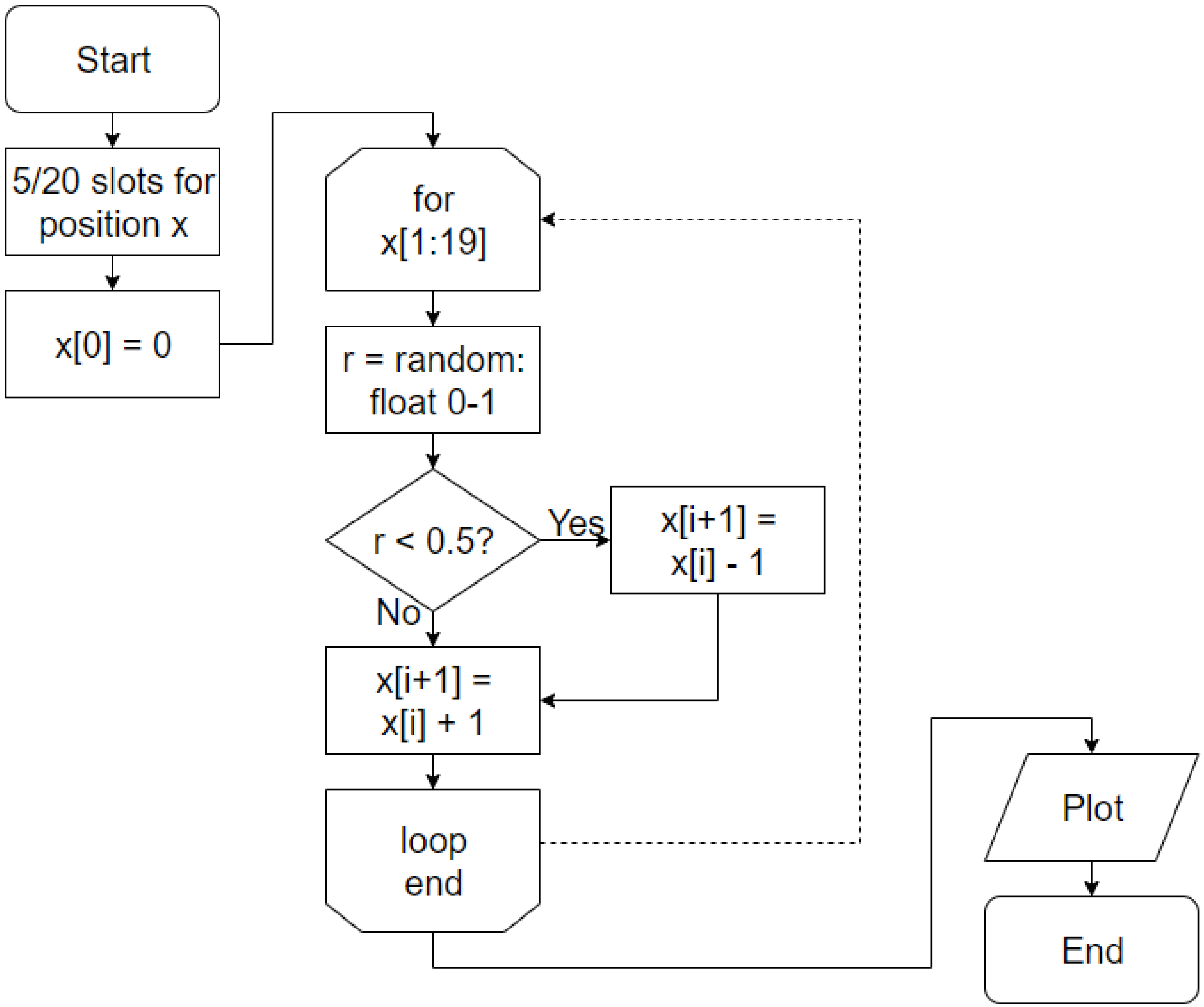
Coding seminar

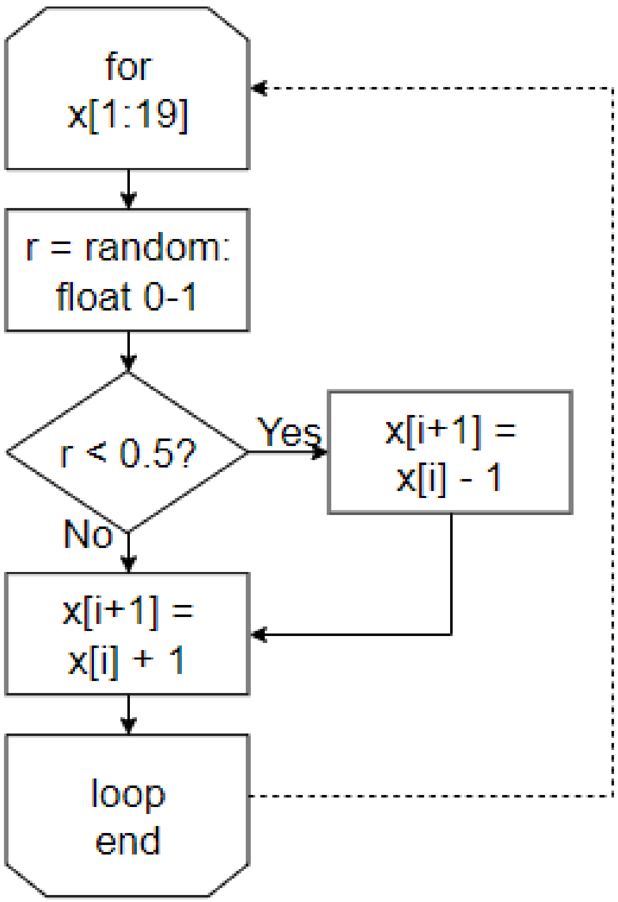
Lesson 3: Handling real-world data

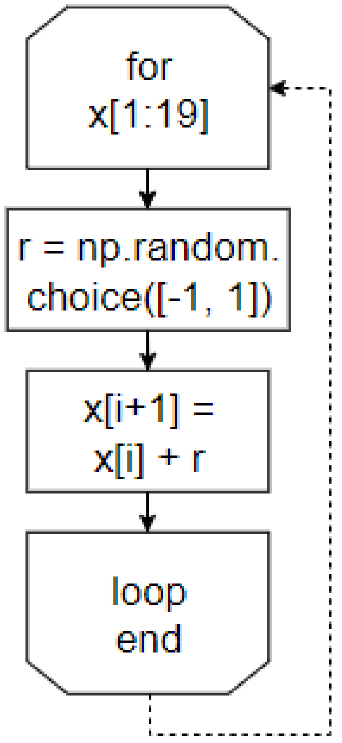
Ikue Hirata, PhD

Exercise model answer: random walk



Make it simple





2-D random walk

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Trusted | Python 3

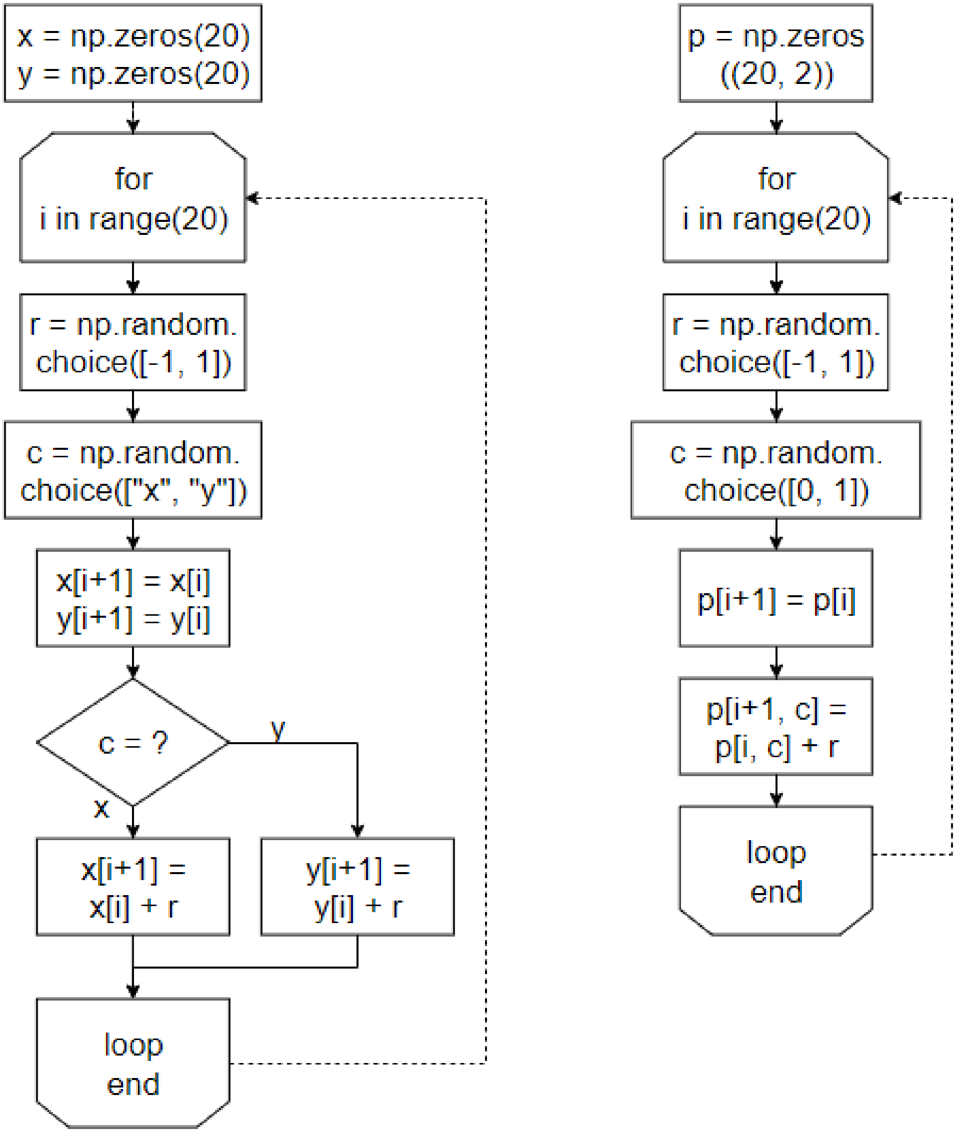
In [2]:

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

p[:,0] p[:,1]

```
[[0. 0.]
 [0. 0.]
 [0. 0.]
 [0. 0.]
 [0. 0.]
 [0. 0.]
 [0. 0.]
```

2-D random walk



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Debugger/debugging

UNIX-based commands for mass-process

Extensions ready?

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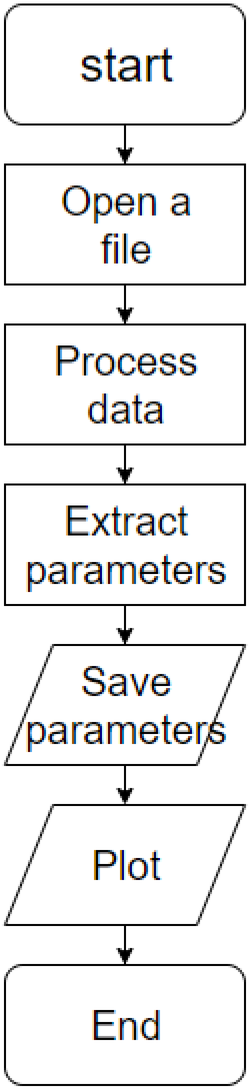
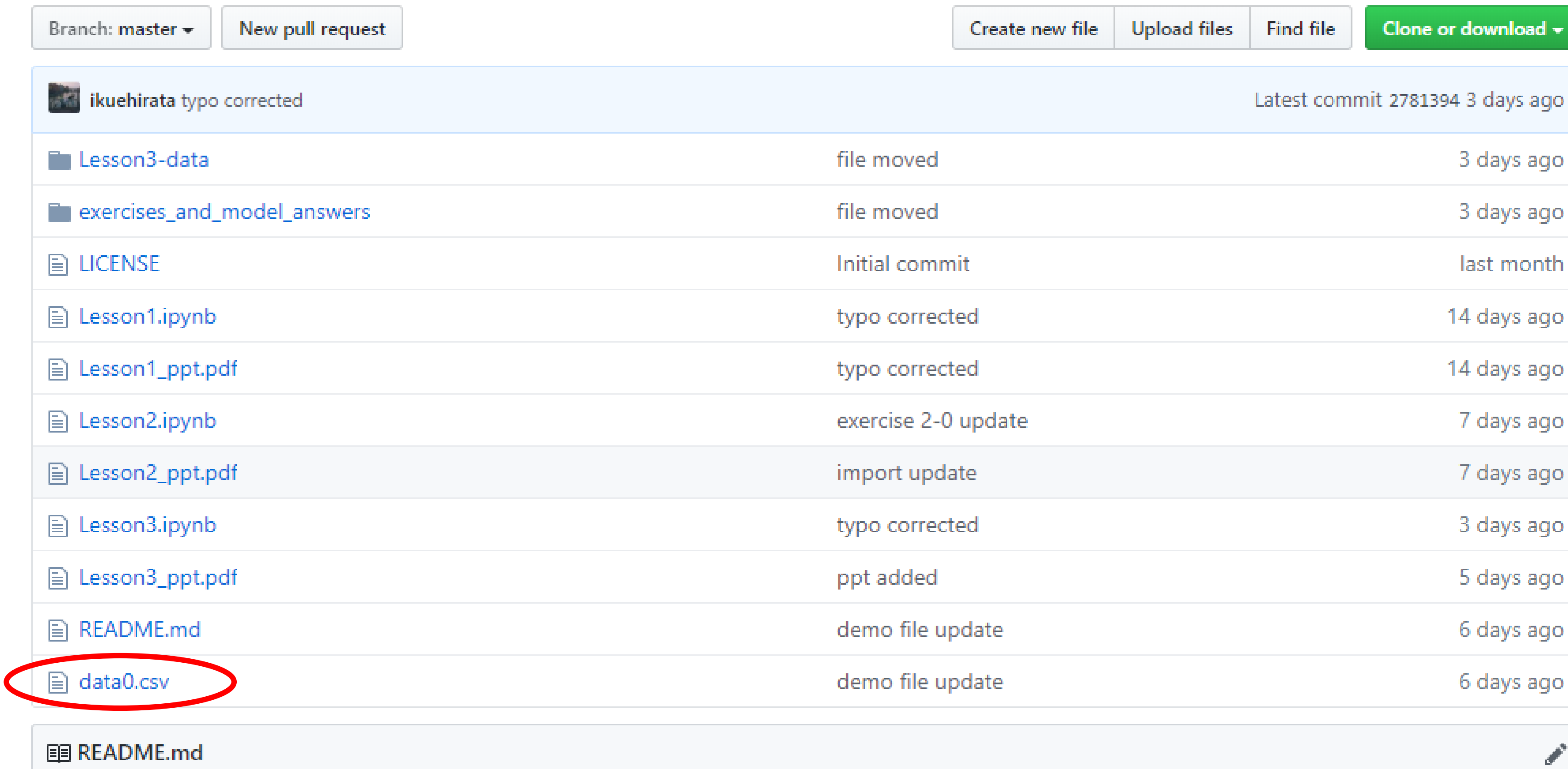
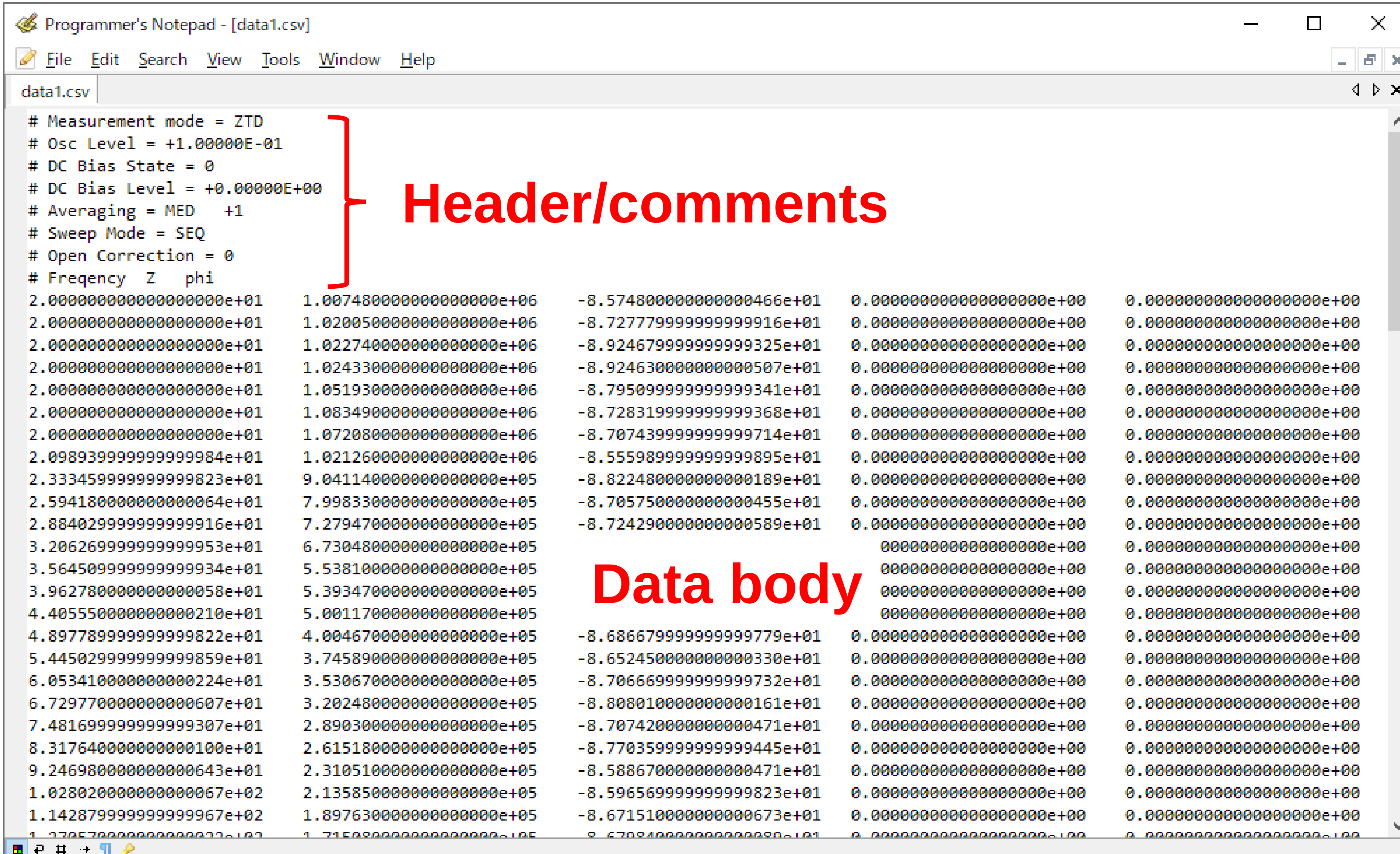
Data analysis process



Download demo files



Sample data



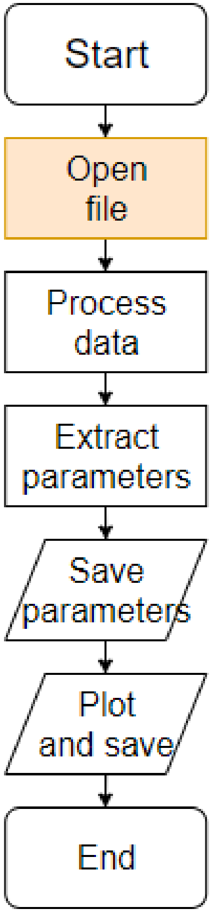

```
# Measurement mode = ZTD
# Osc Level = +1.00000E-01
# DC Bias State = 0
# DC Bias Level = +0.00000E+00
# Averaging = MED    +1
# Sweep Mode = SEQ
# Open Correction = 0
# Freqency  Z   phi
2.000000000000000000e+01    1.007480000000000000e+06    -8.574800000000000466e+01    0.000000000000000000e+00    0.000000000000000000e+00
2.000000000000000000e+01    1.020050000000000000e+06    -8.727779999999999916e+01    0.000000000000000000e+00    0.000000000000000000e+00
2.000000000000000000e+01    1.022740000000000000e+06    -8.924679999999999325e+01    0.000000000000000000e+00    0.000000000000000000e+00
2.000000000000000000e+01    1.024330000000000000e+06    -8.924630000000000507e+01    0.000000000000000000e+00    0.000000000000000000e+00
2.000000000000000000e+01    1.051930000000000000e+06    -8.795099999999999341e+01    0.000000000000000000e+00    0.000000000000000000e+00
2.000000000000000000e+01    1.083490000000000000e+06    -8.728319999999999368e+01    0.000000000000000000e+00    0.000000000000000000e+00
2.000000000000000000e+01    1.072080000000000000e+06    -8.707439999999999714e+01    0.000000000000000000e+00    0.000000000000000000e+00
2.098939999999999984e+01    1.021260000000000000e+06    -8.555989999999999895e+01    0.000000000000000000e+00    0.000000000000000000e+00
2.333459999999999823e+01    9.041140000000000000e+05    -8.822480000000000189e+01    0.000000000000000000e+00    0.000000000000000000e+00
2.594180000000000064e+01    7.998330000000000000e+05    -8.705750000000000455e+01    0.000000000000000000e+00    0.000000000000000000e+00
2.884029999999999916e+01    7.279470000000000000e+05    -8.724290000000000589e+01    0.000000000000000000e+00    0.000000000000000000e+00
3.206269999999999953e+01    6.730480000000000000e+05                                    0000000000000000e+00    0.000000000000000000e+00
3.564509999999999934e+01    5.538100000000000000e+05                                    0000000000000000e+00    0.000000000000000000e+00
3.962780000000000058e+01    5.393470000000000000e+05                                    0000000000000000e+00    0.000000000000000000e+00
4.405550000000000210e+01    5.001170000000000000e+05                                    0000000000000000e+00    0.000000000000000000e+00
4.897789999999999822e+01    4.004670000000000000e+05    -8.686679999999999779e+01    0.000000000000000000e+00    0.000000000000000000e+00
5.445029999999999859e+01    3.745890000000000000e+05    -8.652450000000000330e+01    0.000000000000000000e+00    0.000000000000000000e+00
6.053410000000000224e+01    3.530670000000000000e+05    -8.706669999999999732e+01    0.000000000000000000e+00    0.000000000000000000e+00
6.729770000000000607e+01    3.202480000000000000e+05    -8.808010000000000161e+01    0.000000000000000000e+00    0.000000000000000000e+00
7.481699999999999307e+01    2.890300000000000000e+05    -8.707420000000000471e+01    0.000000000000000000e+00    0.000000000000000000e+00
8.317640000000000100e+01    2.615180000000000000e+05    -8.770359999999999445e+01    0.000000000000000000e+00    0.000000000000000000e+00
9.246980000000000643e+01    2.310510000000000000e+05    -8.588670000000000471e+01    0.000000000000000000e+00    0.000000000000000000e+00
1.028020000000000067e+02    2.135850000000000000e+05    -8.596569999999999823e+01    0.000000000000000000e+00    0.000000000000000000e+00
1.142879999999999967e+02    1.897630000000000000e+05    -8.671510000000000673e+01    0.000000000000000000e+00    0.000000000000000000e+00
```

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



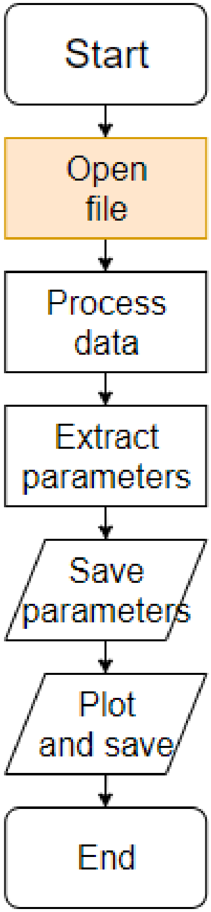
Read data into array

File Edit View Insert Cell Kernel Navigate Widgets Help

In [14]:

```python
import numpy as np
data = np.loadtxt("data0.csv", delimiter='\t')
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]
```



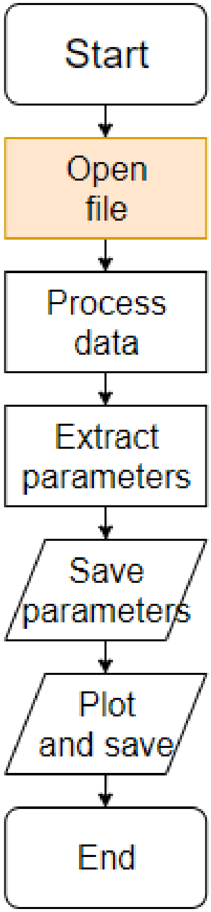
Read data into array

File Edit View Insert Cell Kernel Navigate Widgets Help

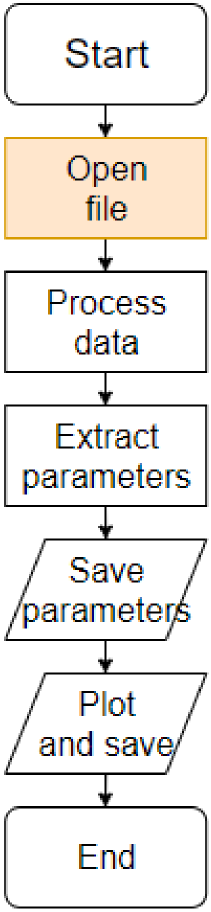
In [2]:

```python
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]
 [ 2.88403e+01  7.27947e+05 -8.72429e+01]
```



For more options…



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Scipy.org | Docs | NumPy v1.17 Manual | NumPy Reference | Routines | Array creation routines | index | next | previous

numpy.loadtxt

numpy.loadtxt(*fname, dtype=<class 'float'>, comments='#', delimiter=None, converters=None, skiprows=0, usecols=None, unpack=False, ndmin=0, encoding='bytes', max_rows=None*) [source]

Load data from a text file.

Each row in the text file must have the same number of values.

Parameters:

fname : *file, str, or pathlib.Path*

File, filename, or generator to read. If the filename extension is `.gz` or `.bz2`, the file is first decompressed. Note that generators should return byte strings for Python 3k.

dtype : *data-type, optional*

Data-type of the resulting array; default: float. If this is a structured data-type, the resulting array will be 1-dimensional, and each row will be interpreted as an element of the array. In this case, the number of columns used must match the number of fields in the data-type.

comments : *str or sequence of str, optional*

The characters or list of characters used to indicate the start of a comment. None implies no comments. For backwards compatibility, byte strings will be decoded as 'latin1'. The default is '#'.

delimiter : *str, optional*

The string used to separate values. For backwards compatibility, byte strings will be decoded as 'latin1'. The default is whitespace.

converters : *dict, optional*

Previous topic

numpy.fromstring

Next topic

numpy.core.records.array

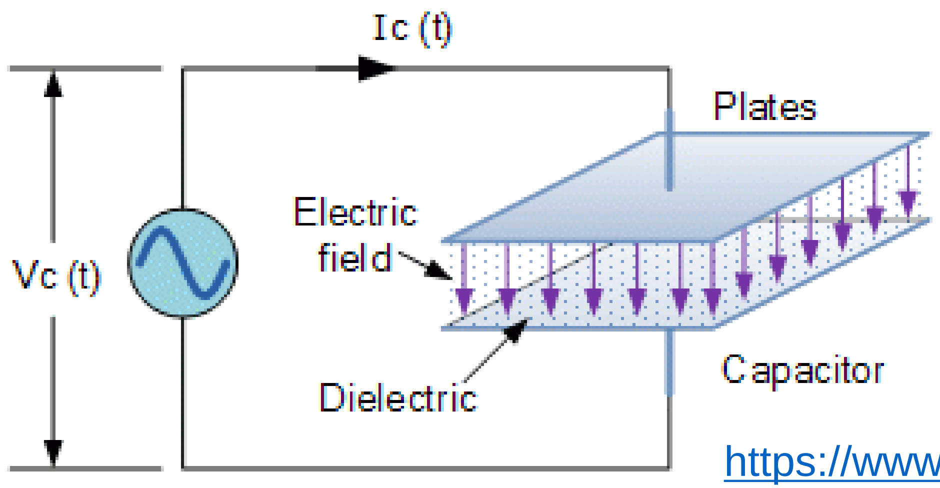
Quick search

search

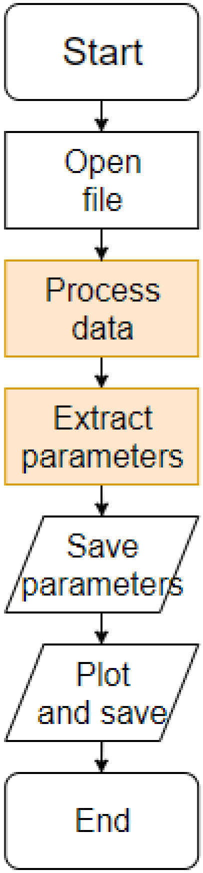
https://docs.scipy.org/doc/numpy/reference/generated/numpy.loadtxt.html

What is this?

Complex impedance of a capacitor



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



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

We want to get this value

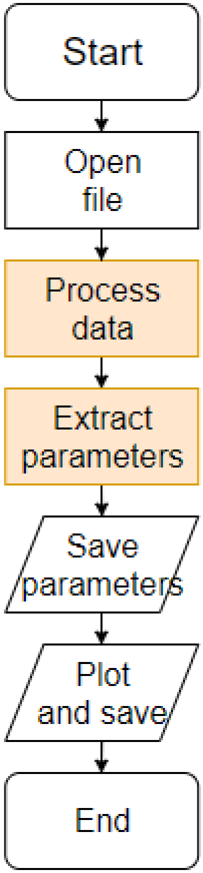
j as imaginary number

Which value is which?

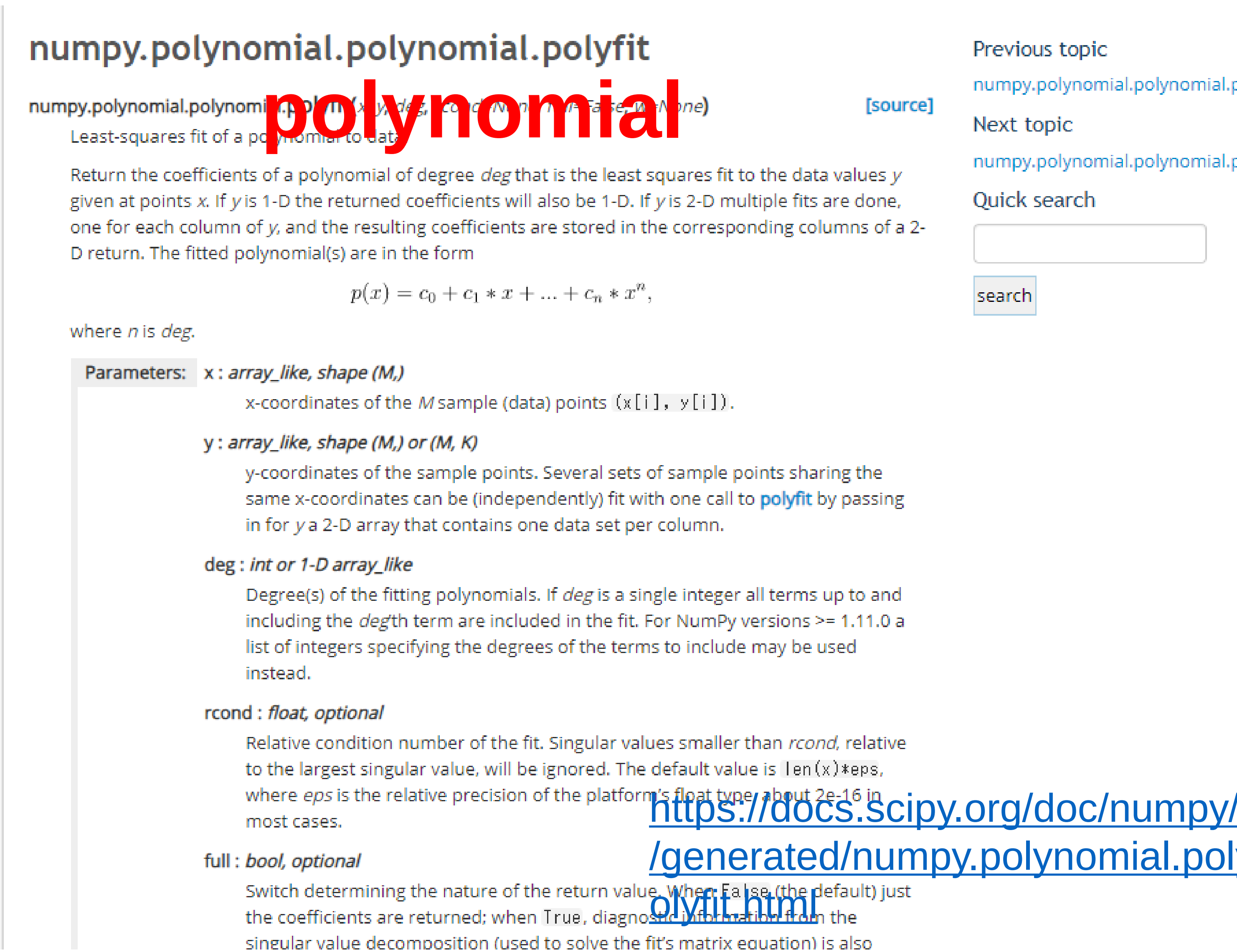
```
3 print(data)
```

```
              f              Z            ϕ
[[ 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]
 [ 2.88403e+01  7.27947e+05 -8.72439e+01]
```

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



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])`.

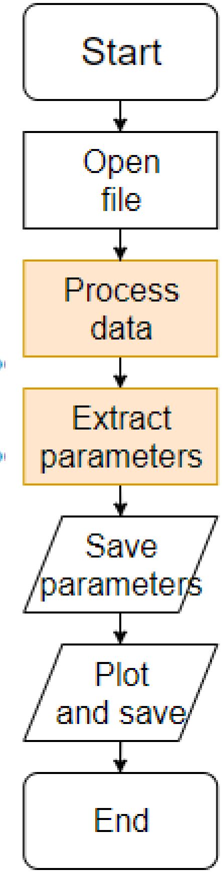
y : *array_like, shape (M,) or (M, K)*
y-coordinates of the sample points. Several sets of sample points sharing the same x-coordinates can be (independently) fit with one call to polyfit by passing in for *y* a 2-D array that contains one data set per column.

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



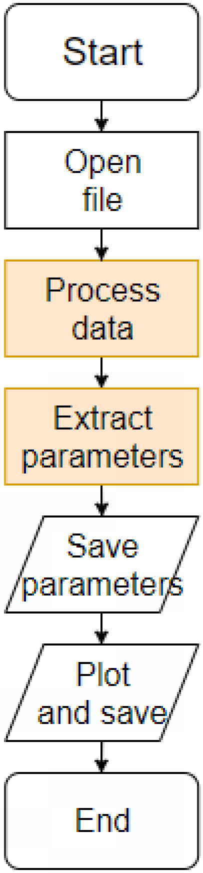
https://docs.scipy.org/doc/numpy/reference/generated/numpy.polynomial.polynomial.polyfit.html

Small trick

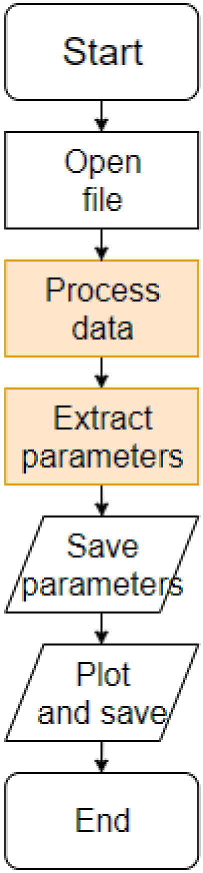
$$Z = \frac{1}{j \cdot 2\pi f C}$$

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

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



Fitting 1 – Exercise 0-1



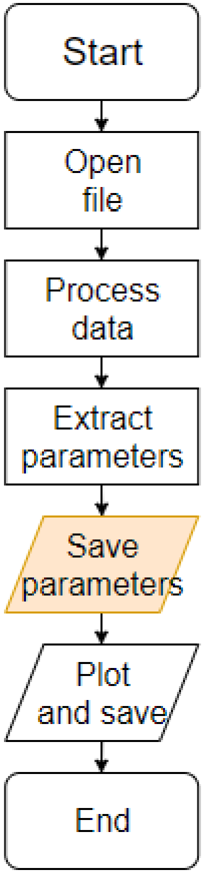
$$y = -0.96x + 16.6$$

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]
```

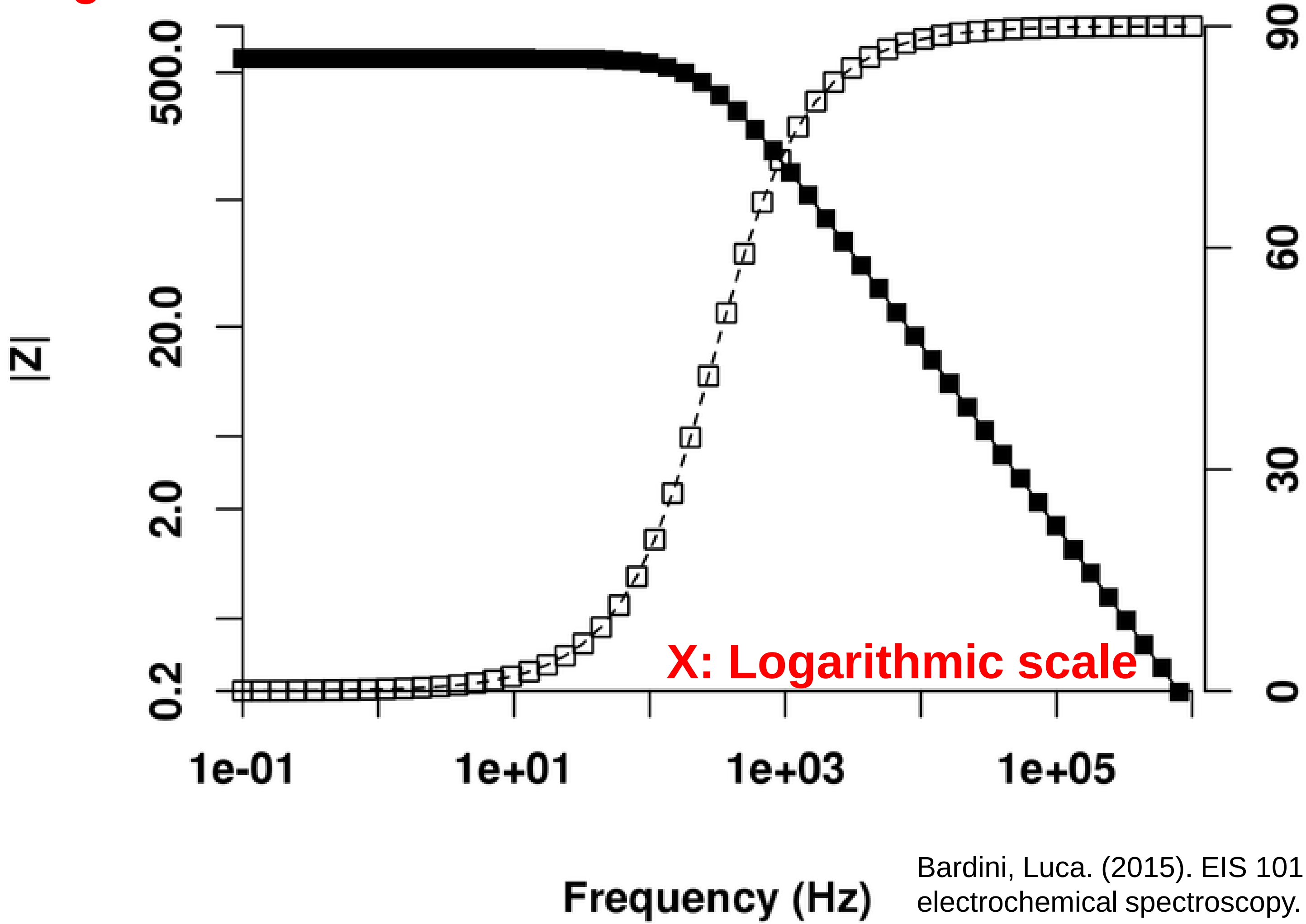
```
In [31]:
np.savetxt("parameters.csv", p, delimiter="\t")
```

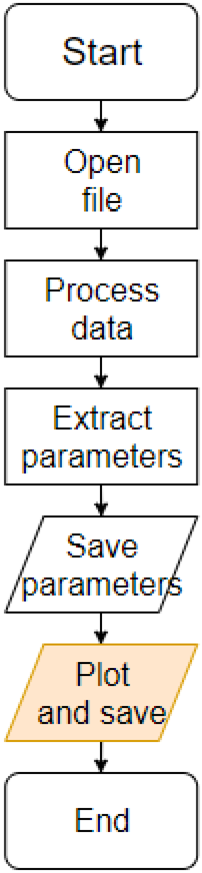


Bode plot

Y2: Linear scale – I prefer ϕ not inverted

Y1: Logarithmic scale

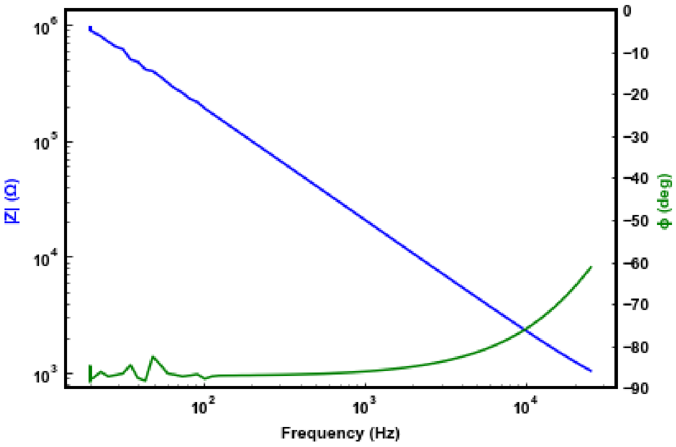


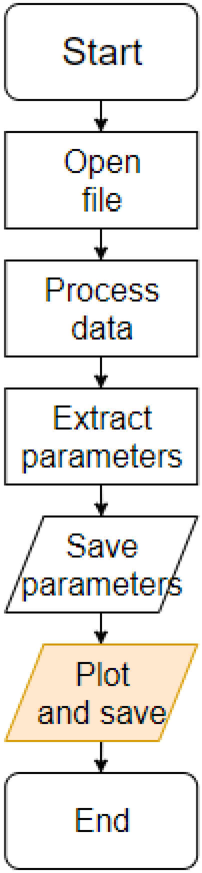


Bardini, Luca. (2015). EIS 101, an introduction to electrochemical spectroscopy. What was a website is now available as a self-contained PDF.

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()
```

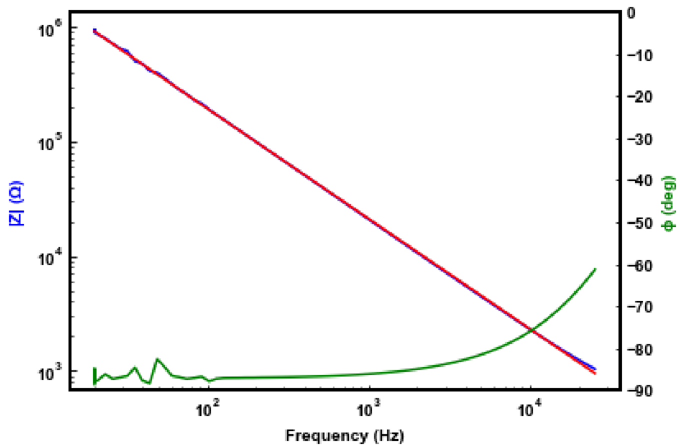




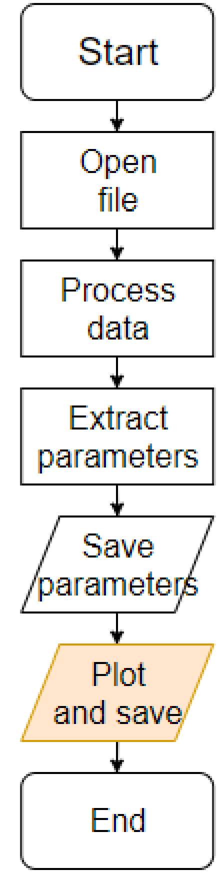
Add fit line

File Edit View Insert Cell Kernel Navigate Widgets Help

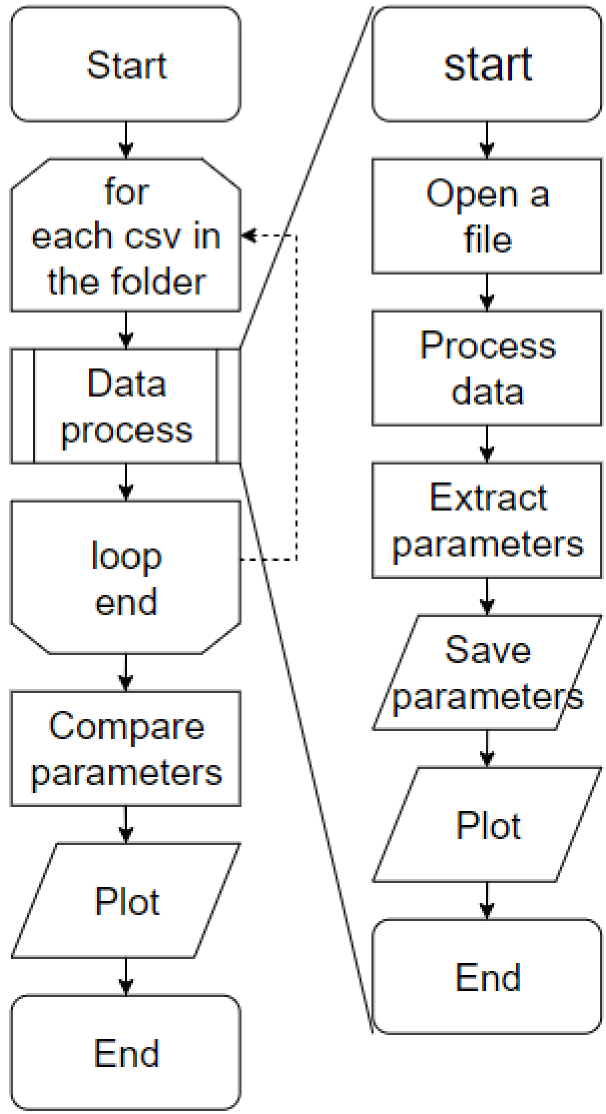
```
fitz = np.exp(p[0] + p[1] * logf)
ax.plot(data[:,0], fitz, color="r")
plt.show()
plt.savefig("impedancefit.png")
```




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

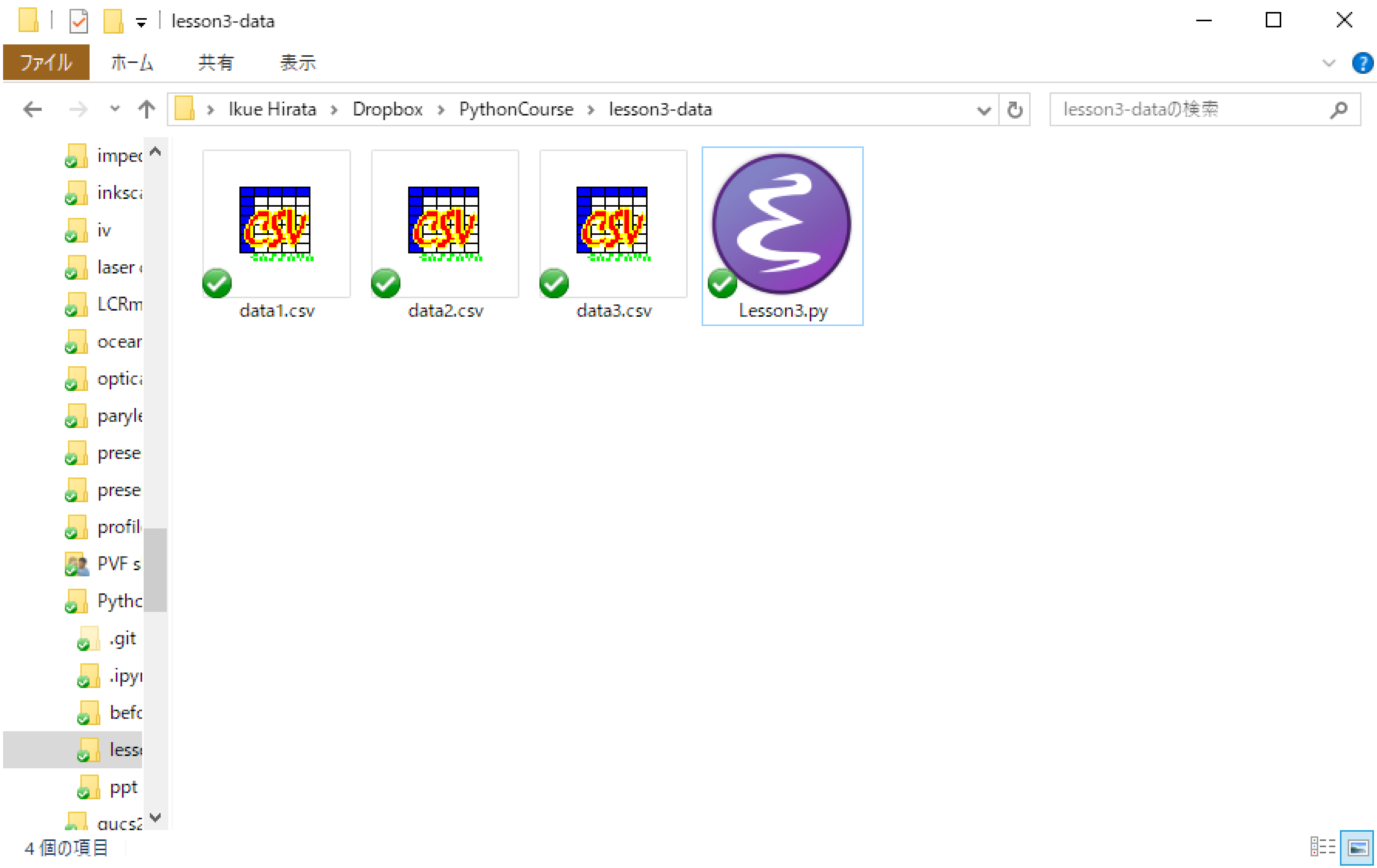


That’s not all!

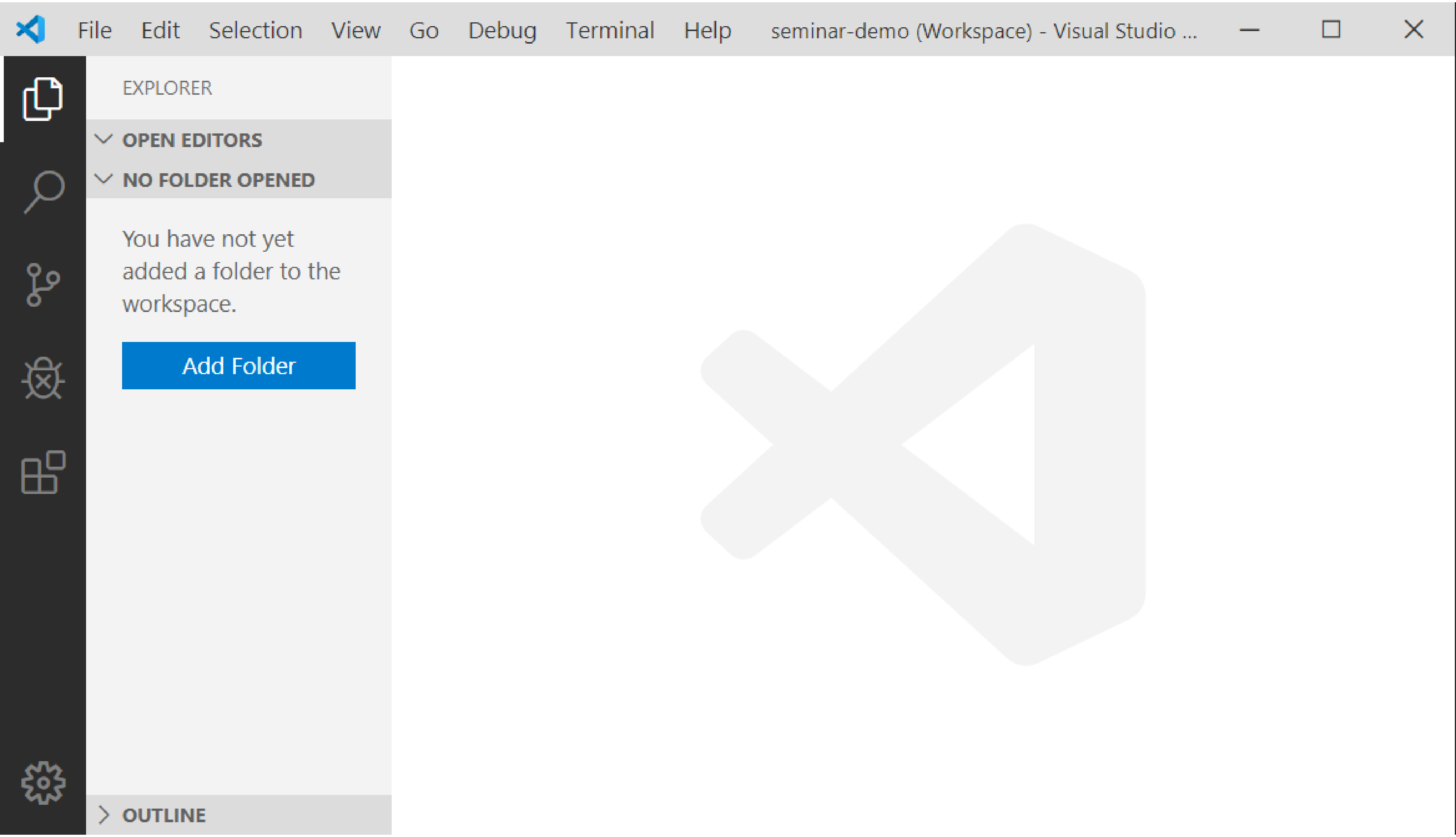


Download the code

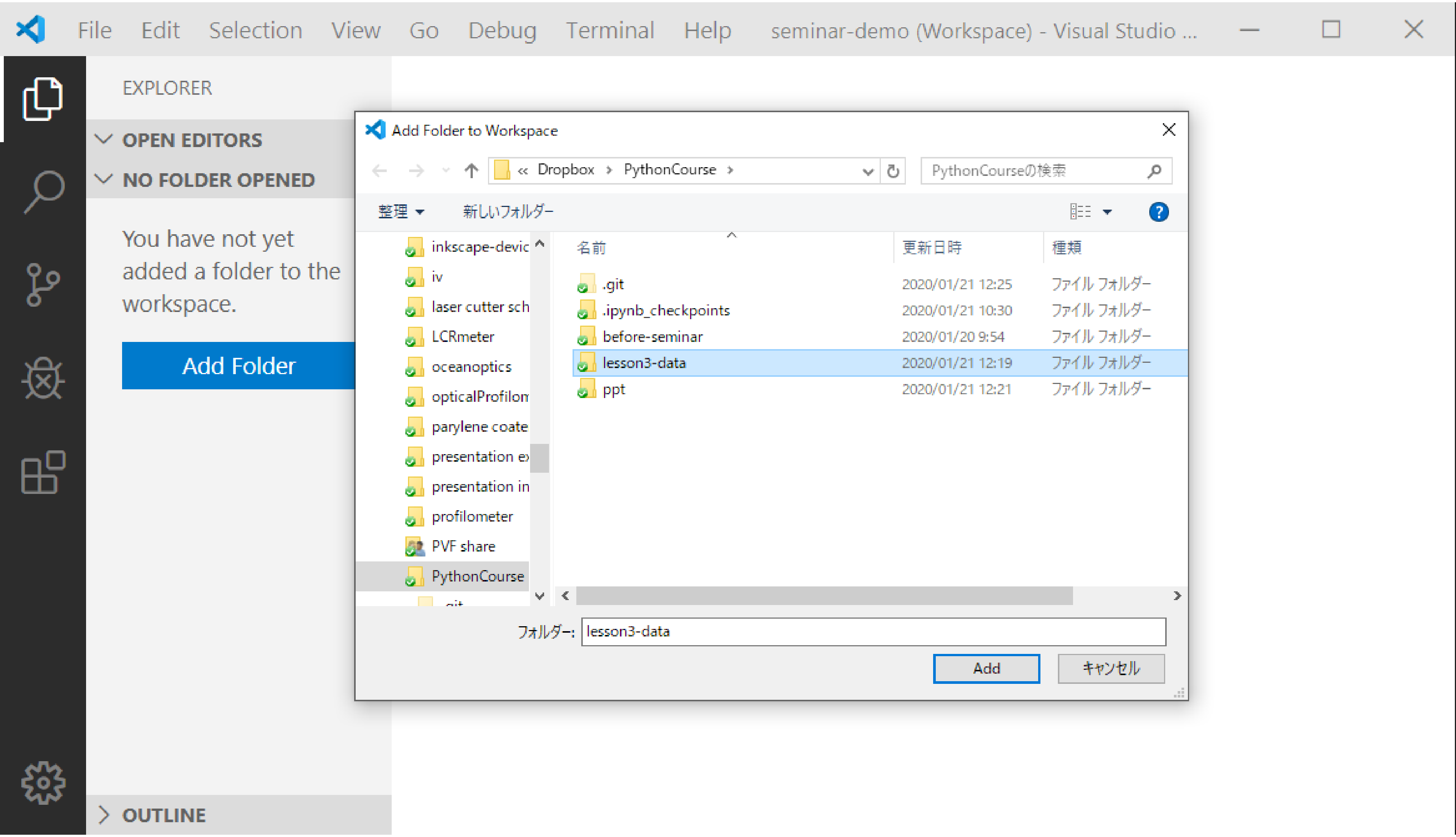
Store it where other data are



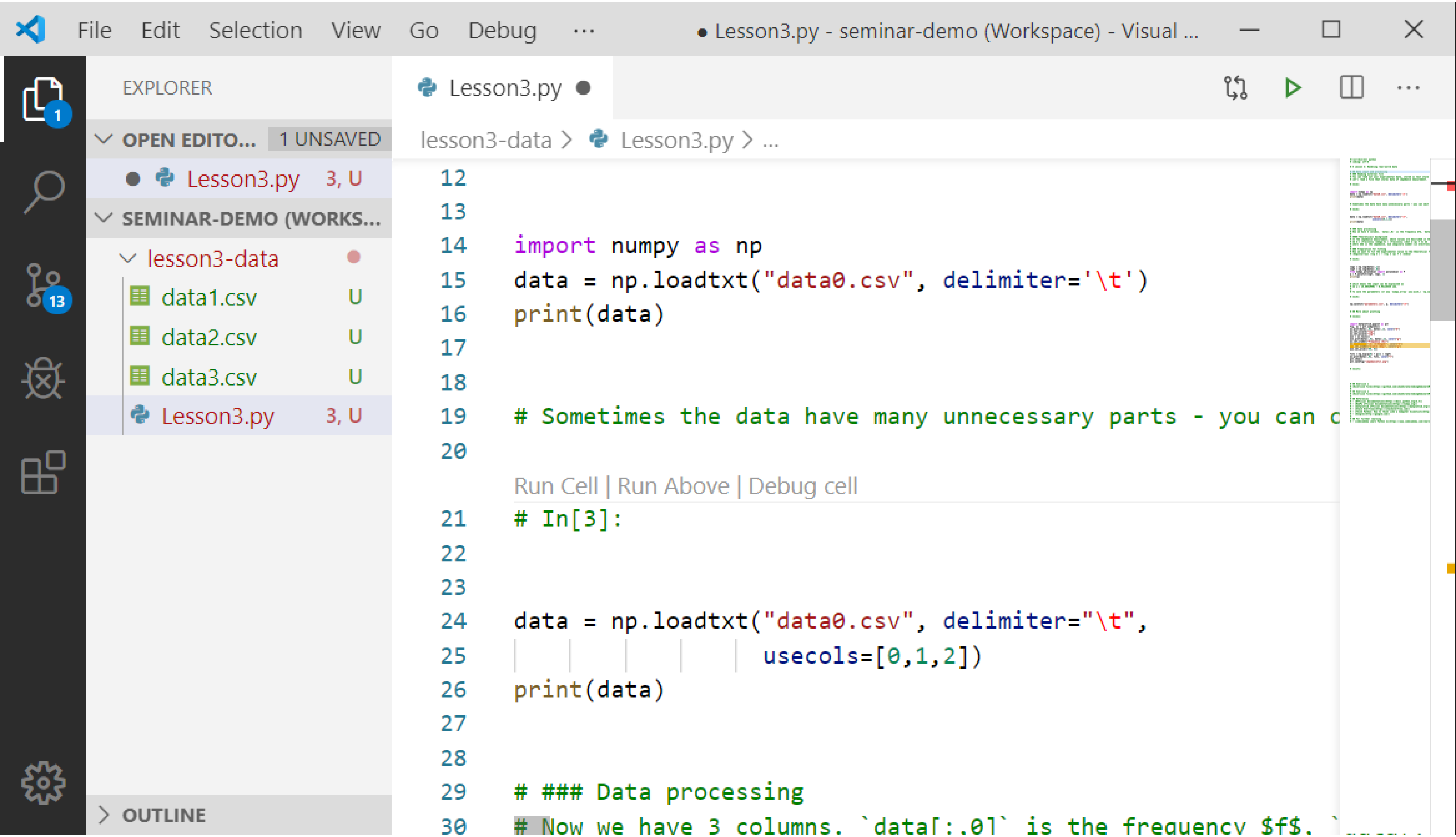
Open Visual Studio Code



Add folder – workspace



Open your code



Code aesthetics – readability

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

Lesson3.py

lesson3-data > Lesson3.py > ...

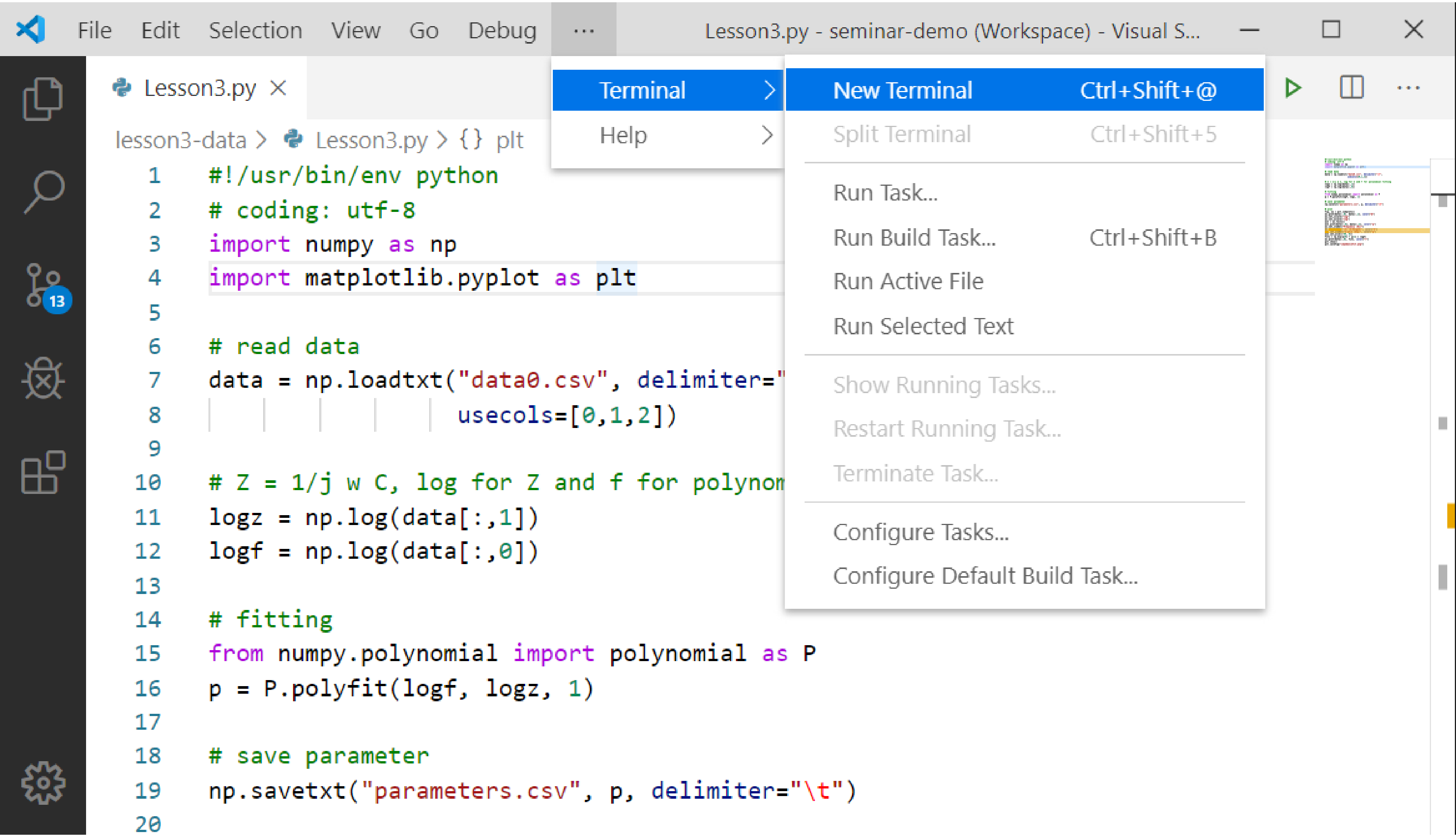
```python
#!/usr/bin/env python
# coding: utf-8
import numpy as np

# read data
data = np.loadtxt("data0.csv", delimiter="\t",
                  usecols=[0,1,2])

# Z = 1/j w C, log for Z and f for polynomial fitting
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="\t")

import matplotlib.pyplot as plt
```

Leave these 2 lines

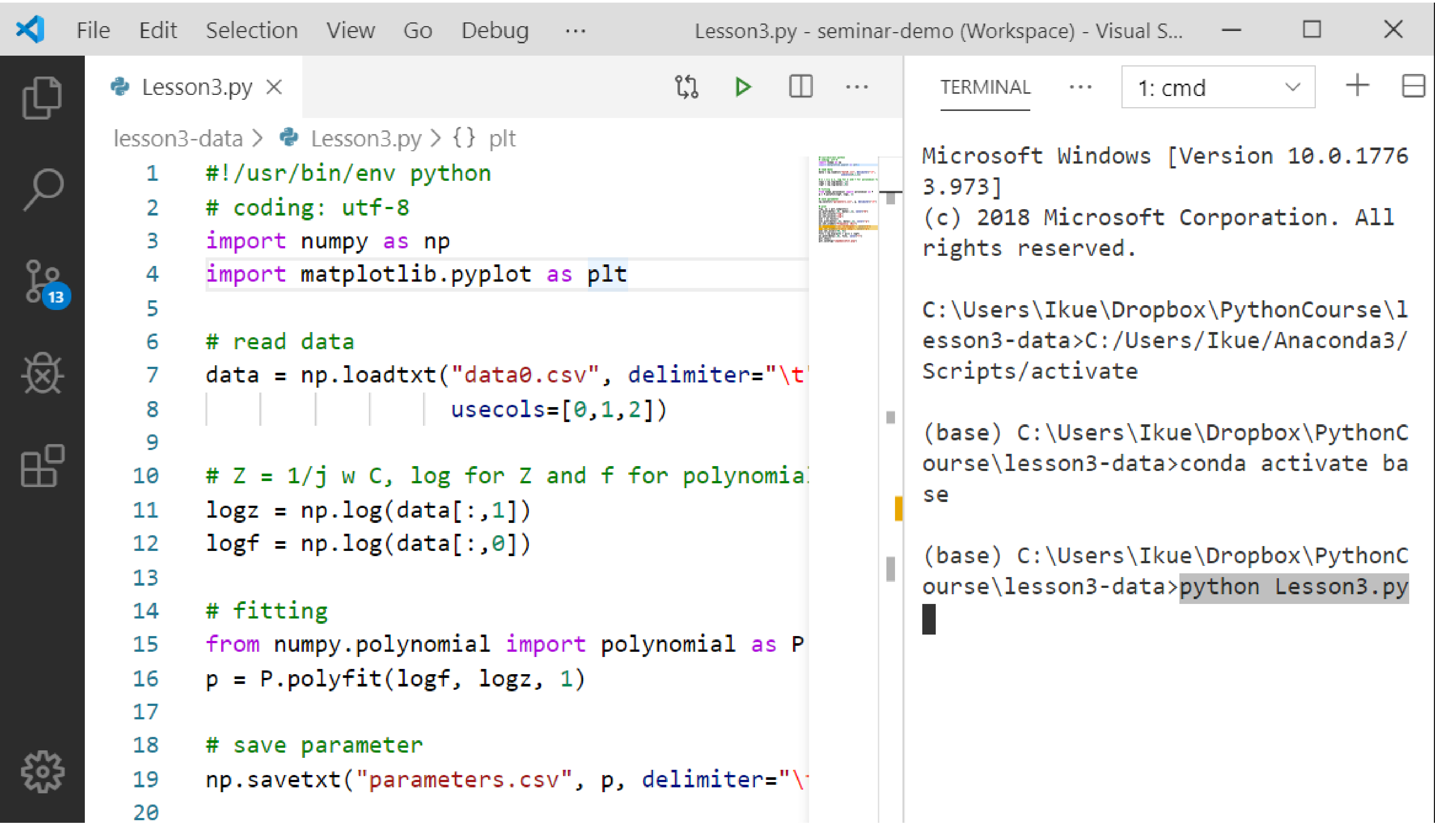
Comments for readability

No extra spaces
No too much/less empty lines

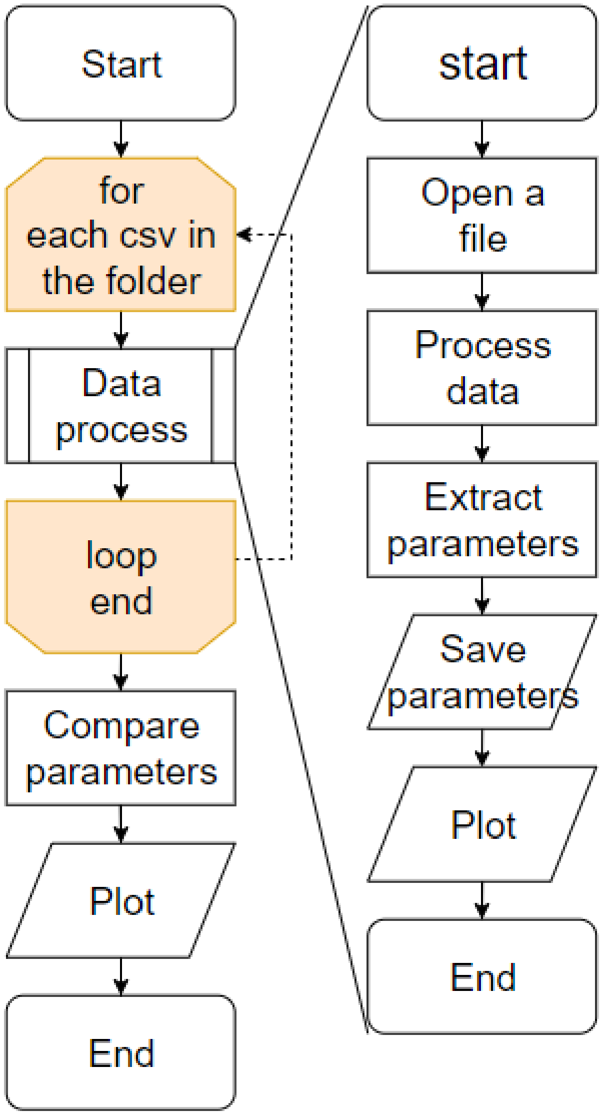
Open Terminal



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 10.0.17763.973]
(c) 2018 Microsoft Corporation. All rights reserved.
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>python Lesson3.py

Getting multiple files



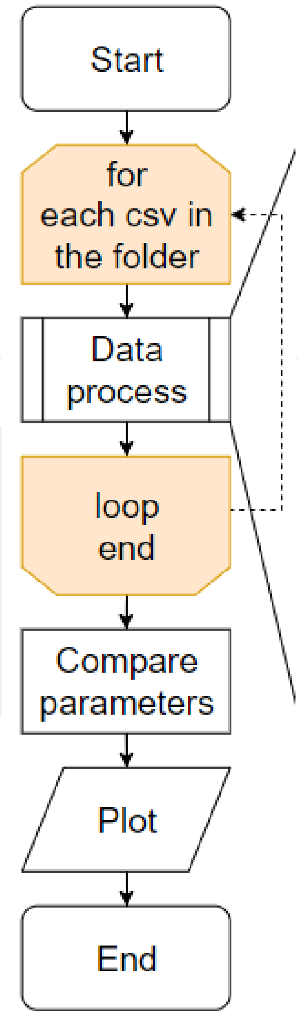
glob

File Edit View Insert Cell Kernel Navigate Widgets Help

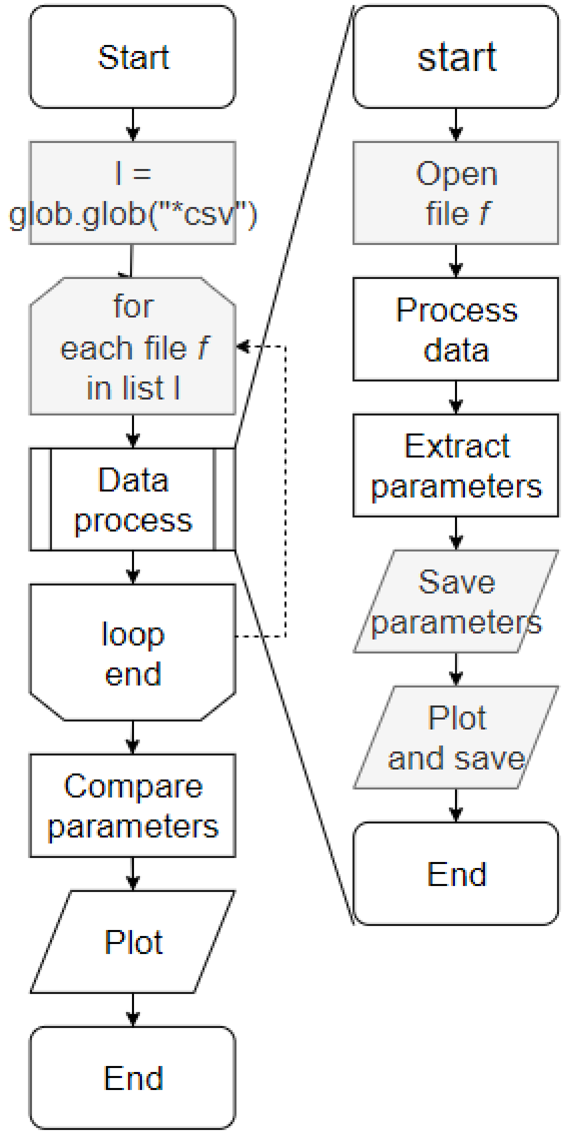
In [1]:

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

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

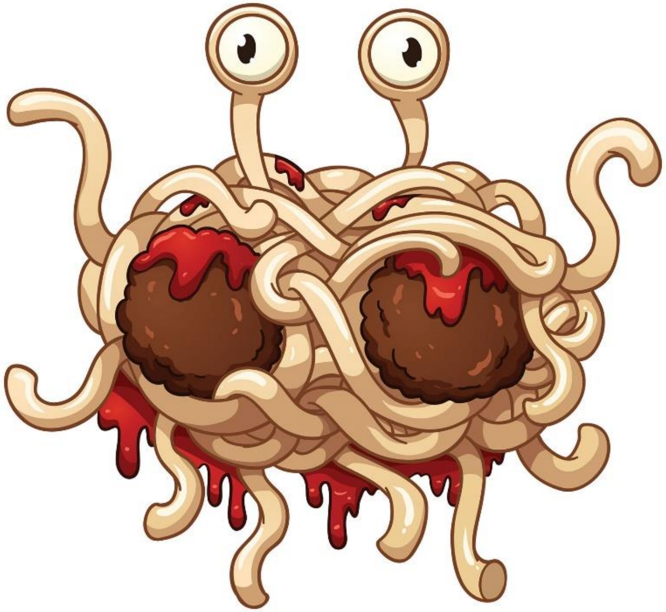


Pay attention to save file name

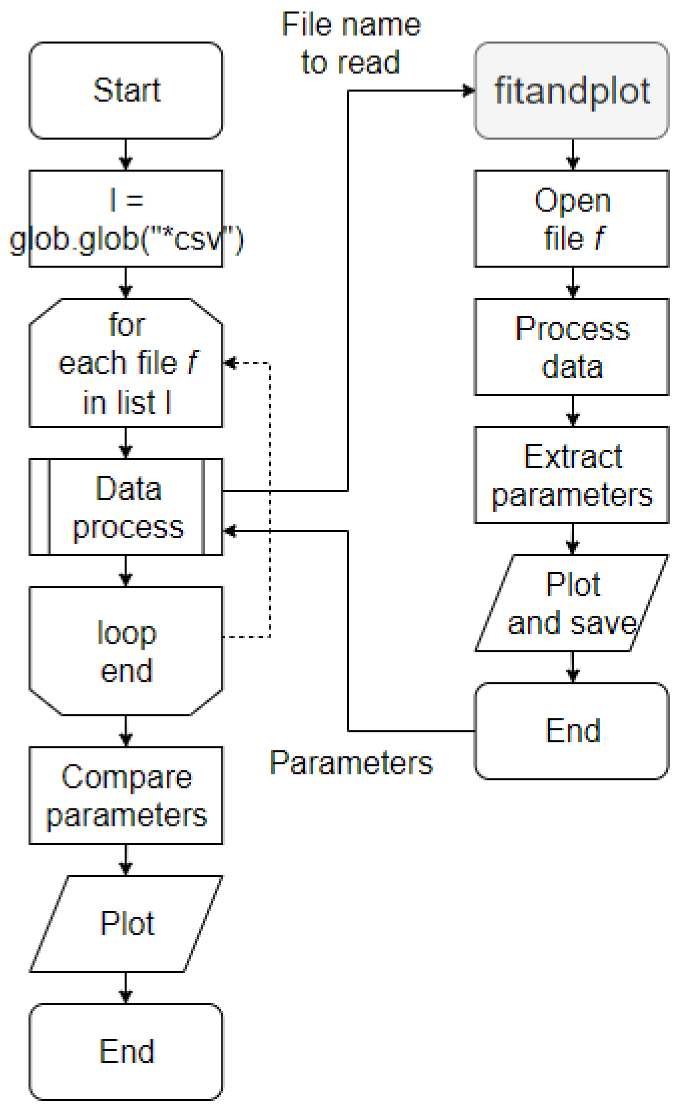


“Spaghetti” code

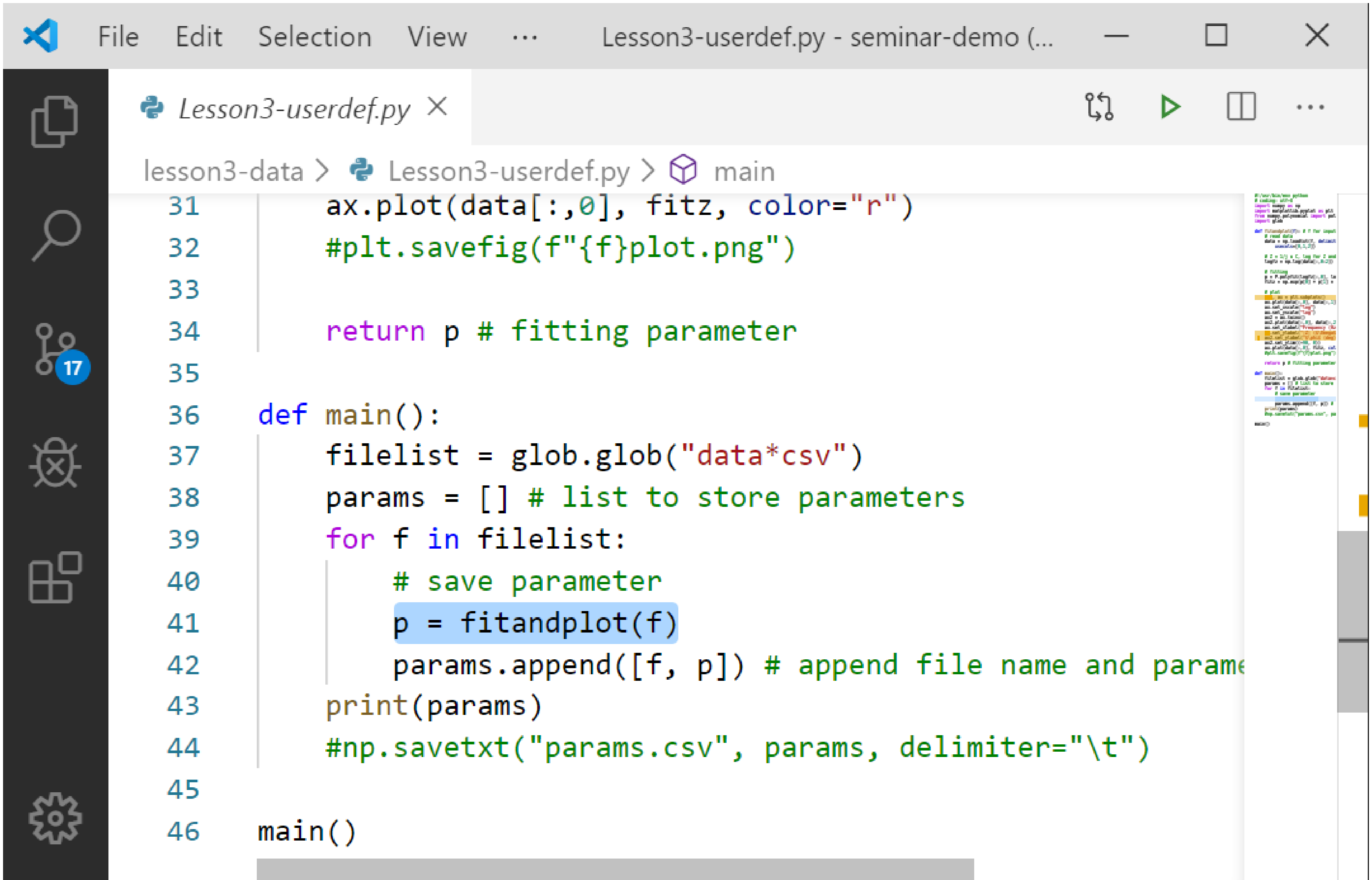
```python
import matplotlib.pyplot as plt
import glob

filelist = glob.glob("*csv")
params = [] # list to store parameters
for f in filelist:
    # 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
    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(f"{f}.csv", p, delimiter="\t") # save file name using original file
    params.append([[f, p]]) # append file name and parameter in the storage

    # plot
    fig, ax = plt.subplots()
    ax.plot(data[:,0], data[:,1], color="b")
    ax.set_xscale("log")
    ax.set_yscale("log")
    ax2 = ax.twinx()
    ax2.plot(data[:,0], data[:,2], color="g")
    ax.set_xlabel("Frequency (Hz)")
    ax.set_ylabel("|Z| ($\Omega$)", color="b")
    ax2.set_ylabel("$\phi$ (deg)", color="g")
    ax2.set_ylim((-90, 0))
    fitz = np.exp(p[0] + p[1] * logf)
    ax.plot(data[:,0], fitz, color="r")
    plt.show()
    plt.savefig(f"{f}.png")
```



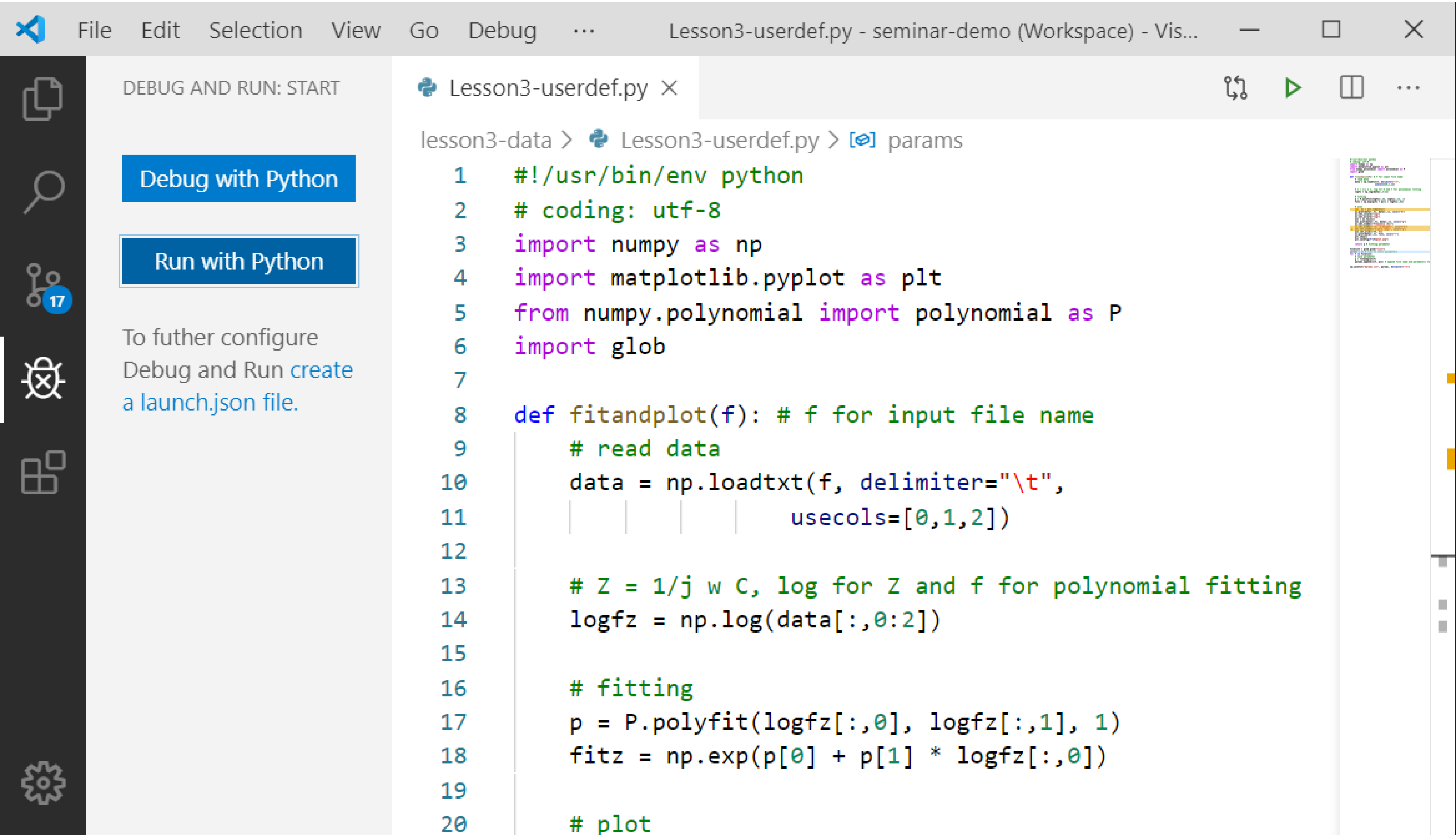
User defined function



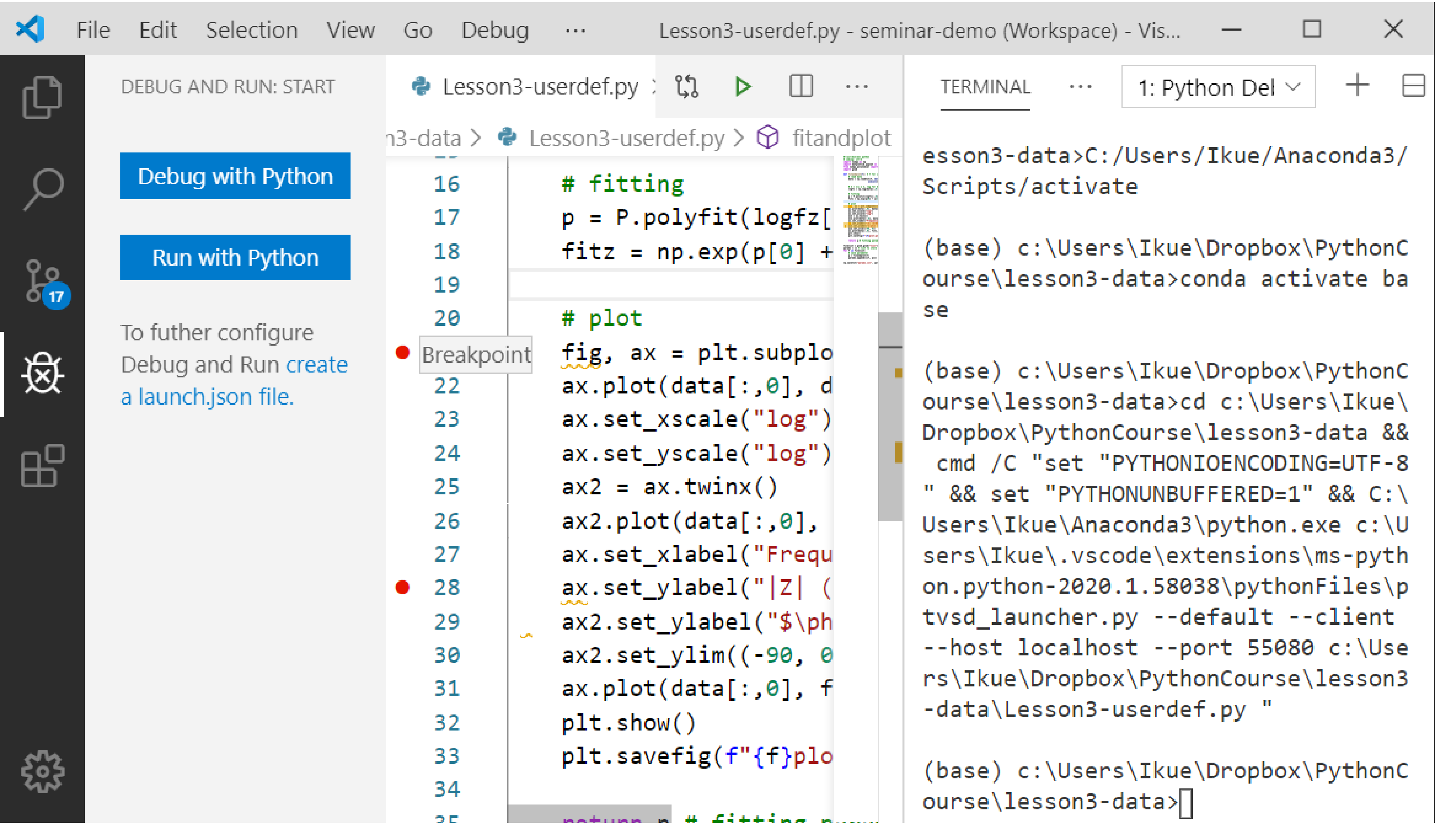
Using user defined function



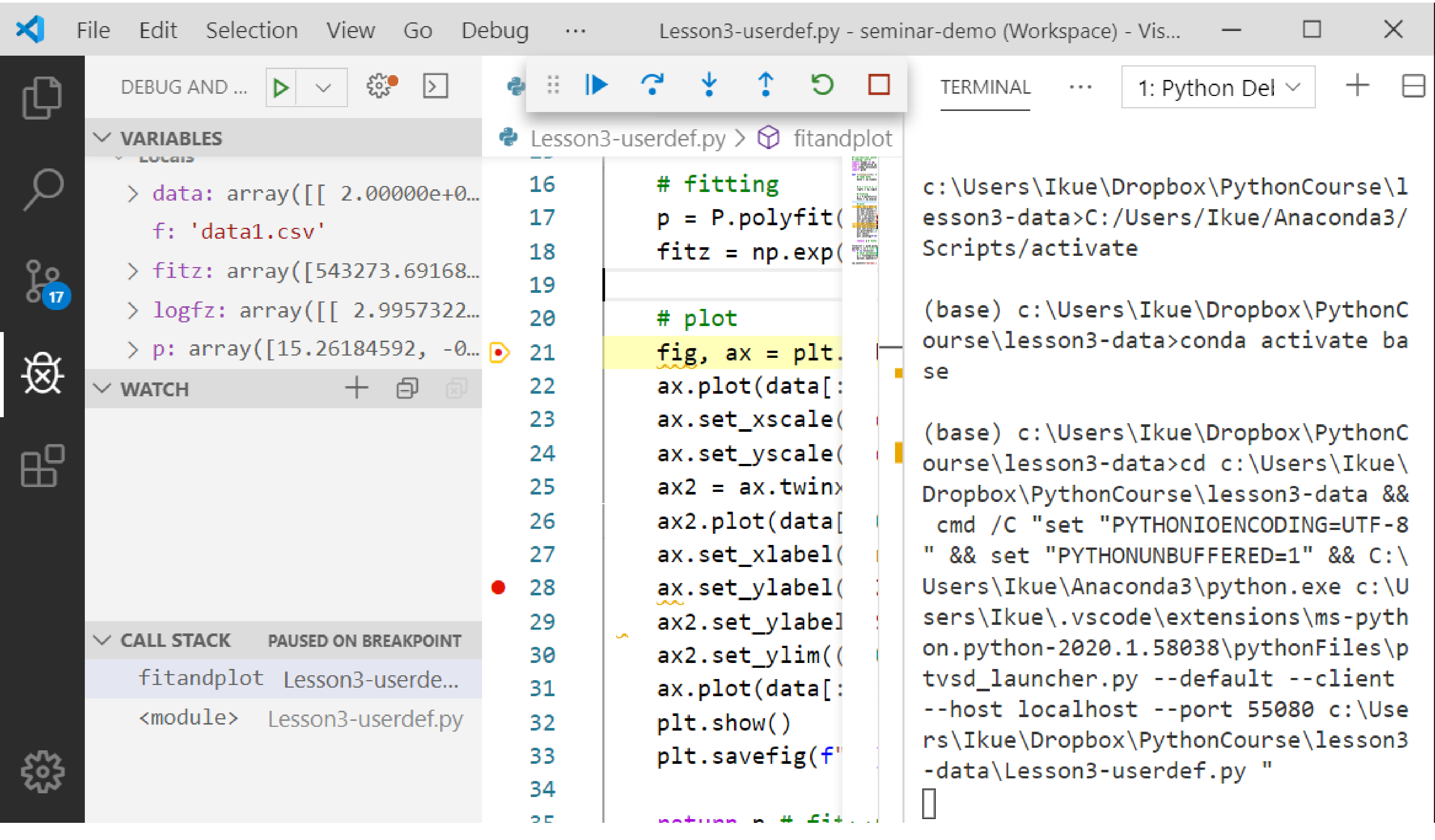
Debugging


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
# fitting
p = P.polyfit(
fitz = np.exp(
# plot
fig, ax = plt.
ax.plot(data[:
ax.set_xscale(
ax.set_yscale(
ax2 = ax.twinx
ax2.plot(data[
ax.set_xlabel(
ax.set_ylabel(
ax2.set_ylabel
ax2.set_ylim((
ax.plot(data[:
plt.show()
plt.savefig(f"
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

File Edit View Insert Cell Kernel Navigate Widgets Help   Trusted | Python 3

In [35]:

```python
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                         Traceback (most recent call last)
<ipython-input-35-89a0c53ab2bc> in <module>
```

try and except

In [51]:

```python
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

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.

To study by yourself: codecademy

*This is outdated Python 2 – `print()` function is a bit different from Python 3