

ch01-code-listing

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1 Chapter 1: Computing with Python

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Source code listings for [Numerical Python - Scientific Computing and Data Science Applications with Numpy, SciPy and Matplotlib](#) (ISBN 979-8-8688-0412-0).

1.1 Interpreter

```
[1]: %%writefile hello.py  
     print("Hello from Python!")
```

Overwriting hello.py

```
[2]: !python hello.py
```

Hello from Python!

```
[3]: !python --version
```

Python 3.10.12

1.2 Input and output caching

(restart the kernel for the same output and cell numbers)

```
[1]: 3 * 3
```

```
[1]: 9
```

```
[2]: In[1]
```

```
[2]: '3 * 3'
```

```
[3]: Out[1]
```

```
[3]: 9
```

```
[4]: In
```

```
[4]: ['', '3 * 3', 'In[1]', 'Out[1]', 'In']
```

```
[5]: Out
```

```
[5]: {1: 9, 2: '3 * 3', 3: 9, 4: ['', '3 * 3', 'In[1]', 'Out[1]', 'In', 'Out']}
```

```
[6]: 1+2
```

```
[6]: 3
```

```
[7]: 1+2;
```

```
[8]: x = 1
```

```
[9]: x = 2; x
```

```
[9]: 2
```

1.3 Documentation

```
[10]: import os
```

```
[11]: # try os.w<TAB>
```

```
[12]: import math
```

```
[13]: math.cos?
```

Signature: `math.cos(x, /)`

Docstring: Return the cosine of x (measured in radians).

Type: builtin_function_or_method

1.4 Interaction with System Shell

```
[14]: !touch file1.py file2.py file3.py
```

```
[15]: !ls file*
```

```
file1.py file2.py file3.py
```

```
[16]: files = !ls file*
```

```
[17]: len(files)
```

```
[17]: 3
```

```
[18]: files
```

```
[18]: ['file1.py', 'file2.py', 'file3.py']
```

```
[19]: file = "file1.py"
```

```
[20]: !ls -l $file
```

```
-rw-----@ 1 rob  staff  0 Nov  2 17:58 file1.py
```

1.5 Running scripts from the IPython console

```
[21]: %%writefile fib.py

def fib(N):
    """
    Return a list of the first N Fibonacci numbers.
    """
    f0, f1 = 0, 1
    f = [1] * N
    for n in range(1, N):
        f[n] = f0 + f1
        f0, f1 = f1, f[n]

    return f

print(fib(10))
```

Overwriting fib.py

```
[22]: !python fib.py
```

```
[1, 1, 2, 3, 5, 8, 13, 21, 34, 55]
```

```
[23]: %run fib.py
```

```
[1, 1, 2, 3, 5, 8, 13, 21, 34, 55]
```

```
[24]: fib(6)
```

```
[24]: [1, 1, 2, 3, 5, 8]
```

1.6 Debugger

```
[25]: fib(1.0)
```

```
-----
TypeError                                Traceback (most recent call last)
Cell In[25], line 1
----> 1 fib(1.0)

File ~/OneDrive/Desktop/npbook-ed3/code/numerical-python-code-ed3-v2-github/fib
.py:7, in fib(N)
     3 """
     4 Return a list of the first N Fibonacci numbers.
     5 """
     6 f0, f1 = 0, 1
----> 7 f = [1] * N
     8 for n in range(1, N):
     9     f[n] = f0 + f1

TypeError: can't multiply sequence by non-int of type 'float'
```

```
[ ]: %debug
```

```
> /Users/rob/OneDrive/Desktop/npbook-ed3/code/numerical-python-code-
ed3-v2-github/fib.py(7)fib()
     5 """
     6     f0, f1 =
0, 1
----> 7     f =
[1] *
N
     8     for n in
range(1,
N):
     9         f[n]
= f0 + f1
```

1.7 Timing and profiling code

```
[27]: %timeit fib(100)
```

```
11.5 µs ± 140 ns per loop (mean ± std. dev. of 7 runs, 100,000 loops each)
```

```
[28]: result = %time fib(100)
```

CPU times: user 27 μ s, sys: 1 μ s, total: 28 μ s

Wall time: 33.1 μ s

```
[29]: len(result)
```

```
[29]: 100
```

```
[30]: import numpy as np

def random_walker_max_distance(M, N):
    """
    Simulate N random walkers taking M steps, and return the largest distance
    from the starting point achieved by any of the random walkers.
    """
    trajectories = [np.random.randn(M).cumsum() for _ in range(N)]
    return np.max(np.abs(trajectories))
```

```
[31]: %prun random_walker_max_distance(400, 10000)
```

20011 function calls in 0.336 seconds

Ordered by: internal time

ncalls	tottime	percall	cumtime	percall	filename:lineno(function)
10000	0.189	0.000	0.189	0.000	{method 'randn' of 'numpy.random. ↳mtrand.RandomState' objects}
10000	0.070	0.000	0.070	0.000	{method 'cumsum' of 'numpy. ↳ndarray' objects}
1	0.047	0.047	0.330	0.330	2615584822.py: ↳3(random_walker_max_distance)
1	0.020	0.020	0.279	0.279	2615584822.py:8(<listcomp>)
1	0.007	0.007	0.336	0.336	<string>:1(<module>)
1	0.004	0.004	0.004	0.004	{method 'reduce' of 'numpy.ufunc' ↳objects}
1	0.000	0.000	0.336	0.336	{built-in method builtins.exec}
1	0.000	0.000	0.004	0.004	fromnumeric.py:71(_wrapreduction)
1	0.000	0.000	0.004	0.004	fromnumeric.py:2692(max)
1	0.000	0.000	0.000	0.000	fromnumeric.py:72(<dictcomp>)
1	0.000	0.000	0.000	0.000	fromnumeric.py: ↳2687(_max_dispatcher)
1	0.000	0.000	0.000	0.000	{method 'disable' of '_lsprof. ↳Profiler' objects}
1	0.000	0.000	0.000	0.000	{method 'items' of 'dict' objects}

1.8 Jupyter notebook

```
[32]: from IPython.display import display, Image, HTML, Math
```

```
[33]: Image(url='http://python.org/images/python-logo.gif')
```

```
[33]: <IPython.core.display.Image object>
```

```
[34]: import scipy, numpy, matplotlib
modules = [numpy, matplotlib, scipy]
row = "<tr> <td>%s</td> <td>%s</td> </tr>"
rows = "\n".join([row % (module.__name__, module.__version__) for module in modules])
s = "<table> <tr><th>Library</th><th>Version</th> </tr> %s</table>" % rows
```

```
[35]: s
```

```
[35]: '<table> <tr><th>Library</th><th>Version</th> </tr> <tr> <td>numpy</td>
<td>1.25.2</td> </tr>\n<tr> <td>matplotlib</td> <td>3.8.0</td> </tr>\n<tr>
<td>scipy</td> <td>1.11.3</td> </tr></table>'
```

```
[36]: HTML(s)
```

```
[36]: <IPython.core.display.HTML object>
```

```
[37]: class HTMLDisplay(object):
    def __init__(self, code):
        self.code = code

    def _repr_html_(self):
        return self.code
```

```
[38]: HTMLDisplayer(s)
```

```
[38]: <__main__.HTMLDisplayer at 0x7fb5a6f03d00>
```

```
[39]: Math(r'\hat{H} = -\frac{1}{2}\epsilon\hat{\sigma}_z - \frac{1}{2}\delta\hat{\sigma}_x
\hat{\sigma}_x')
```

```
[39]: 
$$\hat{H} = -\frac{1}{2}\epsilon\hat{\sigma}_z - \frac{1}{2}\delta\hat{\sigma}_x$$

```

```
[40]: class QubitHamiltonian(object):
    def __init__(self, epsilon, delta):
        self.epsilon = epsilon
        self.delta = delta

    def _repr_latex_(self):
```

```

return "$\hat{H} = -%.2f\hat{\sigma}_z - %.2f\hat{\sigma}_x$" % \
    (self.epsilon/2, self.delta/2)

```

```
[41]: QubitHamiltonian(0.5, 0.25)
```

```
[41]:  $\hat{H} = -0.25\hat{\sigma}_z - 0.12\hat{\sigma}_x$ 
```

```

[42]: import matplotlib.pyplot as plt
import numpy as np
from scipy import stats

def f(mu):
    X = stats.norm(loc=mu, scale=np.sqrt(mu))
    N = stats.poisson(mu)
    x = np.linspace(0, X.ppf(0.999))
    n = np.arange(0, x[-1])

    fig, ax = plt.subplots()
    ax.plot(x, X.pdf(x), color='black', lw=2, label="Normal($\mu=%d, \sigma^2=%d$" % (mu, mu))
    ax.bar(n, N.pmf(n), align='edge', label=r"Poisson($\lambda=%d$" % mu)
    ax.set_ylim(0, X.pdf(x).max() * 1.25)
    ax.legend(loc=2, ncol=2)
    plt.close(fig)
    return fig

```

```

[44]: from ipywidgets import interact
import ipywidgets as widgets

```

```
[45]: interact(f, mu=widgets.FloatSlider(min=1.0, max=20.0, step=1.0));
```

```

interactive(children=(FloatSlider(value=1.0, description='mu', max=20.0, min=1.0, step=1.0), Output()), _dom_c...

```

1.9 Jupyter nbconvert

```
[2]: !jupyter nbconvert --to html ch01-code-listing.ipynb
```

```

[NbConvertApp] Converting notebook ch01-code-listing.ipynb to html
[NbConvertApp] WARNING | Alternative text is missing on 1 image(s).
[NbConvertApp] Writing 341393 bytes to ch01-code-listing.html

```

```
[2]: !jupyter nbconvert --to pdf ch01-code-listing.ipynb
```

```

[NbConvertApp] Converting notebook ch01-code-listing.ipynb to pdf
/Users/rob/miniconda3/envs/py3.10/lib/python3.10/site-packages/nbconvert/utils/pandoc.py:51: RuntimeWarning: You are using an

```

```

unsupported version of pandoc (2.12).
Your version must be at least (2.14.2) but less than (4.0.0).
Refer to https://pandoc.org/installing.html.
Continuing with doubts...
  check_pandoc_version()
[NbConvertApp] Writing 61299 bytes to notebook.tex
[NbConvertApp] Building PDF
[NbConvertApp] Running xelatex 3 times: ['xelatex', 'notebook.tex', '-quiet']
[NbConvertApp] Running bibtex 1 time: ['bibtex', 'notebook']
[NbConvertApp] WARNING | bibtex had problems, most likely because there were no
citations
[NbConvertApp] PDF successfully created
[NbConvertApp] Writing 64876 bytes to ch01-code-listing.pdf

```

```

[8]: %%writefile custom_template.tplx
    ((* extends 'article.tplx' -*))

    ((* block title *)) \title{Document title} ((* endblock title *))
    ((* block author *)) \author{Author's Name} ((* endblock author *))

```

Overwriting custom_template.tplx

```

[ ]: !jupyter nbconvert ch01-code-listing.ipynb --to pdf --template custom_template.
    ↪tplx

```

```

[11]: !jupyter nbconvert ch01-code-listing.ipynb --to python

```

```

[NbConvertApp] Converting notebook ch01-code-listing.ipynb to python
[NbConvertApp] Writing 5142 bytes to ch01-code-listing.py

```

2 Versions

```

[1]: %reload_ext version_information
    %version_information numpy

```

```

[1]:

```

Software	Version
Python	3.10.13 64bit [Clang 14.0.6]
IPython	8.20.0
OS	macOS 10.15.7 x86_64 i386 64bit
numpy	1.24.3
Mon May 06 14:29:51 2024 JST	

```

[ ]:

```