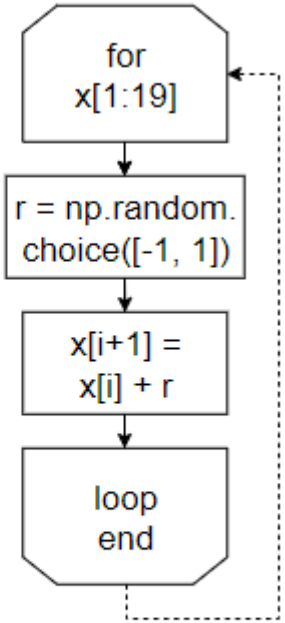
Ikue Hirata, PhD

Exercise model answer: random walk



Make it simple





2-D random walk

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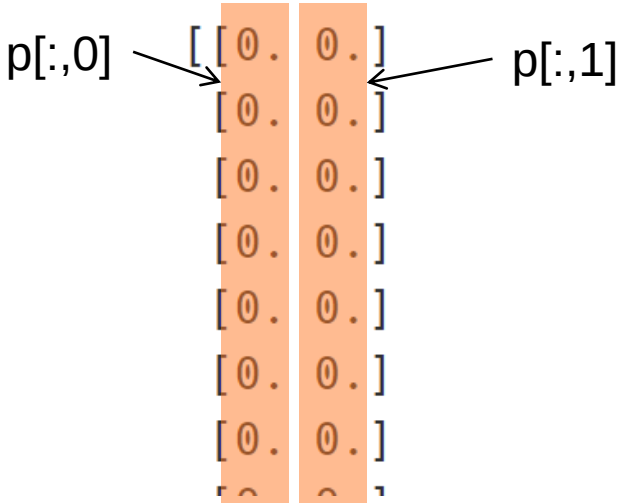
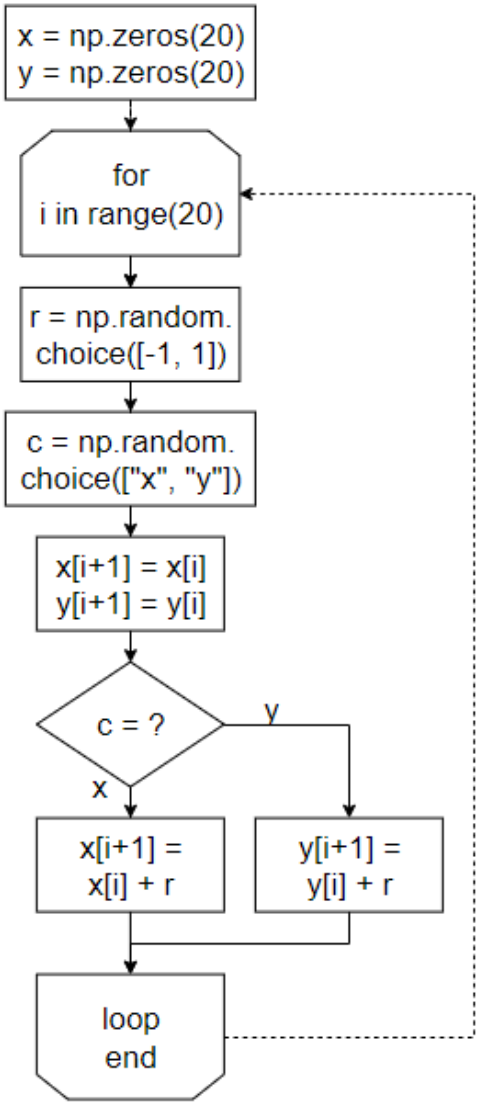
Trusted | Python 3

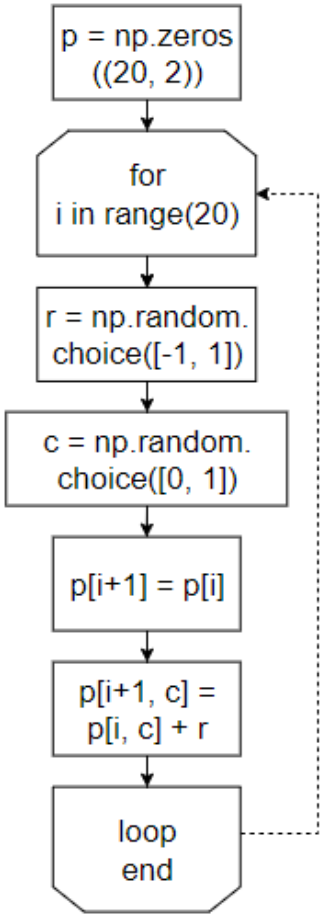
In [2]:

```
import numpy as np
length = 20
t = np.arange(length) # time
p = np.zeros((length, 2)) # position
print(p)
```



2-D random walk





Contents

Modules: More about Numpy

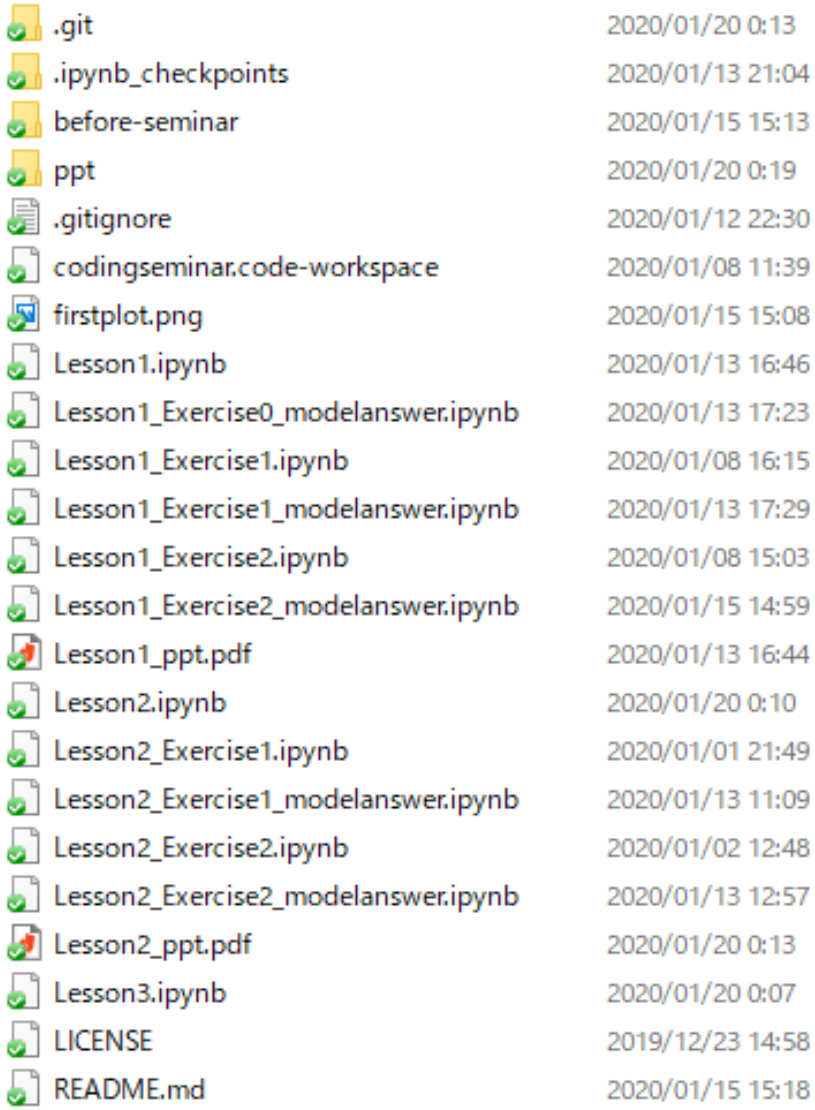
Plotting: More about Matplotlib

Editors

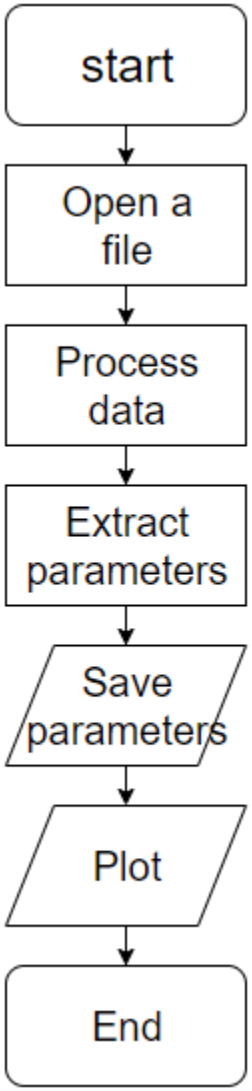
Debugger/debugging

UNIX-based commands for mass-process

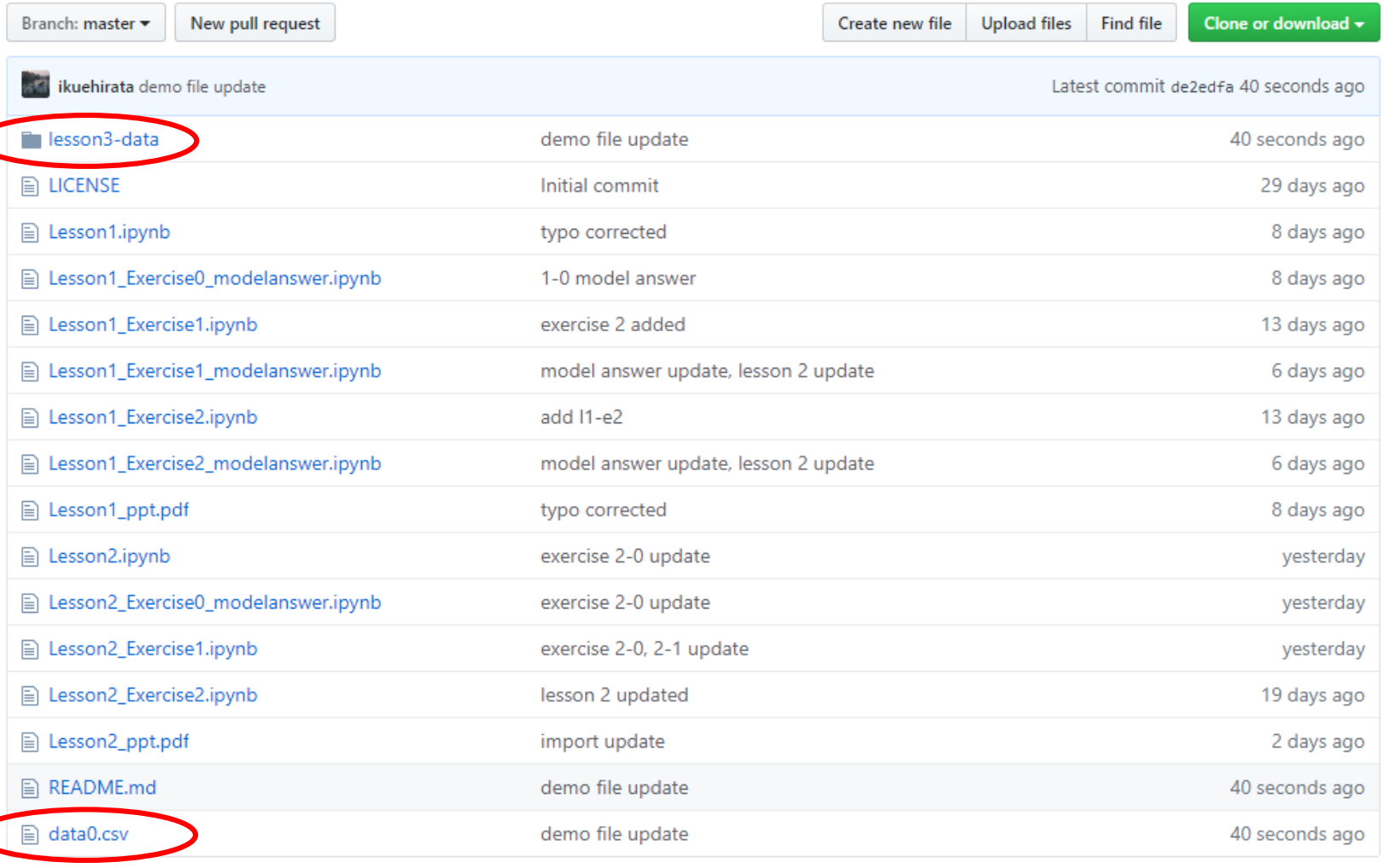
Extensions ready?



Data analysis process



Download demo files



Sample data

Programmer's Notepad - [data1.csv]

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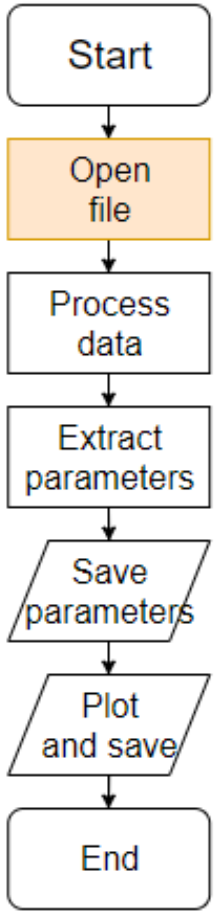
data1.csv

```
# Measurement mode = ZTD
# Osc Level = +1.00000E-01
# DC Bias State = 0
# DC Bias Level = +0.00000E+00
# Averaging = MED   +1
# Sweep Mode = SEQ
# Open Correction = 0
# Freqency  Z   phi
2.0000000000000000e+01    1.0074800000000000e+06    -8.5748000000000466e+01    0.0000000000000000e+00    0.00000000
2.0000000000000000e+01    1.0200500000000000e+06    -8.7277799999999916e+01    0.0000000000000000e+00    0.00000000
2.0000000000000000e+01    1.0227400000000000e+06    -8.9246799999999325e+01    0.0000000000000000e+00    0.00000000
2.0000000000000000e+01    1.0243300000000000e+06    -8.9246300000000507e+01    0.0000000000000000e+00    0.00000000
2.0000000000000000e+01    1.0519300000000000e+06    -8.7950999999999341e+01    0.0000000000000000e+00    0.00000000
2.0000000000000000e+01    1.0834900000000000e+06    -8.7283199999999368e+01    0.0000000000000000e+00    0.00000000
2.0000000000000000e+01    1.0720800000000000e+06    -8.7074399999999714e+01    0.0000000000000000e+00    0.00000000
2.0989399999999984e+01    1.0212600000000000e+06    -8.5559899999999895e+01    0.0000000000000000e+00    0.00000000
2.3334599999999823e+01    9.0411400000000000e+05    -8.8224800000000189e+01    0.0000000000000000e+00    0.00000000
2.5941800000000064e+01    7.9983300000000000e+05    -8.7057500000000455e+01    0.0000000000000000e+00    0.00000000
2.8840299999999916e+01    7.2794700000000000e+05    -8.7242900000000589e+01    0.0000000000000000e+00    0.0000000000000000e+00
3.2062699999999953e+01    6.7304800000000000e+05    -9.                  1    0.0000000000000000e+00    0.0000000000000000e+00
3.5645099999999934e+01    5.5381000000000000e+05    -8.                  1    0.0000000000000000e+00    0.0000000000000000e+00
3.9627800000000058e+01    5.3934700000000000e+05    -8.                  1    0.0000000000000000e+00    0.0000000000000000e+00
4.4055500000000210e+01    5.0011700000000000e+05    -9.0221900000000509e+01    0.0000000000000000e+00    0.0000000000000000e+00
4.8977899999999822e+01    4.0046700000000000e+05    -8.6866799999999779e+01    0.0000000000000000e+00    0.0000000000000000e+00
5.4450299999999859e+01    3.7458900000000000e+05    -8.6524500000000330e+01    0.0000000000000000e+00    0.0000000000000000e+00
6.0534100000000224e+01    3.5306700000000000e+05    -8.7066699999999732e+01    0.0000000000000000e+00    0.0000000000000000e+00
6.7297700000000607e+01    3.2024800000000000e+05    -8.8080100000000161e+01    0.0000000000000000e+00    0.0000000000000000e+00
7.4816999999999307e+01    2.8903000000000000e+05    -8.7074200000000471e+01    0.0000000000000000e+00    0.0000000000000000e+00
8.3176400000000100e+01    2.6151800000000000e+05    -8.7703599999999445e+01    0.0000000000000000e+00    0.0000000000000000e+00
9.2469800000000643e+01    2.3105100000000000e+05    -8.5886700000000471e+01    0.0000000000000000e+00    0.0000000000000000e+00
1.0280200000000067e+02    2.1358500000000000e+05    -8.5965699999999823e+01    0.0000000000000000e+00    0.0000000000000000e+00
1.1428799999999967e+02    1.8976300000000000e+05    -8.6715100000000673e+01    0.0000000000000000e+00    0.0000000000000000e+00
```

Header/comments

Data body

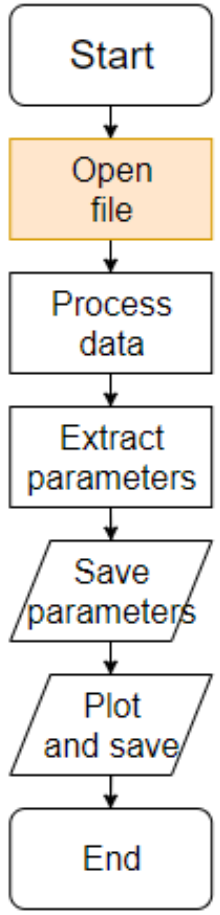


Array data – csv/tsv

comma/tab separated values

	A	B	C	D	E	F
1	# Measurement mode = ZTD					
2	# Osc Level = +1.00000E-01					
3	# DC Bias State = 0					
4	# DC Bias Level = +0.00000E+00					
5	# Averaging = MED	1				
6	# Sweep Mode = SEQ					
7	# Open Correction = 0					
8	# Freqency	Z	phi			
9	2.00E+01	1.01E+06	-8.57E+01	0.00E+00	0.00E+00	
10	2.00E+01	1.02E+06	-8.73E+01	0.00E+00	0.00E+00	
11	2.00E+01	1.02E+06	-8.92E+01	0.00E+00	0.00E+00	
12	2.00E+01	1.02E+06	-8.92E+01	0.00E+00	0.00E+00	
13	2.00E+01	1.05E+06	-8.80E+01	0.00E+00	0.00E+00	
14	2.00E+01	1.08E+06	-8.73E+01	0.00E+00	0.00E+00	
15	2.00E+01	1.07E+06	-8.71E+01	0.00E+00	0.00E+00	
16	2.10E+01	1.02E+06	-8.56E+01	0.00E+00	0.00E+00	
17	2.33E+01	9.04E+05	-8.82E+01	0.00E+00	0.00E+00	
18	2.59E+01	8.00E+05	-8.71E+01	0.00E+00	0.00E+00	
19	2.88E+01	7.28E+05	-8.72E+01	0.00E+00	0.00E+00	
20	3.21E+01	6.73E+05	-9.05E+01	0.00E+00	0.00E+00	
21	3.56E+01	5.54E+05	-8.54E+01	0.00E+00	0.00E+00	
22	3.96E+01	5.39E+05	-8.75E+01	0.00E+00	0.00E+00	
23	4.41E+01	5.00E+05	-9.02E+01	0.00E+00	0.00E+00	
24	4.90E+01	4.00E+05	-8.69E+01	0.00E+00	0.00E+00	
25	5.45E+01	3.75E+05	-8.65E+01	0.00E+00	0.00E+00	
26	6.05E+01	3.53E+05	-8.71E+01	0.00E+00	0.00E+00	

Sheet1



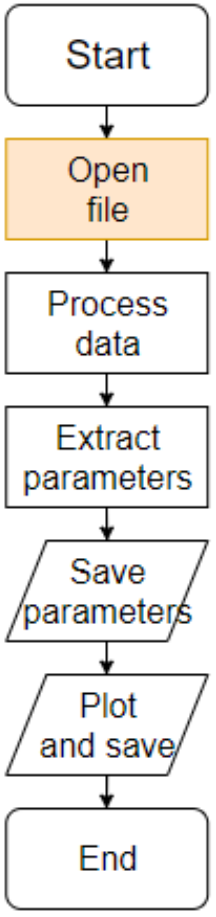
Read data into array

File Edit View Insert Cell Kernel Navigate Widgets Help

In [14]:

```
1 import numpy as np
2 data = np.loadtxt("data0.csv", delimiter='\t')
3 print(data)
```

```
[[ 2.00000e+01  9.04909e+05 -8.85148e+01
0.00000e+00  0.00000e+00]
 [ 2.00000e+01  9.54938e+05 -8.75136e+01
0.00000e+00  0.00000e+00]
 [ 2.00000e+01  9.34201e+05 -8.60863e+01
0.00000e+00  0.00000e+00]
 [ 2.00000e+01  9.25598e+05 -8.47966e+01
0.00000e+00  0.00000e+00]
 [ 2.00000e+01  9.23228e+05 -8.54492e+01
0.00000e+00  0.00000e+00]
```



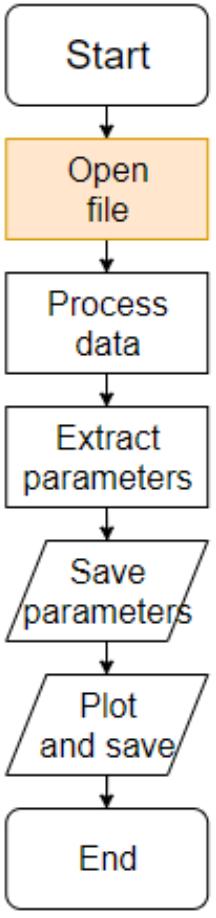
Read data into array

File Edit View Insert Cell Kernel Navigate Widgets Help

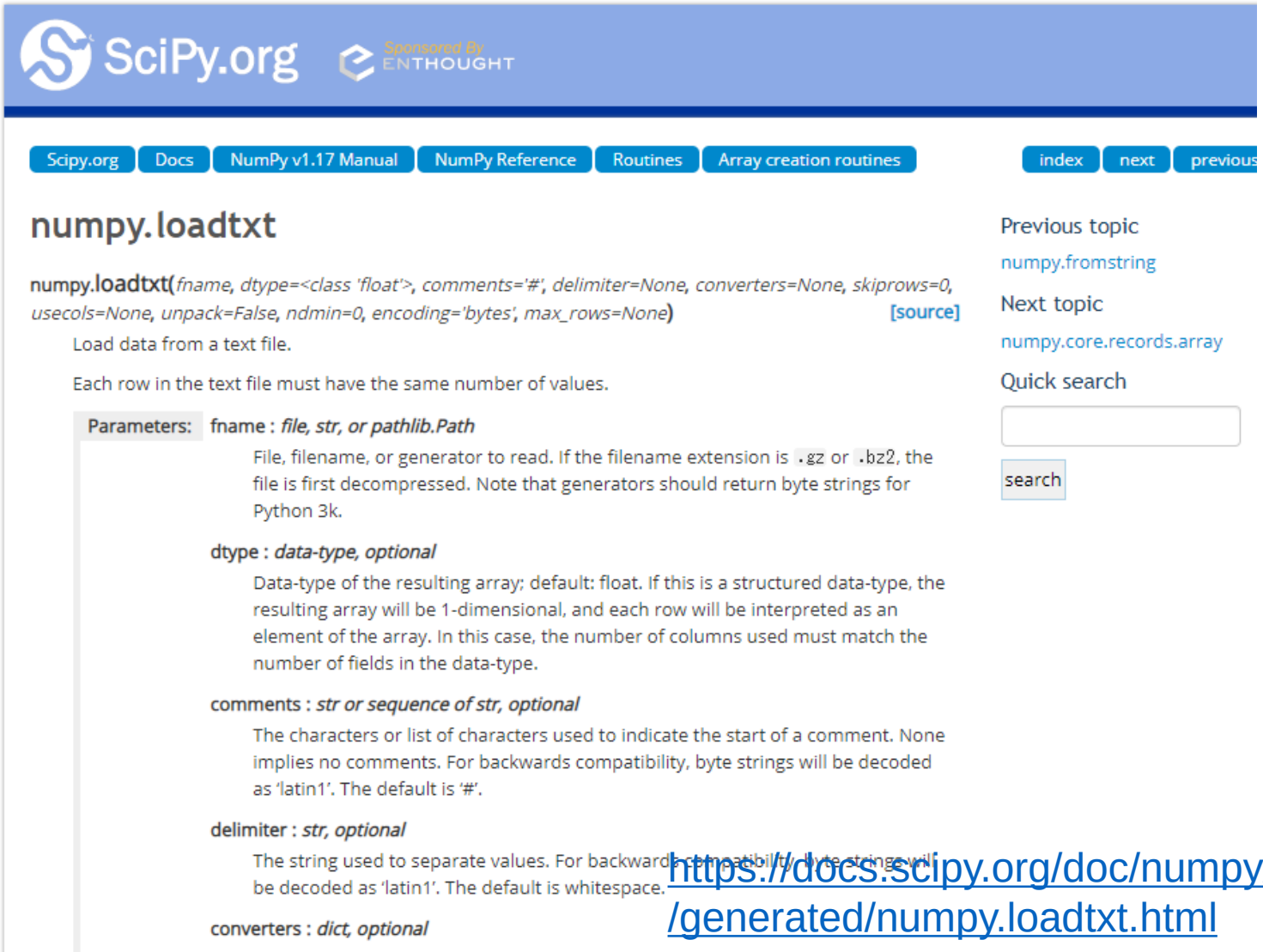
In [2]:

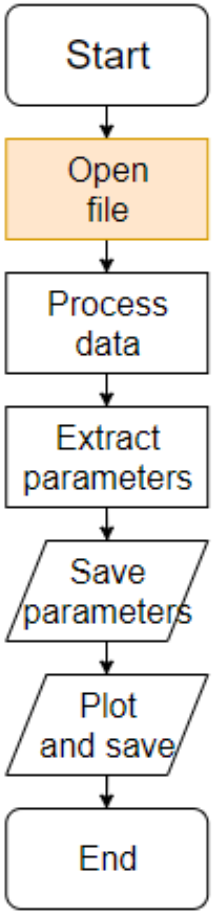
```
data = np.loadtxt("data1.csv", delimiter="\t",
                  usecols=[0,1,2])
print(data)
```

```
[[ 2.00000e+01  1.00748e+06 -8.57480e+01]
 [ 2.00000e+01  1.02005e+06 -8.72778e+01]
 [ 2.00000e+01  1.02274e+06 -8.92468e+01]
 [ 2.00000e+01  1.02433e+06 -8.92463e+01]
 [ 2.00000e+01  1.05193e+06 -8.79510e+01]
 [ 2.00000e+01  1.08349e+06 -8.72832e+01]
 [ 2.00000e+01  1.07208e+06 -8.70744e+01]
 [ 2.09894e+01  1.02126e+06 -8.55599e+01]
 [ 2.33346e+01  9.04114e+05 -8.82248e+01]
 [ 2.59418e+01  7.99833e+05 -8.70575e+01]
```



For more options…

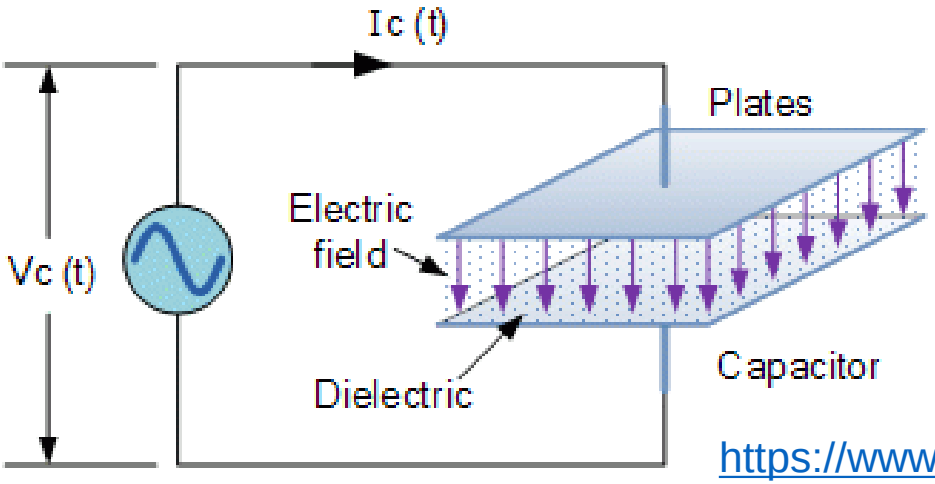




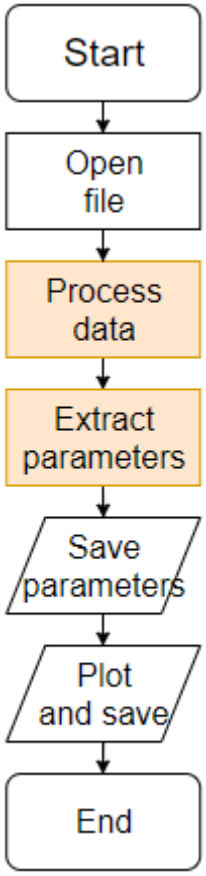
https://docs.scipy.org/doc/numpy/reference/generated/numpy.loadtxt.html

What is this?

Complex impedance of a capacitor



https://www.electronics-tutorials.ws/filter/filter_1.html



$$Z = \frac{1}{j\omega C}, \omega = 2\pi f, \phi = \arg Z$$

We want to get this value

j as imaginary number

Fitting function

numpy.polynomial.polynomial.polyfit

numpy.polynomial.polynomial.**polyfit**(*x*, *y*, *deg*, *rcond=None*, *full=False*, *w=None*) [source]

Least-squares fit of a polynomial to data.

Return the coefficients of a polynomial of degree *deg* that is the least squares fit to the data values *y* given at points *x*. If *y* is 1-D the returned coefficients will also be 1-D. If *y* is 2-D multiple fits are done, one for each column of *y*, and the resulting coefficients are stored in the corresponding columns of a 2-D return. The fitted polynomial(s) are in the form

$$p(x) = c_0 + c_1 * x + ... + c_n * x^n,$$

where *n* is *deg*.

Parameters:

x : *array_like, shape (M,)*

x-coordinates of the *M* sample (data) points `(x[i], y[i])`.

y : *array_like, shape (M,) or (M, K)*

y-coordinates of the sample points. Several sets of sample points sharing the same x-coordinates can be (independently) fit with one call to polyfit by passing in for *y* a 2-D array that contains one data set per column.

deg : *int or 1-D array_like*

Degree(s) of the fitting polynomials. If *deg* is a single integer all terms up to and including the *deg*'th term are included in the fit. For NumPy versions >= 1.11.0 a list of integers specifying the degrees of the terms to include may be used instead.

rcond : *float, optional*

Relative condition number of the fit. Singular values smaller than *rcond*, relative to the largest singular value, will be ignored. The default value is `len(x)*eps`, where *eps* is the relative precision of the platform's float type, about 2e-16 in most cases.

full : *bool, optional*

Switch determining the nature of the return value. When `False` (the default) just the coefficients are returned; when `True`, diagnostic information from the singular value decomposition (used to solve the fit's matrix equation) is also

Previous topic

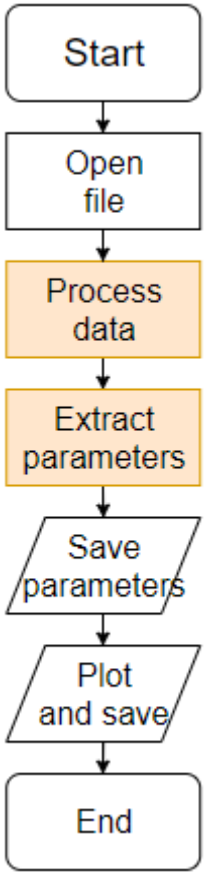
numpy.polynomial.polynomial.p

Next topic

numpy.polynomial.polynomial.p

Quick search

search



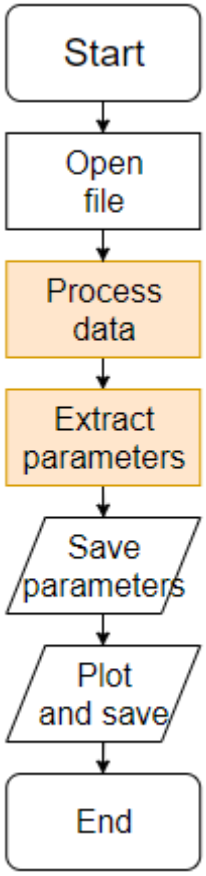
https://docs.scipy.org/doc/numpy/reference/generated/numpy.polynomial.polynomial.polyfit.html

Small trick

$$Z = \frac{1}{j \cdot 2\pi f \omega C}$$

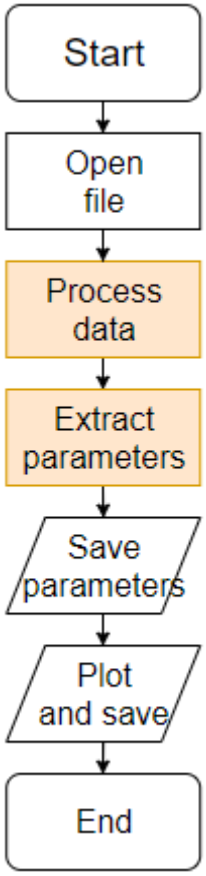
$$\log(Z) = -\log(2\pi f C)$$

$$\log(Z) = -\log(2\pi C) - \log(f)$$

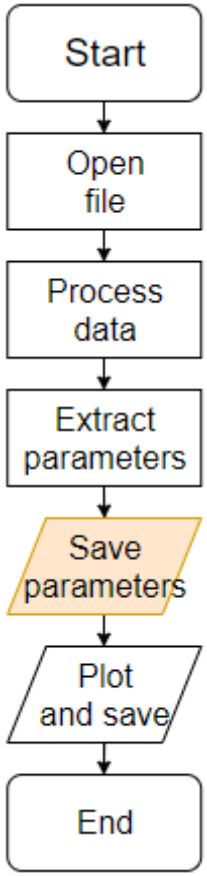


Fitting 1 – Exercise 0-1

$$y = -0.96x + 16.6$$



Save parameter



In [30]:
```
logz = np.log(data[:,1])
logf = np.log(data[:,0])
from numpy.polynomial import polynomial as P
p = P.polyfit(logf, logz, 1)
print(p)
```

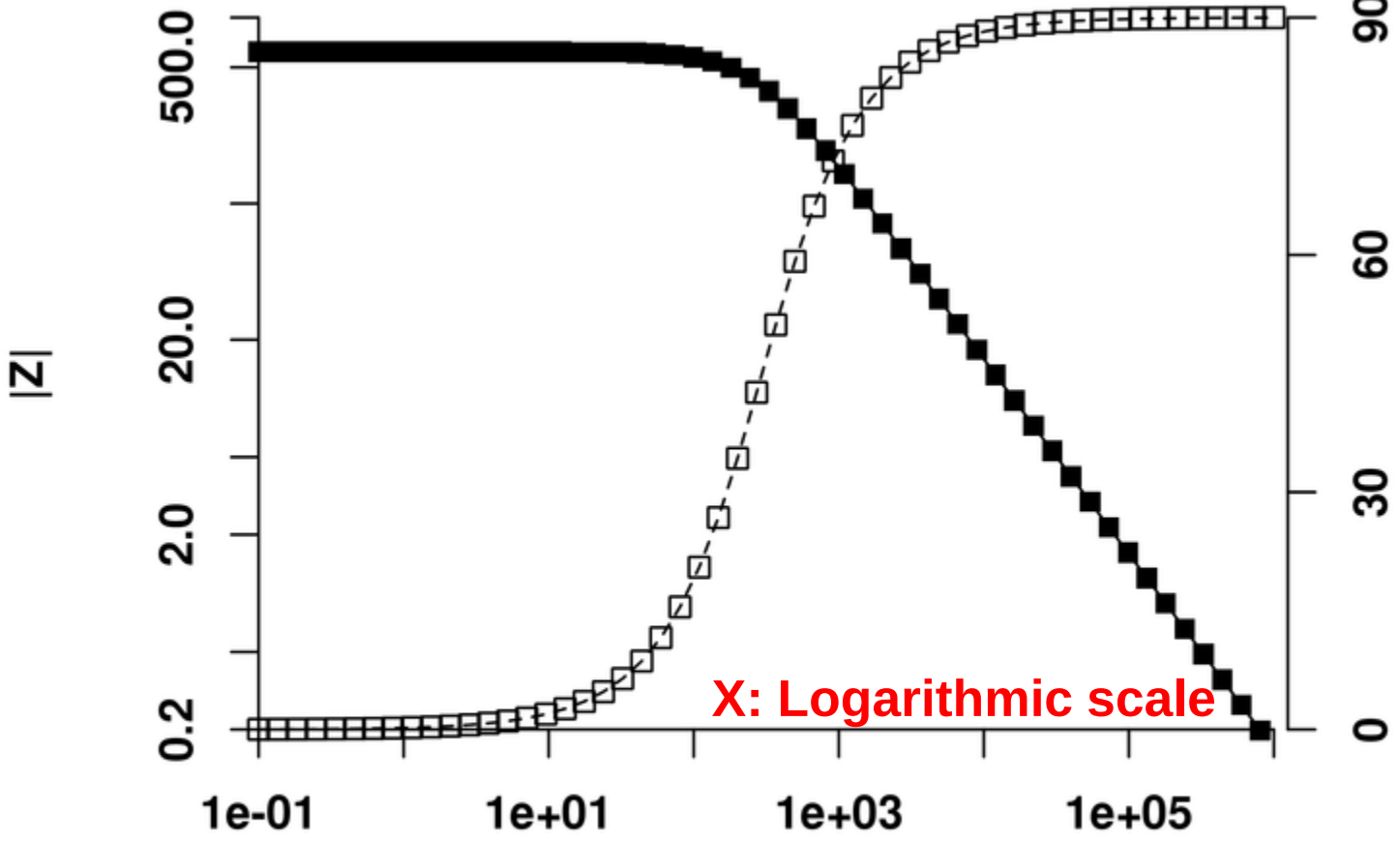
```
[16.60429901 -0.96116536]
```

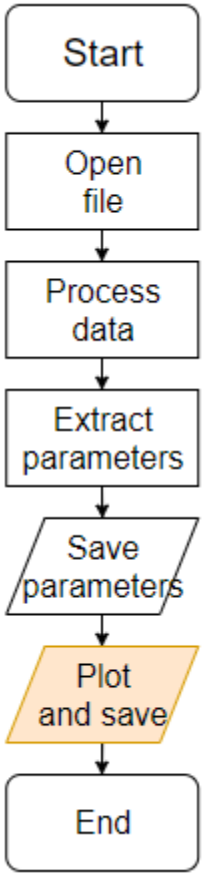
In [31]:
```
np.savetxt("parameters.csv", p, delimiter="\t")
```

Bode plot

Y1: Logarithmic scale

Y2: Linear scale –
I prefer ϕ not inverted

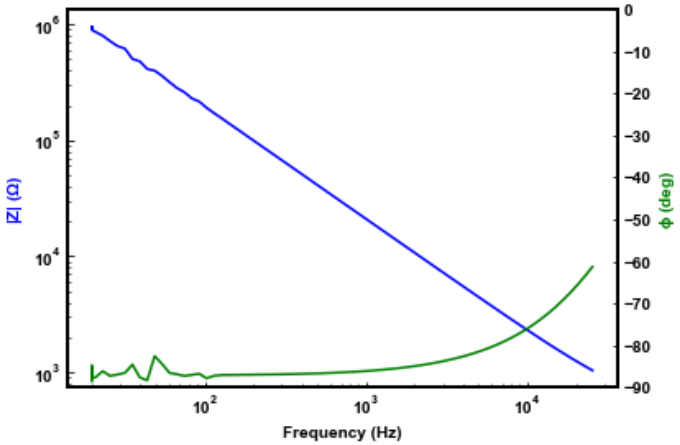


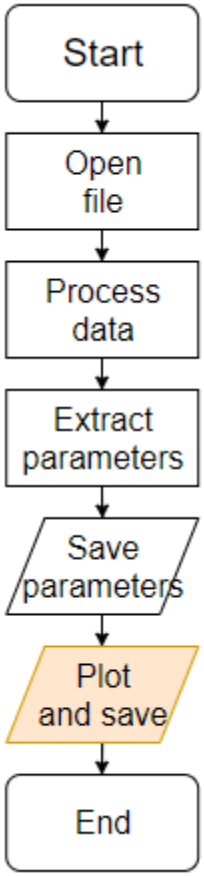


Bardini, Luca. (2015). EIS 101, an introduction to electrochemical spectroscopy. What was a website is now available as a self-contained PDF.

Plotting – Exercise 0-2

```
ax.set_xlabel("Frequency (Hz)")
ax.set_ylabel("|Z| ($\Omega$)", color="b")
ax2.set_ylabel("$\phi$ (deg)", color="g")
ax2.set_ylim((-90, 0))
plt.show()
```





Add fit line

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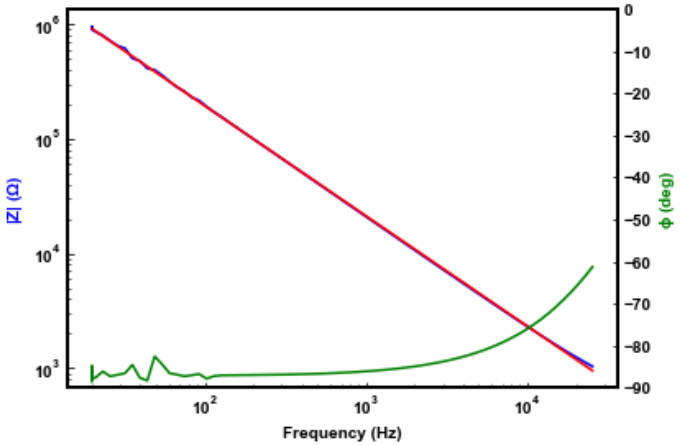
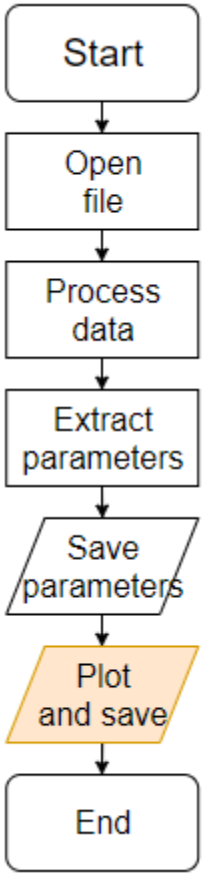
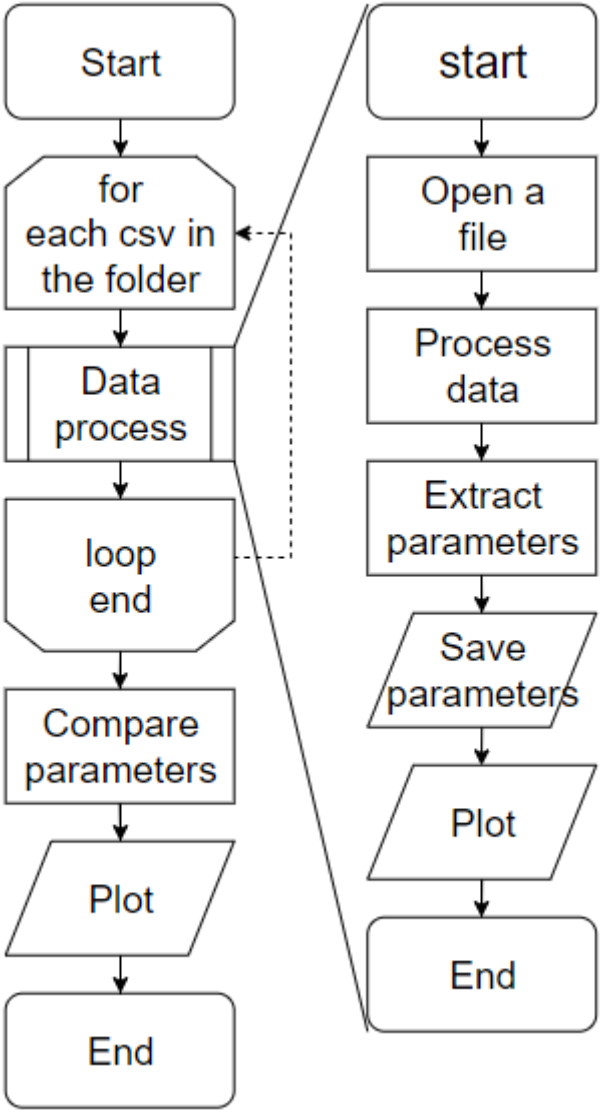
```
fitz = np.exp(p[0] + p[1] * logf)
ax.plot(data[:,0], fitz, color="r")
plt.show()
plt.savefig("impedancefit.png")
```




```
<Figure size 432x288 with 0 Axes>
```



That’s not all!



Download the code

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Trusted | Python 3

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Save as...
Rename...
Save and Checkpoint
Revert to Checkpoint
Print Preview
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Close and Halt

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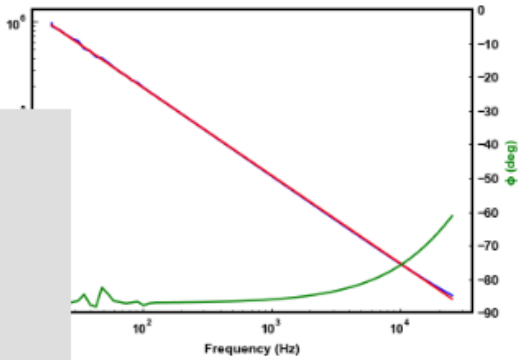
- HTML (.html)
- HTML with toc (.html)
- LaTeX (.tex)
- Markdown (.md)
- Notebook (.ipynb)
- PDF via LaTeX (.pdf)
- reST (.rst)
- Python (.py)
- Reveal.js slides (.slides.html)

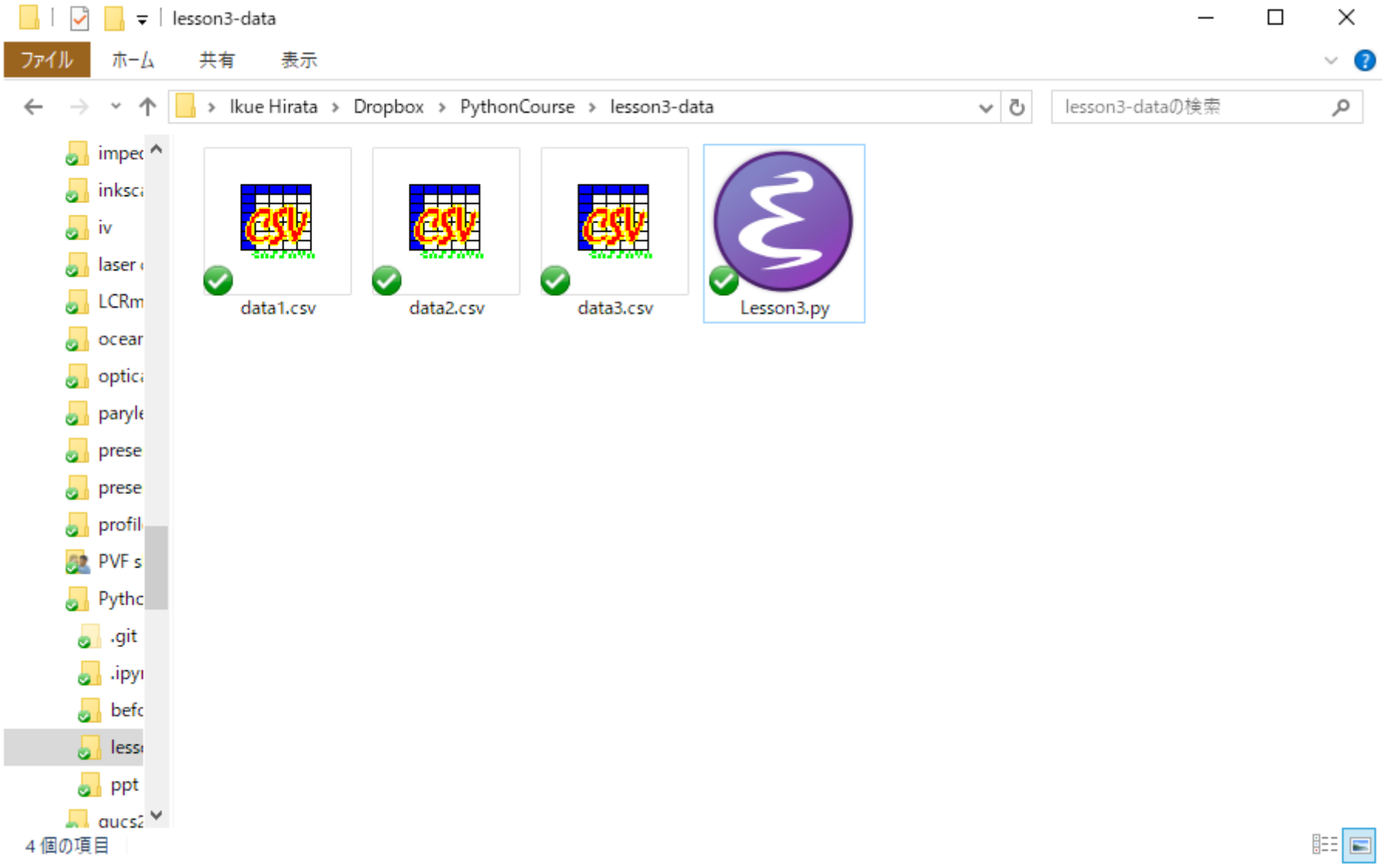
```
fitz = np.exp(p[0] + p[1] * logf)
ax.plot(data[:,0], fitz, color="r")
plt.show()
plt.savefig("impedancefit.png")
```



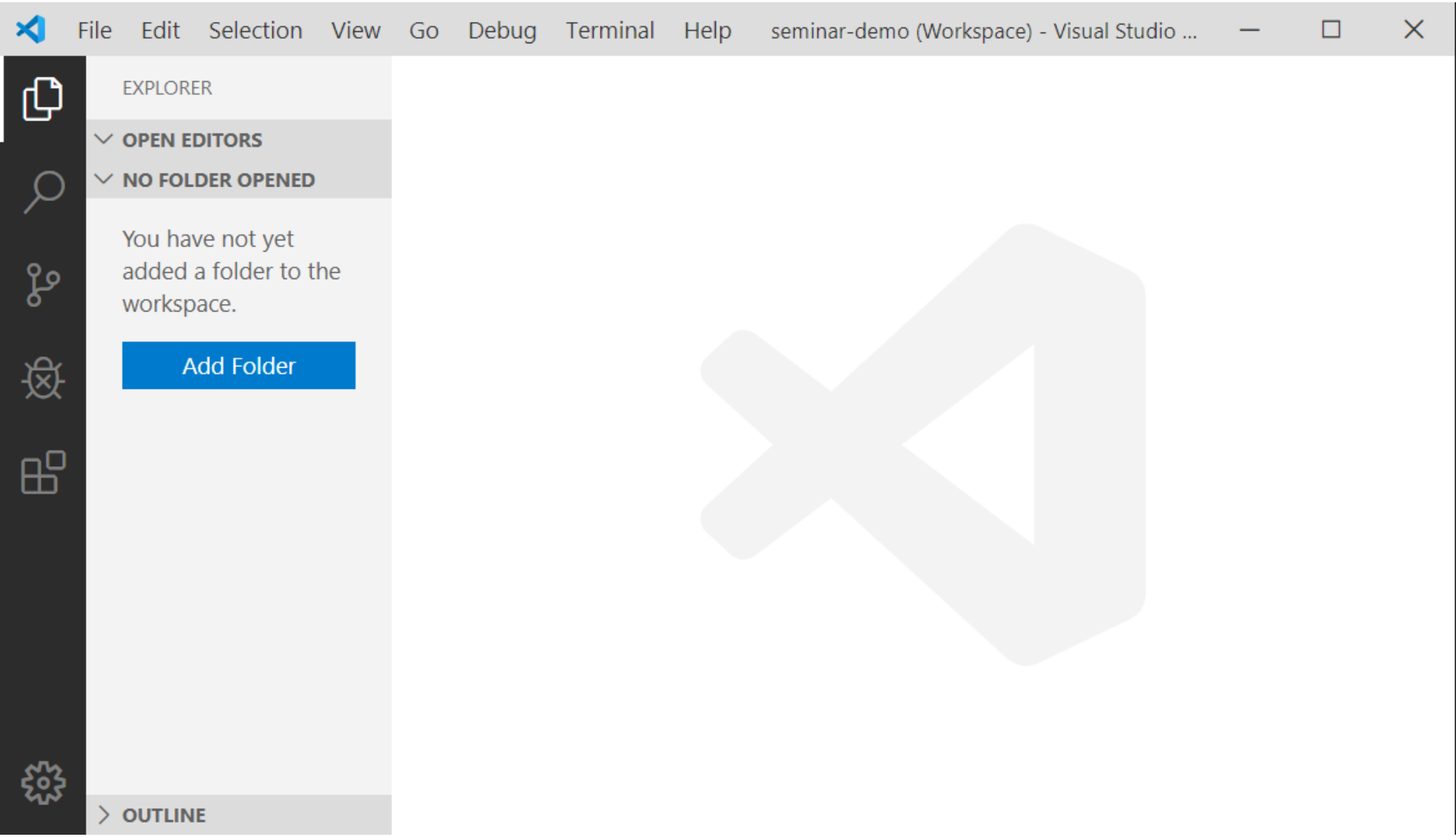

```
gure size 432x288 with 0 Axes>
```

3. Exercise 1

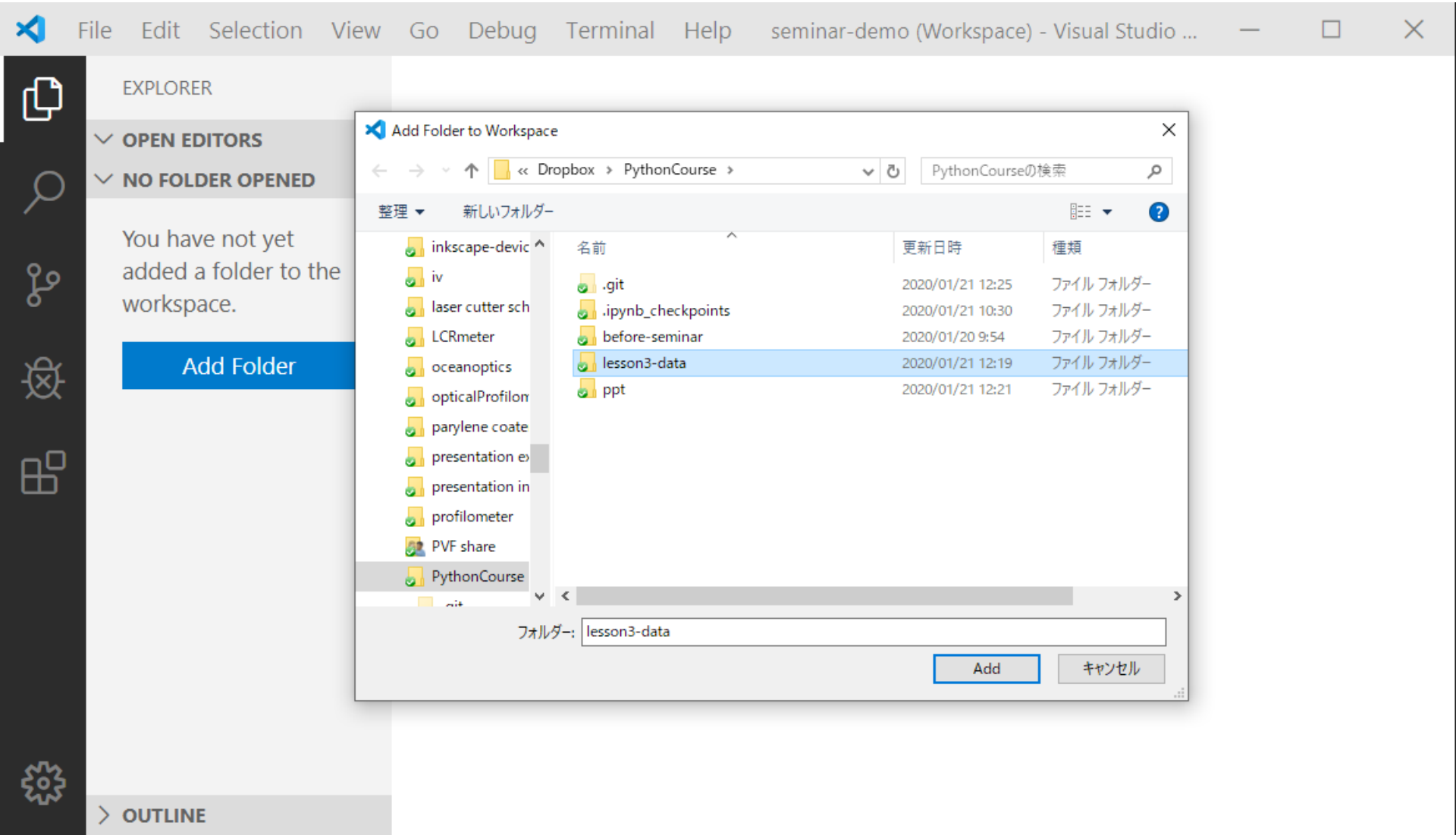
Store it where other data are



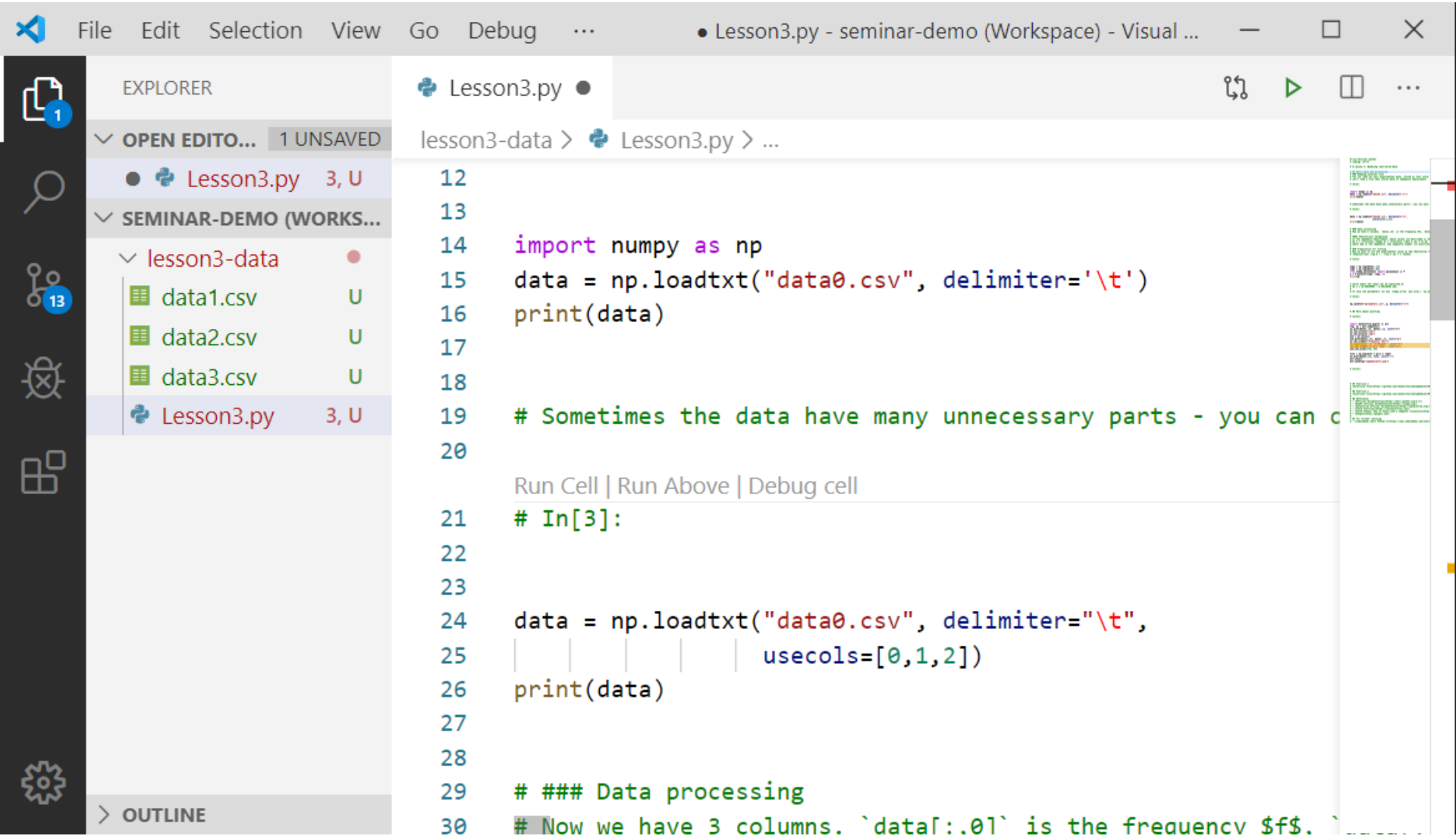
Open Visual Studio Code



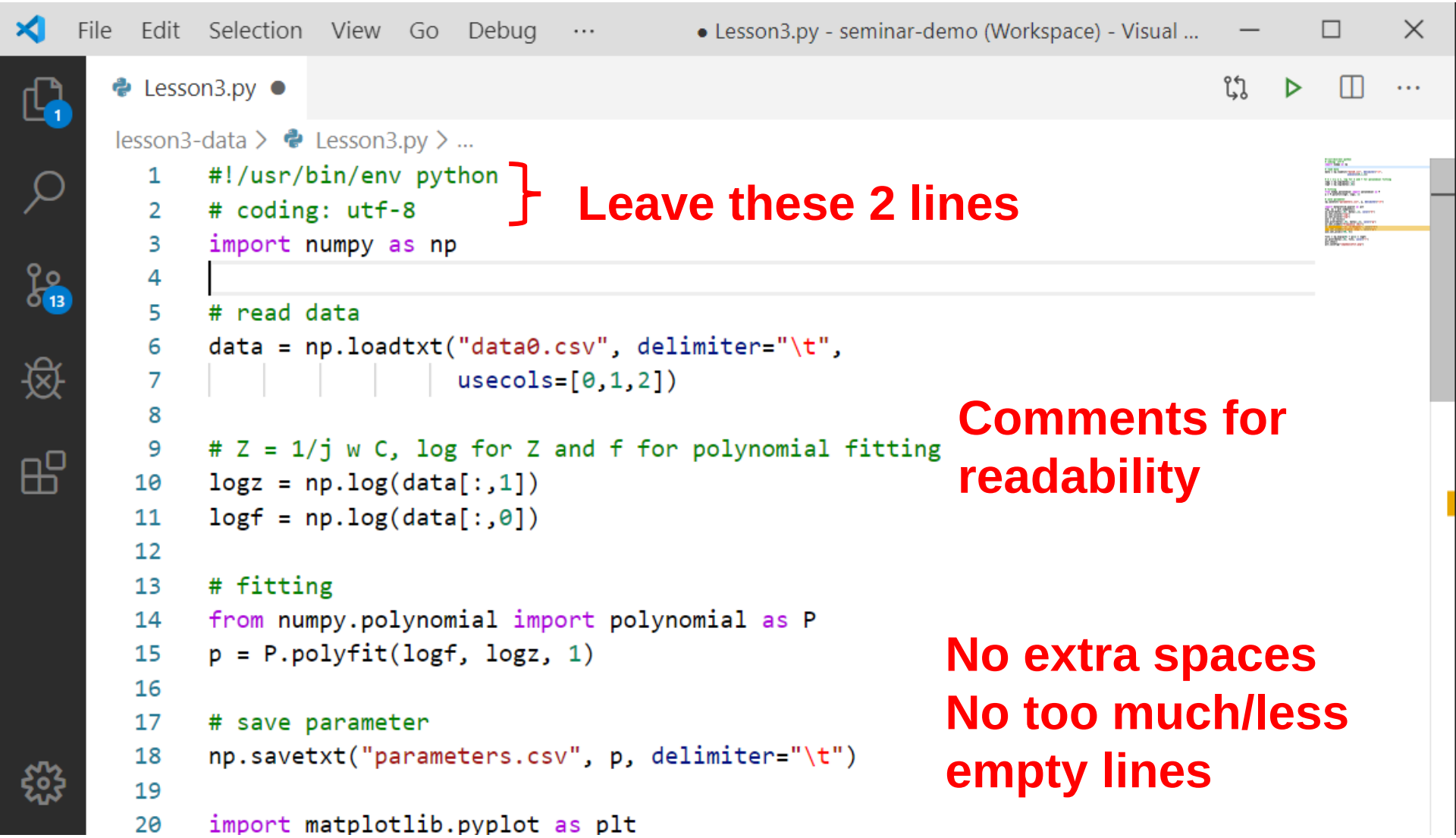
Add folder – workspace



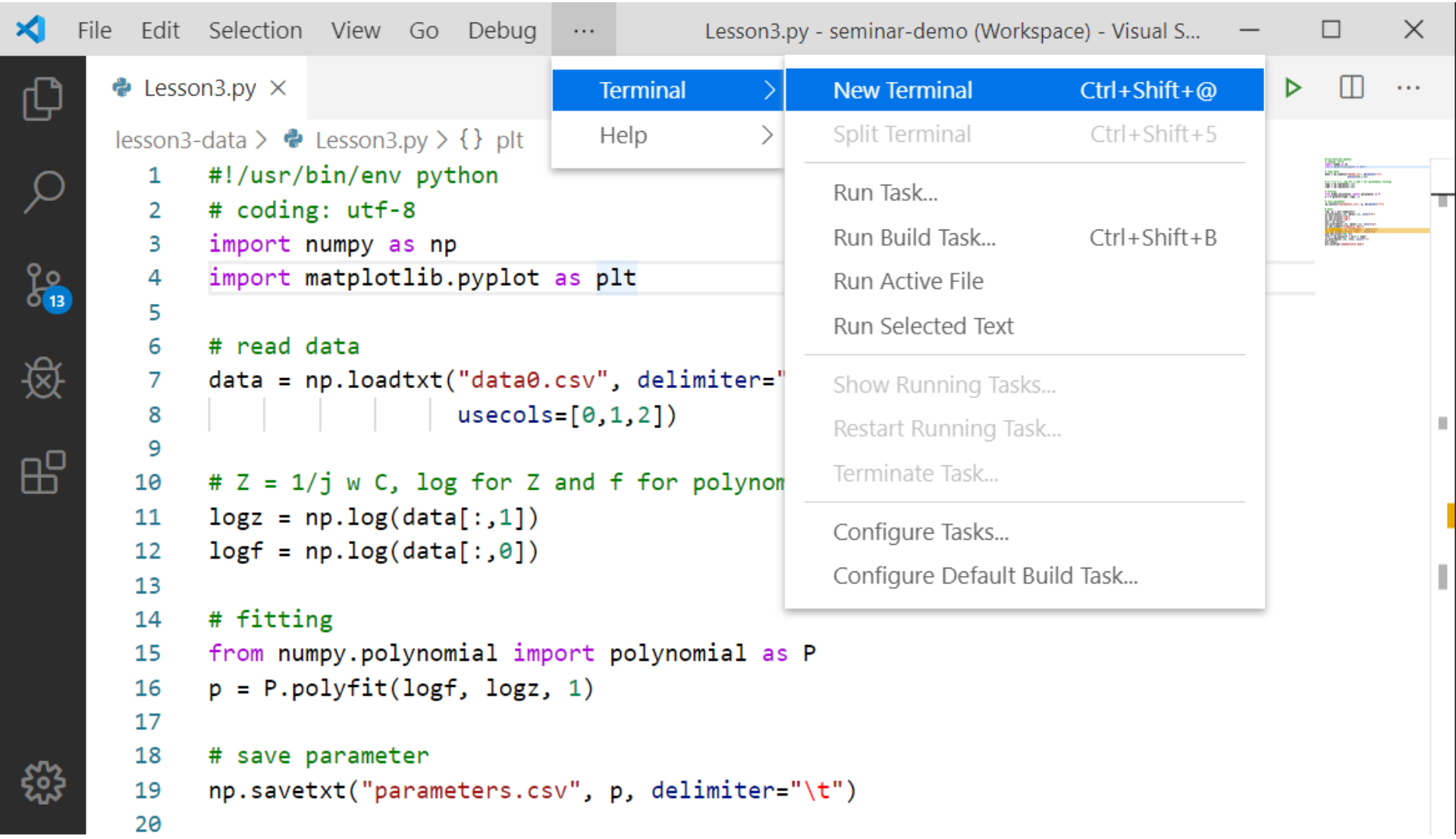
Open your code



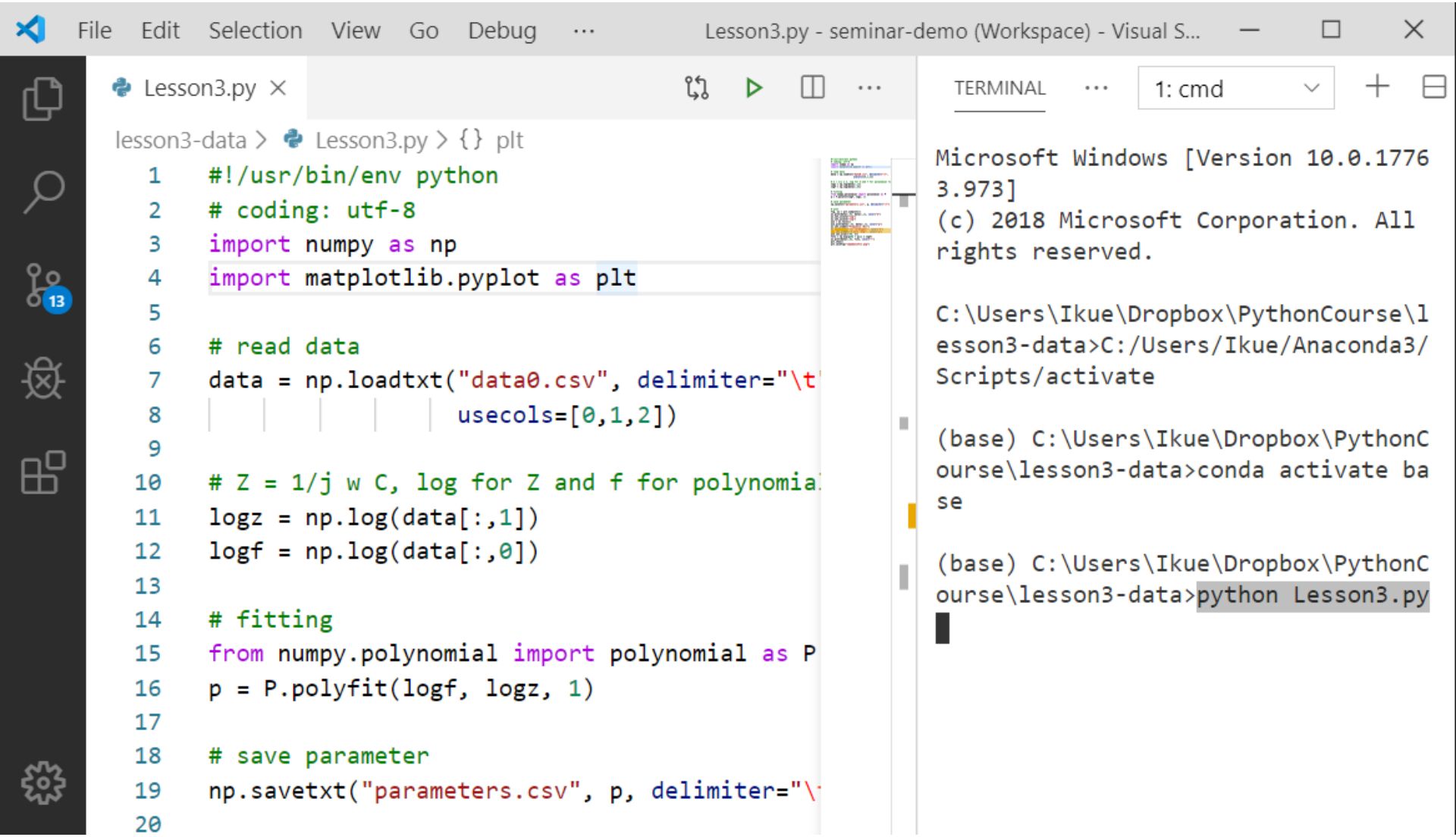
Code aesthetics – readability



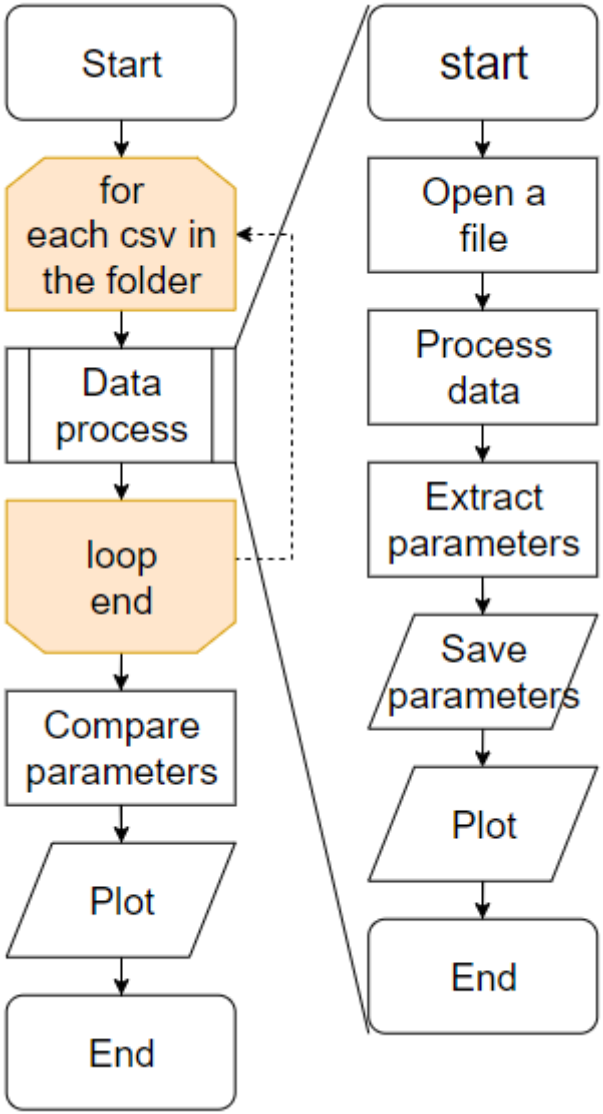
Open Terminal



Run the code


File Edit Selection View Go Debug ···
Lesson3.py - seminar-demo (Workspace) - Visual S...
Lesson3.py
lesson3-data > Lesson3.py > { } plt
#!/usr/bin/env python
# coding: utf-8
import numpy as np
import matplotlib.pyplot as plt
# read data
data = np.loadtxt("data0.csv", delimiter="\t
usecols=[0,1,2])
# Z = 1/j w C, log for Z and f for polynomia
logz = np.log(data[:,1])
logf = np.log(data[:,0])
# fitting
from numpy.polynomial import polynomial as P
p = P.polyfit(logf, logz, 1)
# save parameter
np.savetxt("parameters.csv", p, delimiter="\
TERMINAL
1: cmd
Microsoft Windows [Version 10.0.1776
3.973]
(c) 2018 Microsoft Corporation. All
rights reserved.
C:\Users\Ikue\Dropbox\PythonCourse\l
esson3-data>C:/Users/Ikue/Anaconda3/
Scripts/activate
(base) C:\Users\Ikue\Dropbox\PythonC
ourse\lesson3-data>conda activate ba
se
(base) C:\Users\Ikue\Dropbox\PythonC
ourse\lesson3-data>python Lesson3.py

Getting multiple files



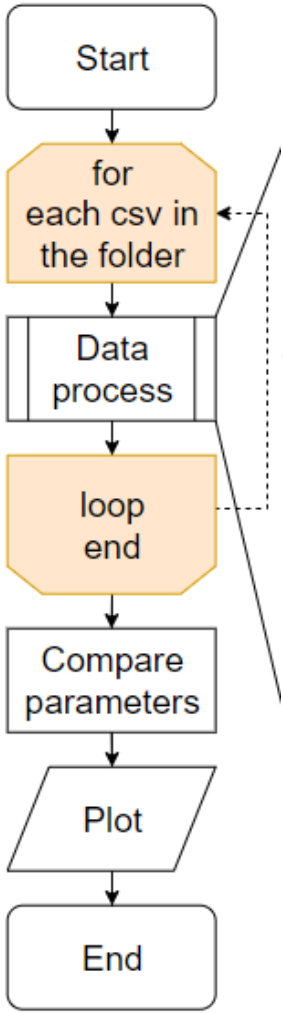
glob

File Edit View Insert Cell Kernel Navigate Widgets Help

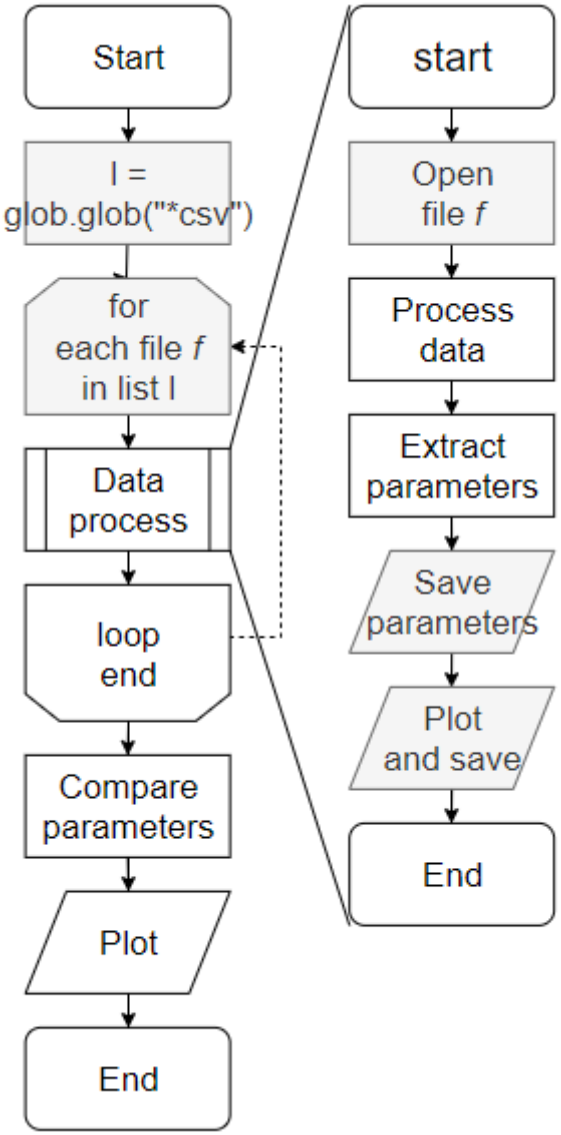
In [1]:

```
import glob
l = glob.glob("*csv")
print(l)
```

```
['data1.csv', 'data2.csv', 'data3.csv']
```



Pay attention to save file name



“Spaghetti” code

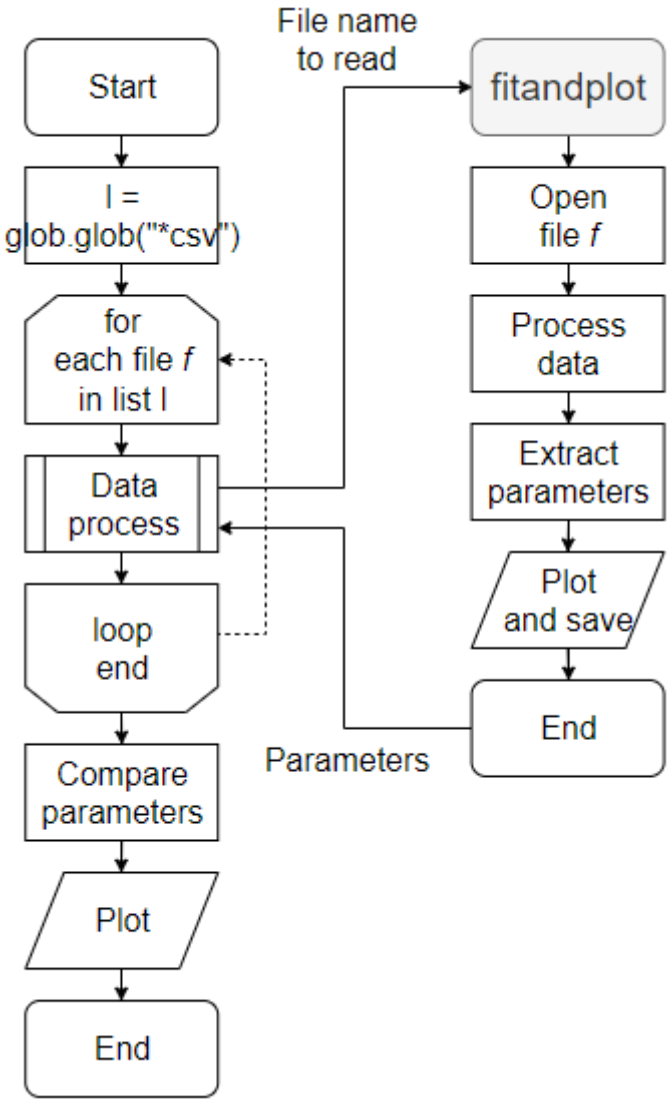
File Edit Selection View Go Debug Terminal Help — Lesson3.py - seminar-demo (Workspace) - Visual Studio Code

Lesson3.py

lesson3-data > Lesson3.py > ...

```
4   import matplotlib.pyplot as plt
5   import glob
6
7   filelist = glob.glob("*csv")
8   params = [] # list to store parameters
9   for f in filelist:
10      # read data
11      data = np.loadtxt(f, delimiter="\t",
12                        usecols=[0,1,2])
13
14      # Z = 1/j w C, log for Z and f for polynomial fitting
15      logz = np.log(data[:,1])
16      logf = np.log(data[:,0])
17
18      # fitting
19      from numpy.polynomial import polynomial as P
20      p = P.polyfit(logf, logz, 1)
21
22      # save parameter
23      np.savetxt(f"{f}.csv", p, delimiter="\t") # save file name using original file
24      params.append([[f, p]]) # append file name and parameter in the storage
25
26      # plot
27      fig, ax = plt.subplots()
28      ax.plot(data[:,0], data[:,1], color="b")
29      ax.set_xscale("log")
30      ax.set_yscale("log")
31      ax2 = ax.twinx()
32      ax2.plot(data[:,0], data[:,2], color="g")
33      ax.set_xlabel("Frequency (Hz)")
34      ax.set_ylabel("|Z| ($\Omega$)", color="b")
35      ax2.set_ylabel("$\phi$ (deg)", color="g")
36      ax2.set_ylim((-90, 0))
37      fitz = np.exp(p[0] + p[1] * logf)
38      ax.plot(data[:,0], fitz, color="r")
39      plt.show()
40      plt.savefig(f"{f}.png")
41
```

User defined function



Using user defined function

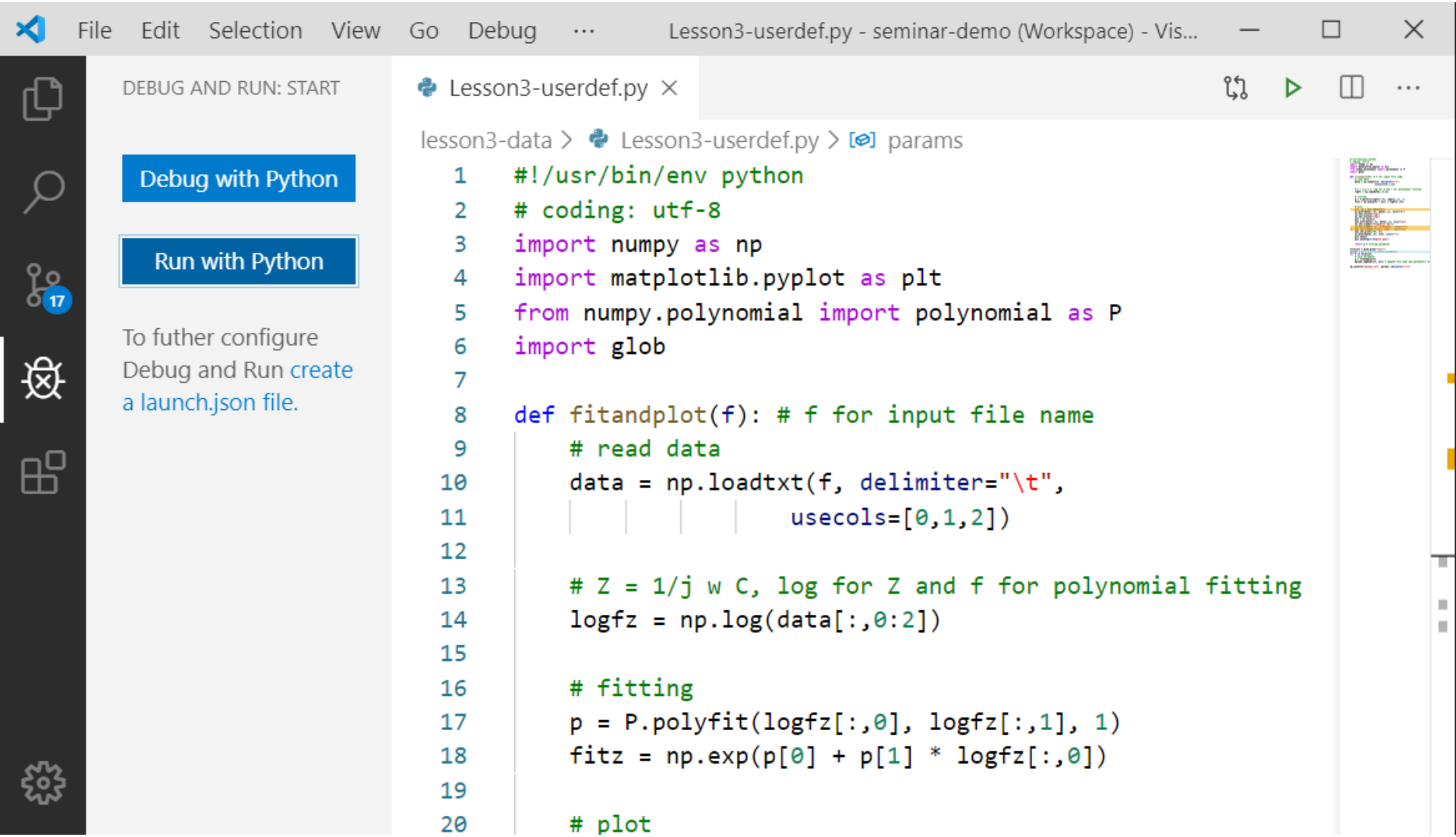
File Edit Selection View Go Debug ··· Lesson3-userdef.py - seminar-demo (Workspace) - Vis...

Lesson3-userdef.py

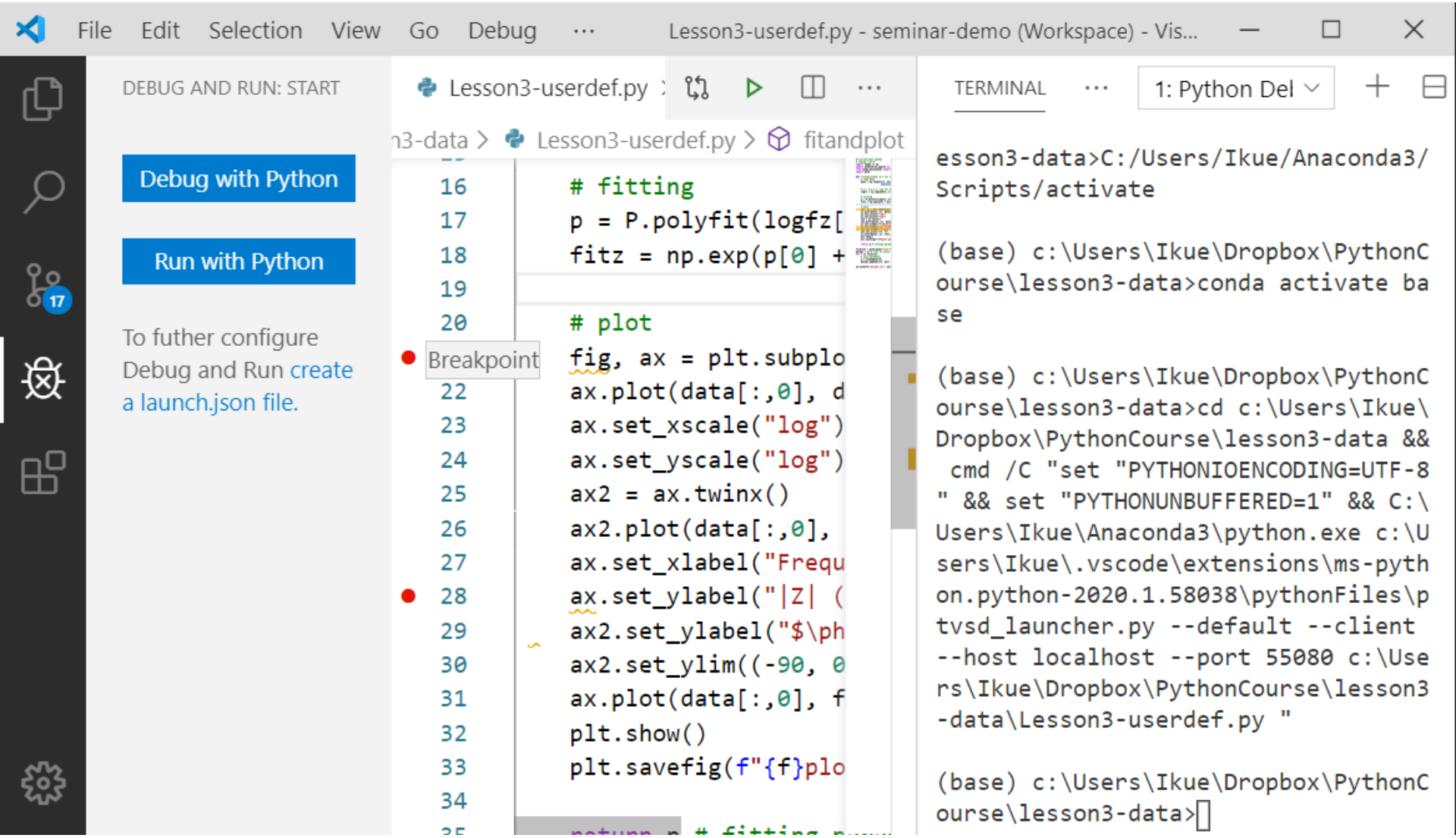
lesson3-data > Lesson3-userdef.py > ...

```
33      plt.savefig(f"{f}plot.png")
34
35      return p # fitting parameter
36
37  filelist = glob.glob("*csv")
38  params = [] # list to store parameters
39  for f in filelist:
40      # save parameter
41      p = fitandplot(f)
42      params.append([[f, p]]) # append file name and parameters to the storage
43
44  np.savetxt("params.csv", params, delimiter="\t")
```

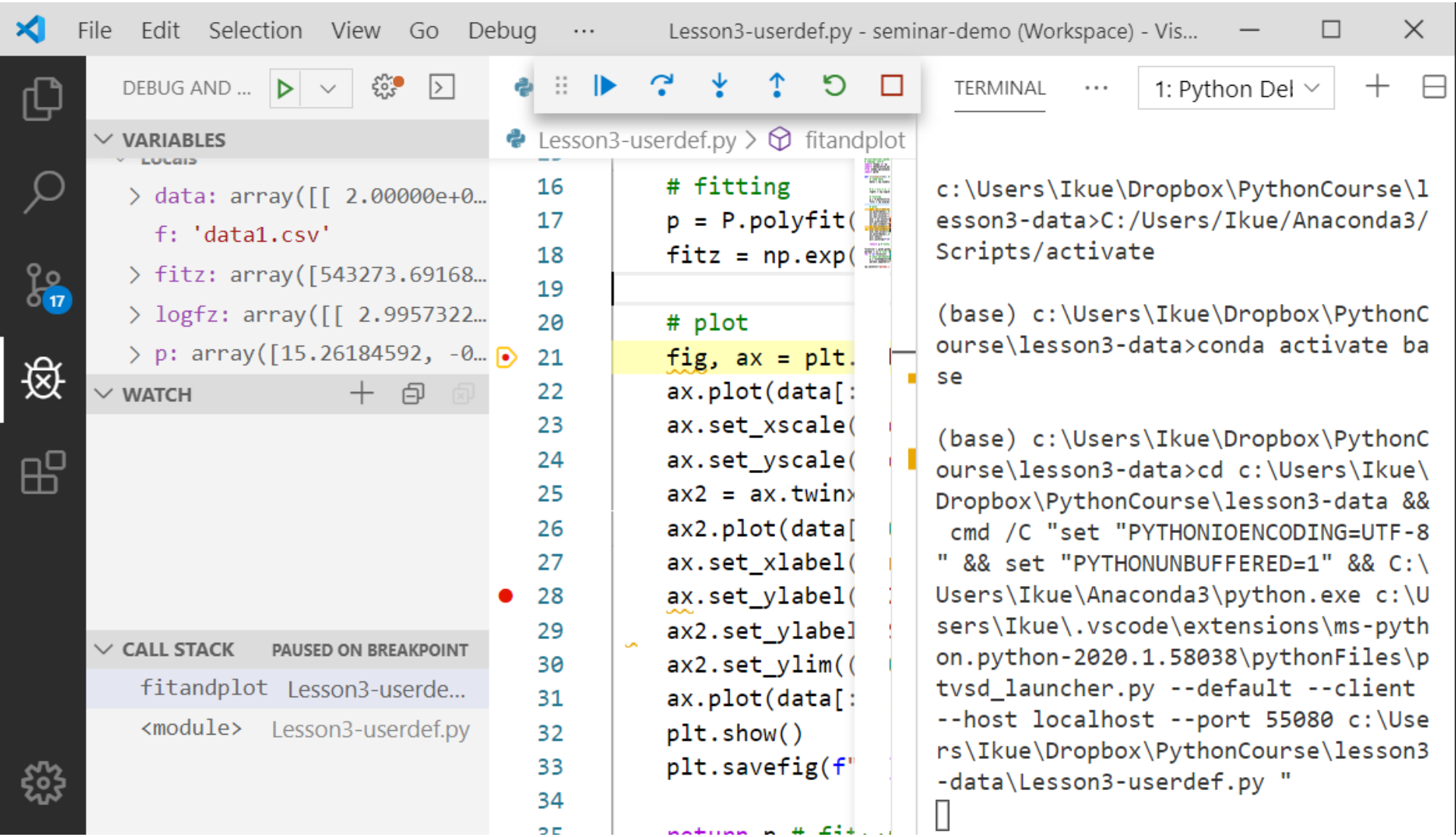
Debugging


File Edit Selection View Go Debug ···
Lesson3-userdef.py - seminar-demo (Workspace) - Vis...
DEBUG AND RUN: START
Debug with Python
Run with Python
To futher configure Debug and Run create a launch.json file.
Lesson3-userdef.py
lesson3-data > Lesson3-userdef.py > params
#!/usr/bin/env python
# coding: utf-8
import numpy as np
import matplotlib.pyplot as plt
from numpy.polynomial import polynomial as P
import glob
def fitandplot(f): # f for input file name
# read data
data = np.loadtxt(f, delimiter="\t",
usecols=[0,1,2])
# Z = 1/j w C, log for Z and f for polynomial fitting
logfz = np.log(data[:,0:2])
# fitting
p = P.polyfit(logfz[:,0], logfz[:,1], 1)
fitz = np.exp(p[0] + p[1] * logfz[:,0])
# plot

Breakpoints



Run


File Edit Selection View Go Debug ···
Lesson3-userdef.py - seminar-demo (Workspace) - Vis...
DEBUG AND ...
VARIABLES
data: array([[2.00000e+0...
f: 'data1.csv'
fitz: array([543273.69168...
logfz: array([[2.9957322...
p: array([15.26184592, -0...
WATCH
CALL STACK PAUSED ON BREAKPOINT
fitandplot Lesson3-userde...
<module> Lesson3-userdef.py
Lesson3-userdef.py > fitandplot
16 # fitting
17 p = P.polyfit(
18 fitz = np.exp(
19
20 # plot
21 fig, ax = plt.
22 ax.plot(data[:
23 ax.set_xscale(
24 ax.set_yscale(
25 ax2 = ax.twinx
26 ax2.plot(data[
27 ax.set_xlabel(
28 ax.set_ylabel(
29 ax2.set_ylabel
30 ax2.set_ylim((
31 ax.plot(data[:
32 plt.show()
33 plt.savefig(f'
34
TERMINAL
1: Python Del
c:\Users\Ikue\Dropbox\PythonCourse\lesson3-data>C:/Users/Ikue/Anaconda3/Scripts/activate
(base) c:\Users\Ikue\Dropbox\PythonCourse\lesson3-data>conda activate base
(base) c:\Users\Ikue\Dropbox\PythonCourse\lesson3-data>cd c:\Users\Ikue\Dropbox\PythonCourse\lesson3-data && cmd /C "set "PYTHONIOENCODING=UTF-8" && set "PYTHONUNBUFFERED=1" && C:\Users\Ikue\Anaconda3\python.exe c:\Users\Ikue\.vscode\extensions\ms-python.python-2020.1.58038\pythonFiles\ptvsd_launcher.py --default --client --host localhost --port 55080 c:\Users\Ikue\Dropbox\PythonCourse\lesson3-data\Lesson3-userdef.py "

Exception handling

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Trusted | Python 3

In [35]:

```
num = [1, 2, 3, 0]
for n in num:
    print(n, 1/n)
print("process end")
```

```
1 1.0
2 0.5
3 0.3333333333333333


---------------------------------------
---------------------------------
ZeroDivisionError                         T
raceback (most recent call last)
<ipython-input-35-89a0c53ab2bc> in <module>
```

try and except

In [51]:

```
for n in num:
    try:
        print(n, 1/n)
    except Exception as e:
        print(f"there's an error: {e}")
print("process end")
```

```
1 1.0
2 0.5
3 0.3333333333333333
there's an error: division by zero
process end
```

Exercise 1

Code | Issues 0 | Pull requests 0 | Actions | Projects 0 | Wiki | Security | Insights | Settings

Branch: master ▾ CodingSeminarCMBR / exercises_and_model_answers / Lesson3_Exercise1.ipynb Find file Copy path

ikuehirata Lesson 3 added cda8712 1 hour ago

1 contributor

62 lines (62 sloc) | 2.15 KB Raw Blame History

Lesson 3 - Exercise 1

1. Using the impedance measurement data `.csv` provided in lesson3-data in GitHub fit the values to the formula

$$Z = \frac{1}{j\omega C}$$

where $C = 2\pi f$, j is the imaginary number, and extract C value. The first column of the data is the frequency f, the second the impedance Z, the third the phase $\phi = \arg(Z)$. Plot the experimental value in Bode plot. Add the fit value of $|Z|$.
Hint: use the range range where the experimental fits the theoretical value.

2. The experimental value does not follow the theoretical value explicitly because of some parasite resistances. Capacitor model can be explained as

$$Z = \frac{1}{j\omega C} \text{ !/mkern-5mu/! } R_p + R_s$$

where R_p is parallel resistance, R_s series resistance, operator !/mkern-5mu/!

$$a \text{ !/mkern-5mu/! } b = \frac{1}{\frac{1}{a} + \frac{1}{b}}$$

, meaning a parallel circuit. Plot the experimental value in Bode plot. Add the fit value of $|Z|$.
Hint: if R_p is huge, it can be ignored.

3. Plot C vs file name to visually compare the extracted C value.

Exercise 2

Plan, code, and run your own program for your own experiments.