Applied Mathematics: an introduction to Scientific Computing by Numerical Analysis

Lecture 04 - Numpy, Scipy, and Matplotlib (lecture notes taken from Sven Schmit)

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Numpy

- Fundamental package for scientific computing with Python
- N-dimensional array object
- Linear algebra, Fourier transform, random number capabilities
- Building block for other packages (e.g. Scipy)
- Open source

import numpy as np

Basics:

```
import numpy as np

A = np.array([[1, 2, 3], [4, 5, 6]])
print A
# [[1 2 3]
#  [4 5 6]]

Af = np.array([1, 2, 3], float)
```

Slicing as usual.

More basics

```
np.arange(0, 1, 0.2)
# array ([ 0.  ,      0.2,    0.4,    0.6,    0.8])

np.linspace(0, 2*np.pi, 4)
# array ([ 0.0,      2.09,     4.18, 6.28])

A = np.zeros((2,3))
# array ([[ 0.,       0.,     0.],
#          [ 0.,      0.,     0.]])
# np . ones , np . diag
A.shape
# (2, 3)
```

More basics

```
np.random.random((2,3))
# array([[ 0.78084261,    0.64328818,    0.55380341],
#        [ 0.24611092,    0.37011213,    0.83313416]])

a = np.random.normal(loc=1.0, scale=2.0, size=(2,2))
# array([[ 2.87799514,    0.6284259 ],
#        [ 3.10683164,    2.05324587]])

np.savetxt("a_out.txt", a)
# save to file
b = np.loadtxt("a_out.txt")
# read from file
```

Arrays are mutable

```
A = np.zeros((2, 2))
# array([[ 0.,       0.],
#        [ 0.,       0.]])
C = A
C[0, 0] = 1

print A
# [[ 1.     0.]
#  [ 0.     0.]]
```

Array attributes

```
a = np.arange(10).reshape((2,5))

a.ndim      # 2 dimension
a.shape     # (2, 5) shape of array
a.size      # 10 # of elements
a.T         # transpose
a.dtype     # data type
```

Basic operations

Arithmetic operators: **elementwise** application

```
a = np.arange(4)
# array ([0, 1, 2, 3])

b = np.array([2, 3, 2, 4])

a * b    # array ([ 0,      3,    4, 12])
b - a    # array ([2, 2, 0, 1])

c = [2, 3, 4, 5]
a * c    # array ([ 0,      3,    8, 15])
```

Also, we can use += and *= .

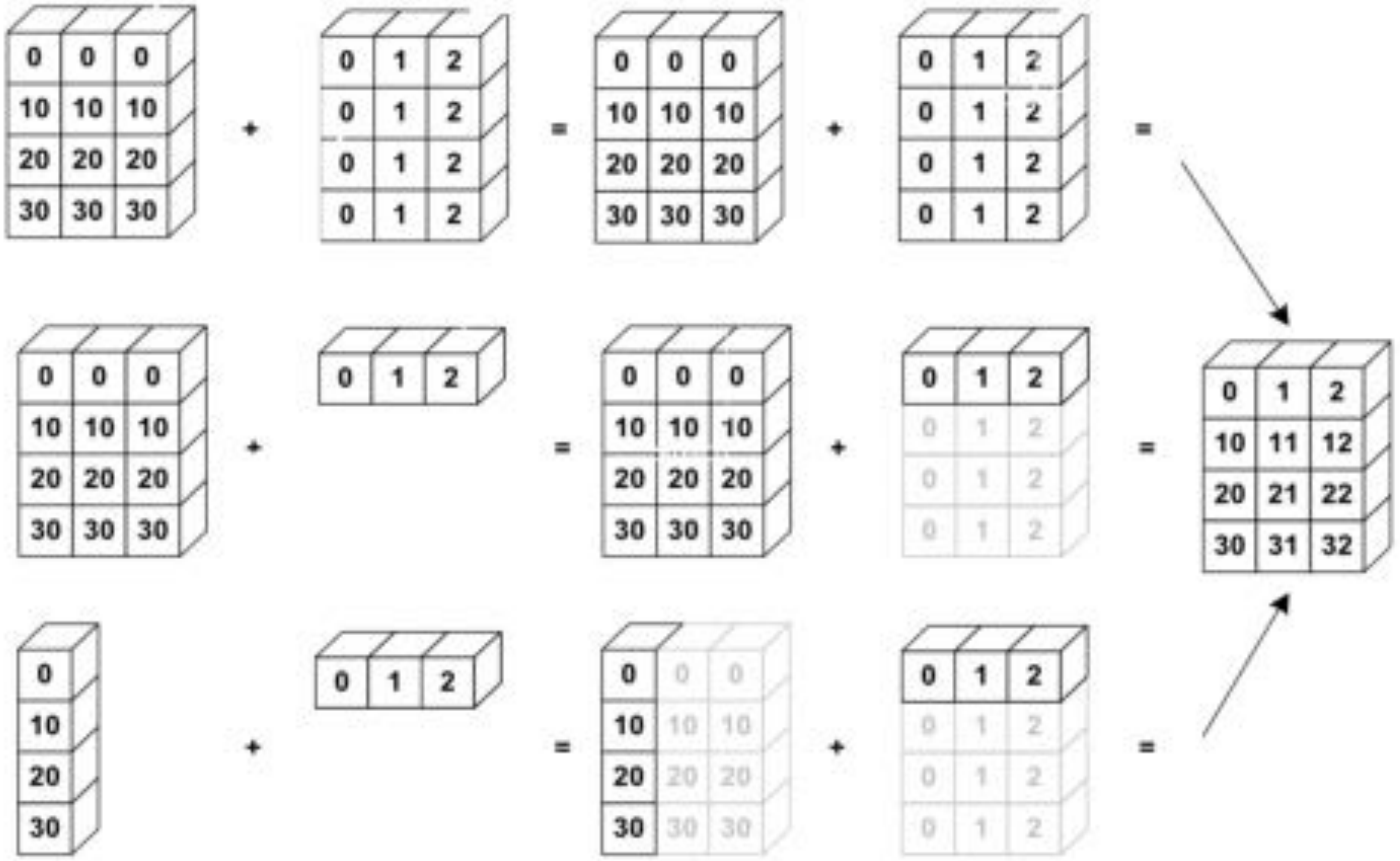
Array broadcasting

When operating on two arrays, numpy compares shapes. Two dimensions are compatible when

1. They are of equal size

2. One of them is 1

Array broadcasting



Array broadcasting with scalars

This also allows us to add a constant to a matrix or multiply a matrix by a constant

```
A = np.ones((3,3))

print 3 * A - 1
# [[ 2.     2.    2.]
#   [ 2.     2.    2.]
#   [ 2.     2.    2.]]
```

Vector operations

- inner product
- outer product
- dot product (matrix multiplication)

```
# note : numpy automatically converts lists
u = [1, 2, 3]
v = [1, 1, 1]

np.inner(u, v)
# 6
np.outer(u, v)
# array ([[1, 1, 1],
#         [2, 2, 2],
#         [3, 3, 3]])
np.dot(u, v)
# 6
```

Matrix operations

First, define some matrices:

```
A = np.ones((3, 2))
# array([[ 1.,    1.],
#        [ 1.,    1.],
#        [ 1.,    1.]])
A.T
# array([[ 1.,    1.,    1.],
#        [ 1.,    1.,    1.]])

B = np.ones((2, 3))
# array([[ 1.,    1.,    1.],
#        [ 1.,    1.,    1.]])
```

Matrix operations

```
np.dot(A, B)
# array([[ 2.,    2.,   2.],
#        [ 2.,    2.,   2.],
#        [ 2.,    2.,   2.]])

np.dot(B, A)
# array([[ 3.,    3.],
#        [ 3.,    3.]])

np.dot(B.T, A.T)
# array([[ 2.,    2.,   2.],
#        [ 2.,    2.,   2.],
#        [ 2.,    2.,   2.]])

np.dot(A, B.T)
# Traceback (most recent call last):
#   File "<stdin>", line 1, in <module>
# ValueError: shapes (3,2) and (3,2) not aligned:          ...
# ... 2 (dim 1) != 3 (dim 0)
```

Operations along axes

```
a = np.random.random((2,3))
# array([[ 0.9190687 ,  0.36497813,  0.75644216],
#        [ 0.91938241,  0.08599547,  0.49544003]])
a.sum()
# 3.5413068994445549
a.sum(axis=0)   # column sum
# array([ 1.83845111,  0.4509736 ,  1.25188219])
a.cumsum()
# array([ 0.9190687 ,  1.28404683,  2.04048899,  2.9598714 ,
#         3.04586687,  3.5413069 ])
a.cumsum(axis=1)   # cumulative row sum
# array([[ 0.9190687 ,  1.28404683,  2.04048899],
#        [ 0.91938241,  1.00537788,  1.50081791]])
a.min()
# 0.0859954690403677
a.max(axis=0)
# array([ 0.91938241,  0.36497813,  0.75644216])
```

Slicing arrays

More advanced slicing

```
a = np.random.random((4,5))

a[2, :]
# third row, all columns
a[1:3]
# 2nd, 3rd row, all columns
a[:, 2:4]
# all rows, columns 3 and 4
```

Iterating over arrays

- Iterating over multidimensional arrays is done with respect to the first axis: `for row in A`
- Looping over all elements: `for element in A.flat`

Reshaping

Reshape using reshape. Total size must remain the same.

Resize using resize , always works: chopping or appending zeros

First dimension has ‘priority’, so beware of unexpected results

Try it!

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Reshaping

Reshape using reshape. Total size must remain the same.

Resize using resize , always works: chopping or appending zeros

First dimension has ‘priority’, so beware of unexpected results

Try it!

Matrix operations

import numpy.linalg

eye(3)	Identity matrix
trace(A)	Trace
column_stack((A,B))	Stack column wise
row_stack((A,B,A))	Stack row wise

Linear algebra

import numpy.linalg

qr	Computes the QR decomposition
cholesky	Computes the Cholesky decomposition
inv(A)	Inverse
solve(A,b)	Solves $Ax = b$ for A full rank
lstsq(A,b)	Solves argmin $_x \quad Ax - b \quad _2$
eig(A)	Eigenvalue decomposition
eig(A)	Eigenvalue decomposition for symmetric or hermitian
eigvals(A)	Computes eigenvalues.
svd(A, full)	Singular value decomposition
pinv(A)	Computes pseudo-inverse of A

Fourier transform

import numpy.fft

- fft 1-dimensional DFT
- fft2 2-dimensional DFT
- fftn N-dimensional DFT
- ifft 1-dimensional inverse DFT (etc.)
- rfft Real DFT (1-dim)
- ifft Imaginary DFT (1-dim)

Random sampling

import numpy.random

rand(d0,d1,...,dn)	Random values in a given shape
randn(d0, d1, ...,dn)	Random standard normal
randint(lo, hi, size)	Random integers [lo, hi)
choice(a, size, repl, p)	Sample from a
shuffle(a)	Permutation (in-place)
permutation(a)	Permutation (new array)

Distributions in random

import numpy.random

The list of distributions to sample from is quite long, and includes

- beta
- binomial
- chisquare
- exponential
- dirichlet
- gamma
- laplace
- lognormal
- pareto
- poisson
- power

Contents

What is SciPy?

SciPy is a library of algorithms and mathematical tools built to work with NumPy arrays.

- linear algebra - *scipy.linalg*
- statistics - *scipy.stats*
- optimization - *scipy.optimize*
- sparse matrices - *scipy.sparse*
- signal processing - *scipy.signal*
- etc.

Scipy Linear Algebra

Slightly different from numpy.linalg. Always uses BLAS/LAPACK support, so could be faster.

Some more functions.

Functions can be slightly different.

Scipy Optimization

- General purpose minimization: CG, BFGS, least-squares
- Constrainted minimization; non-negative least-squares
- Minimize using simulated annealing
- Scalar function minimization
- Root finding
- Check gradient function
- Line search

Scipy Statistics

- Mean, median, mode, variance, kurtosis
- Pearson correlation coefficient
- Hypothesis tests (ttest, Wilcoxon signed-rank test, Kolmogorov-Smirnov)
- Gaussian kernel density estimation

See also SciKits (or scikit-learn).

Scipy sparse

- Sparse matrix classes: CSC, CSR, etc.
- Functions to build sparse matrices
- sparse.linalg module for sparse linear algebra
- sparse.csgraph for sparse graph routines

Scipy signal

- Convolutions
- B-splines
- Filtering
- Continuous-time linear system
- Wavelets
- Peak finding

Scipy IO

Methods for loading and saving data

- Matlab files
- Matrix Market files (sparse matrices)
- Wav files

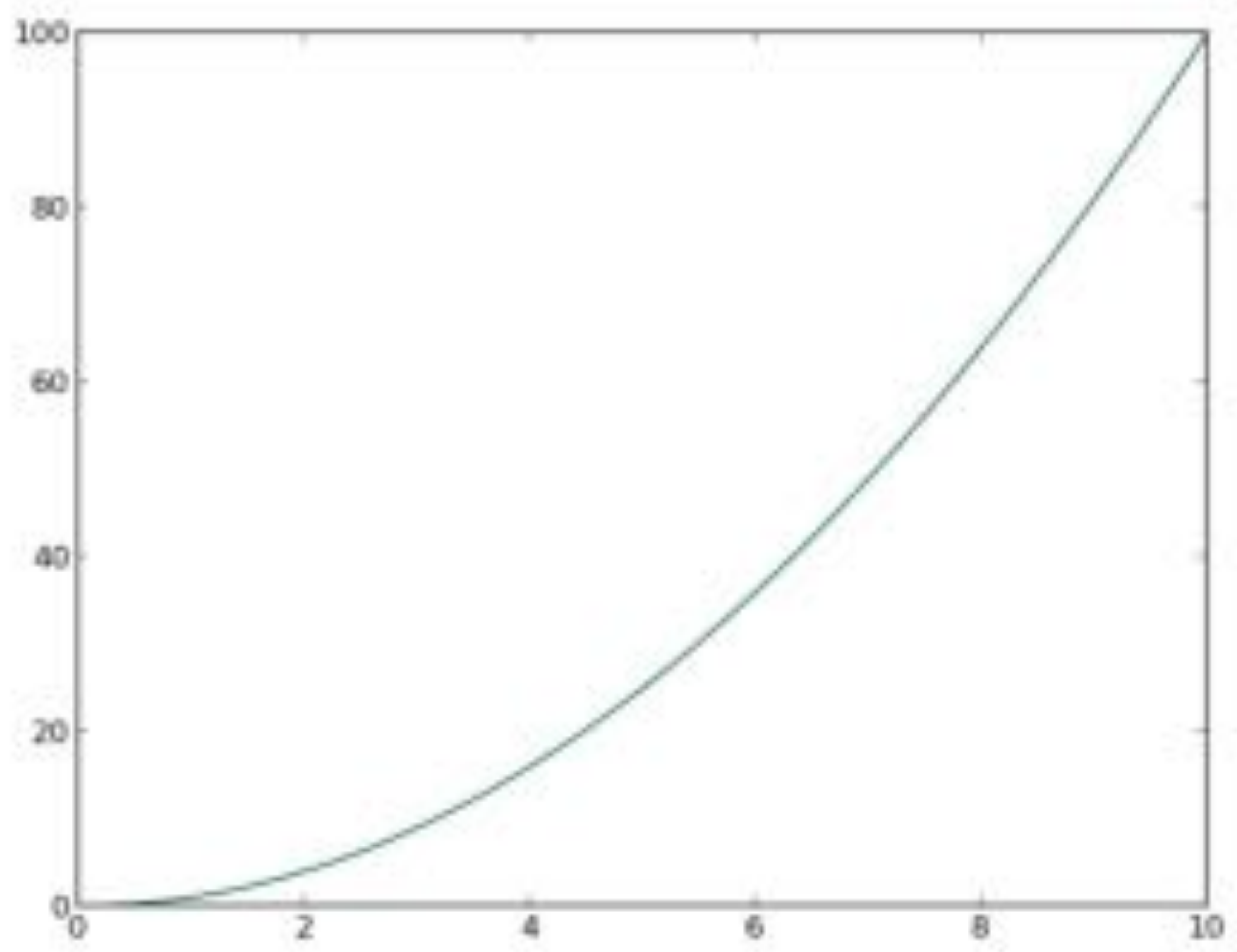
Contents

What is Matplotlib?

- Plotting library for Python
- Works well with Numpy
- Syntax similar to Matlab

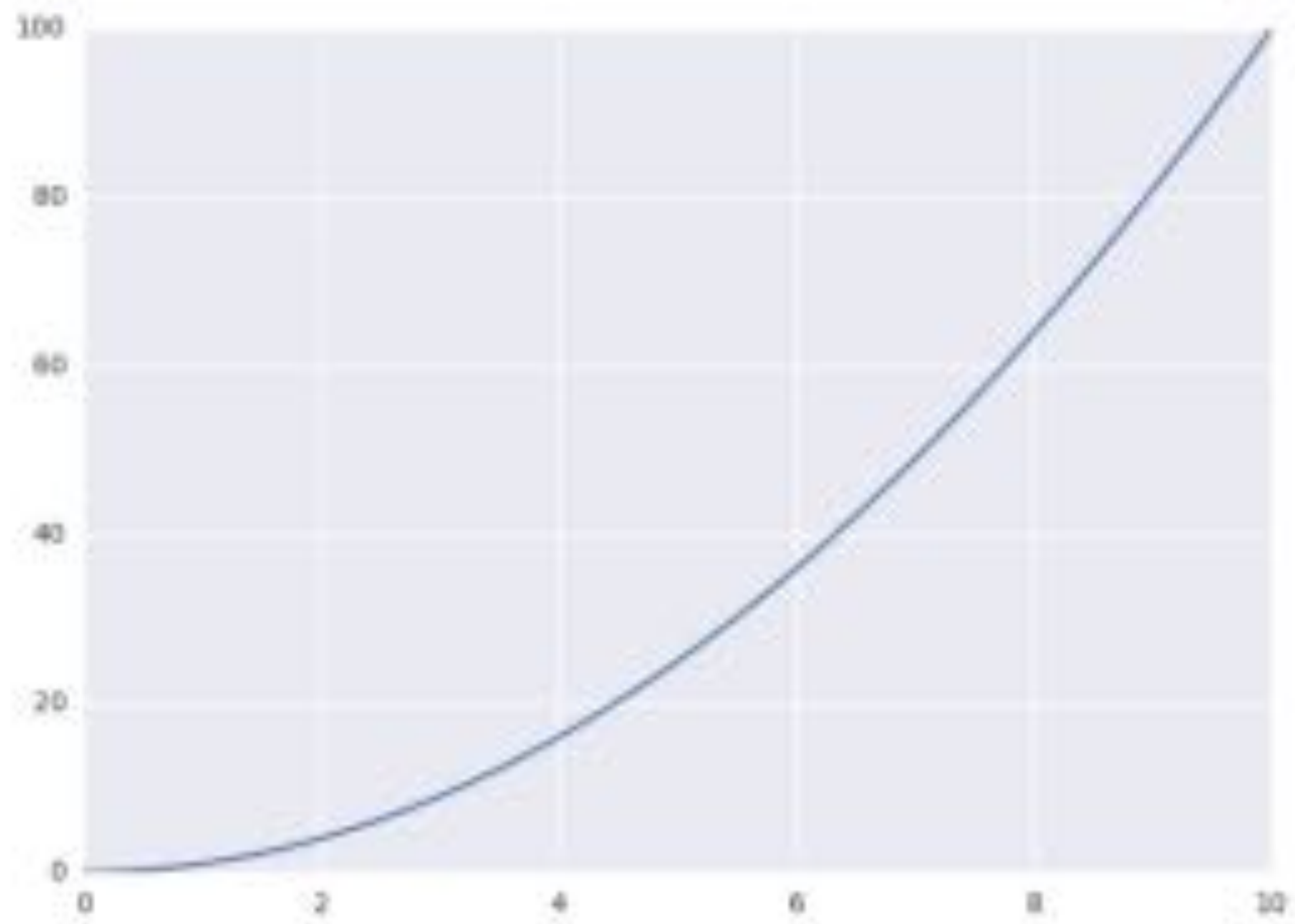
Scatter Plot

```
import numpy as np
import matplotlib.pyplot as plt

x = np. linspace(0, 10, 1000)
y = np.power(x, 2)
plt . plot(x, y)
plt .show()
```



Seaborn makes plot pretty

```
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

x = np. linspace(0, 10, 1000)
y = np.power(x, 2)
plt . plot(x, y)
plt .show()
```

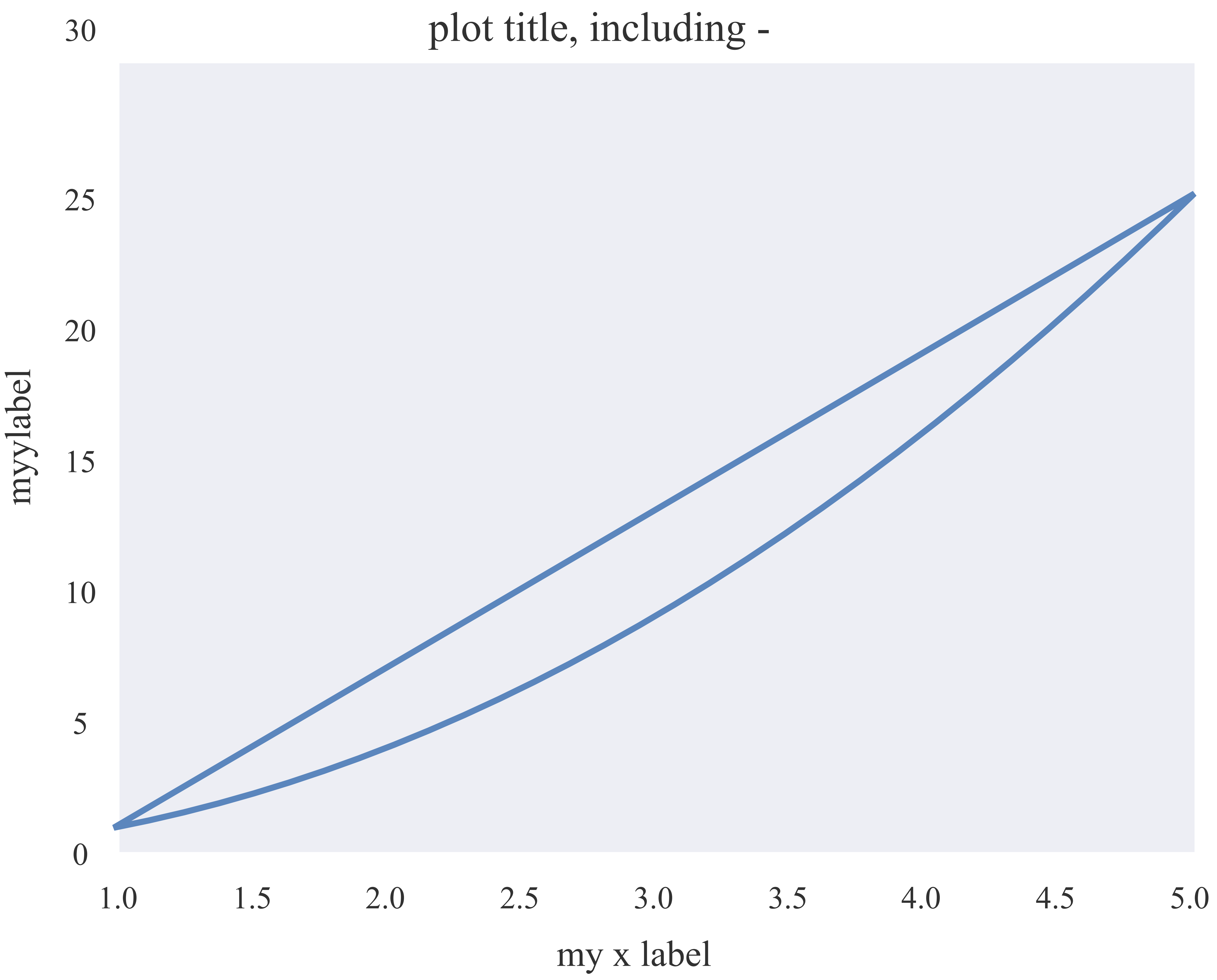


Scatter Plot

Adding titles and labels

```
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

f, ax = plt.subplots(1, 1, figsize=(5,4))

x = np.linspace(0, 10, 1000)
y = np.power(x, 2)
ax.plot(x, y)
ax.set_xlim((1, 5))
ax.set_ylim((0, 30))
ax.set_xlabel('my x label')
ax.set_ylabel('my y label')
ax.set_title('plot title, including $\Omega$')

plt.tight_layout()
plt.savefig('line_plot_plus.pdf')
```

Scatter Plot

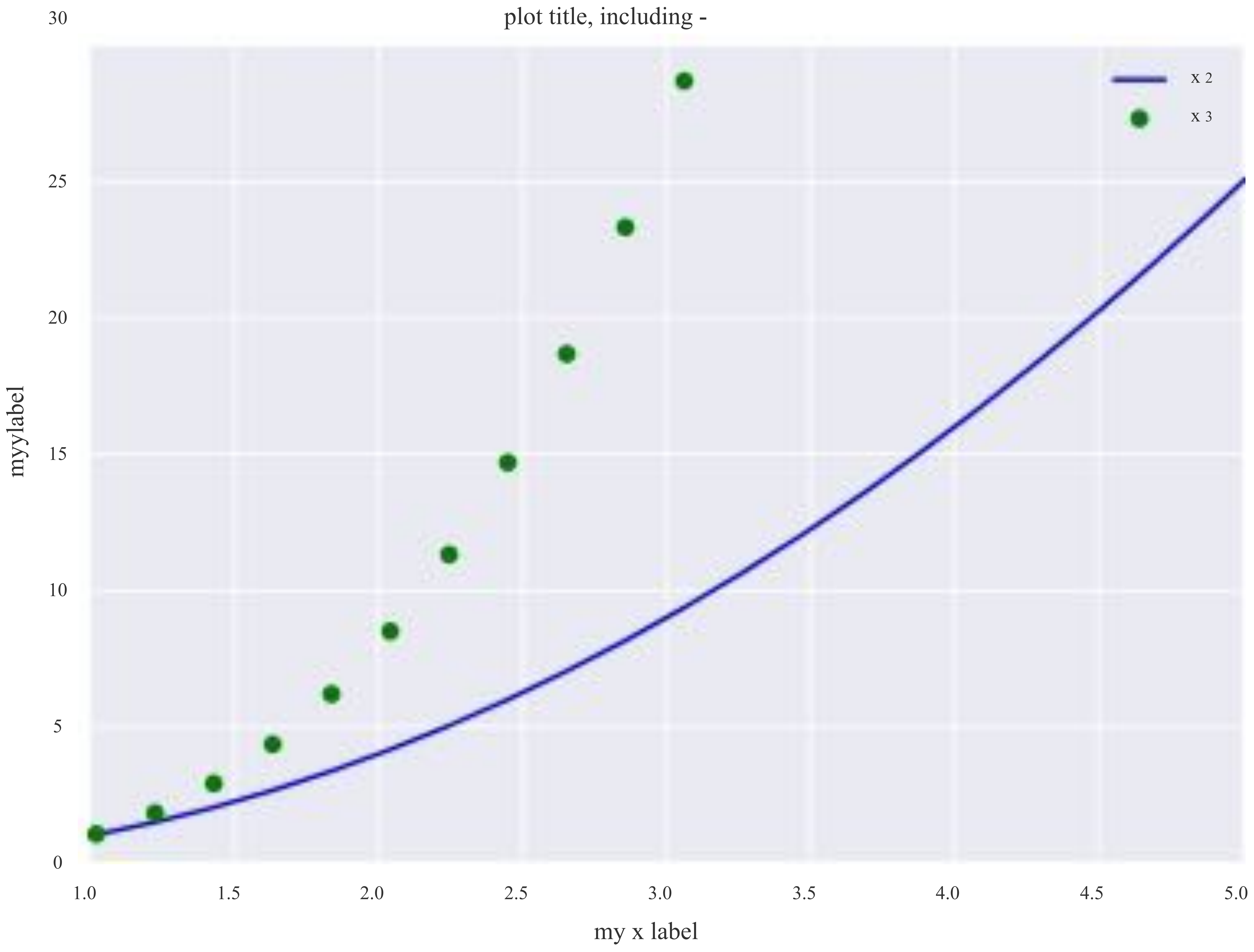


Scatter Plot

Adding multiple lines and a legend

```
x = np.linspace(0, 10, 50)
y1 = np.power(x, 2)
y2 = np.power(x, 3)


plt.plot(x, y1, 'b-', label='$x^2$')
plt.plot(x, y2, 'go', label='$x^3$')
plt.xlim((1, 5))
plt.ylim((0, 30))
plt.xlabel('my x label')
plt.ylabel('my y label')
plt.title('plot title, including $\Omega$')
plt.legend()

plt.savefig('line_plot_plus2.pdf')
```

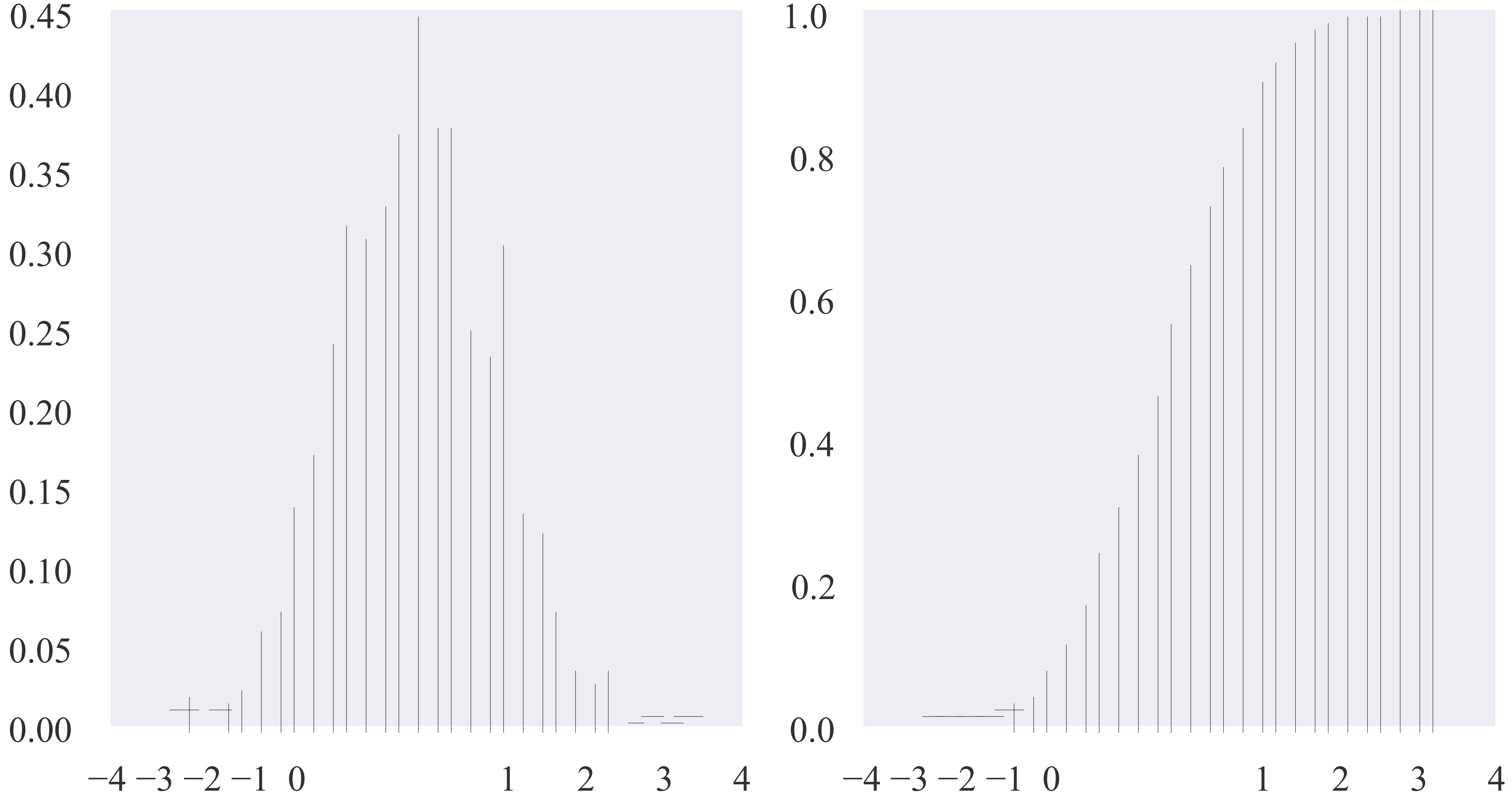
Scatter Plot



Histogram

```
data = np.random.randn(1000)

f, (ax1, ax2) = plt.subplots(1, 2, figsize=(6,3))

# histogram (pdf)
ax1.hist(data, bins=30, normed=True, color='b')

# empirical cdf
ax2.hist(data, bins=30, normed=True, color='r',
            cumulative=True)

plt.savefig('histogram.pdf')
```

Histogram


0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
−4 −3 −2 −1 0 1 2 3 4
1.0
0.8
0.6
0.4
0.2
0.0
−4 −3 −2 −1 0 1 2 3 4

Box Plot

```
samp1 = np.random.normal(loc=0., scale=1., size=100)
samp2 = np.random.normal(loc=1., scale=2., size=100)
samp3 = np.random.normal(loc=0.3, scale=1.2, size=100)

f, ax = plt.subplots(1, 1, figsize=(5,4))

ax.boxplot((samp1, samp2, samp3))
ax.set_xticklabels(['sample 1', 'sample 2', 'sample 3'])
plt.savefig('boxplot.pdf')
```

Box Plot

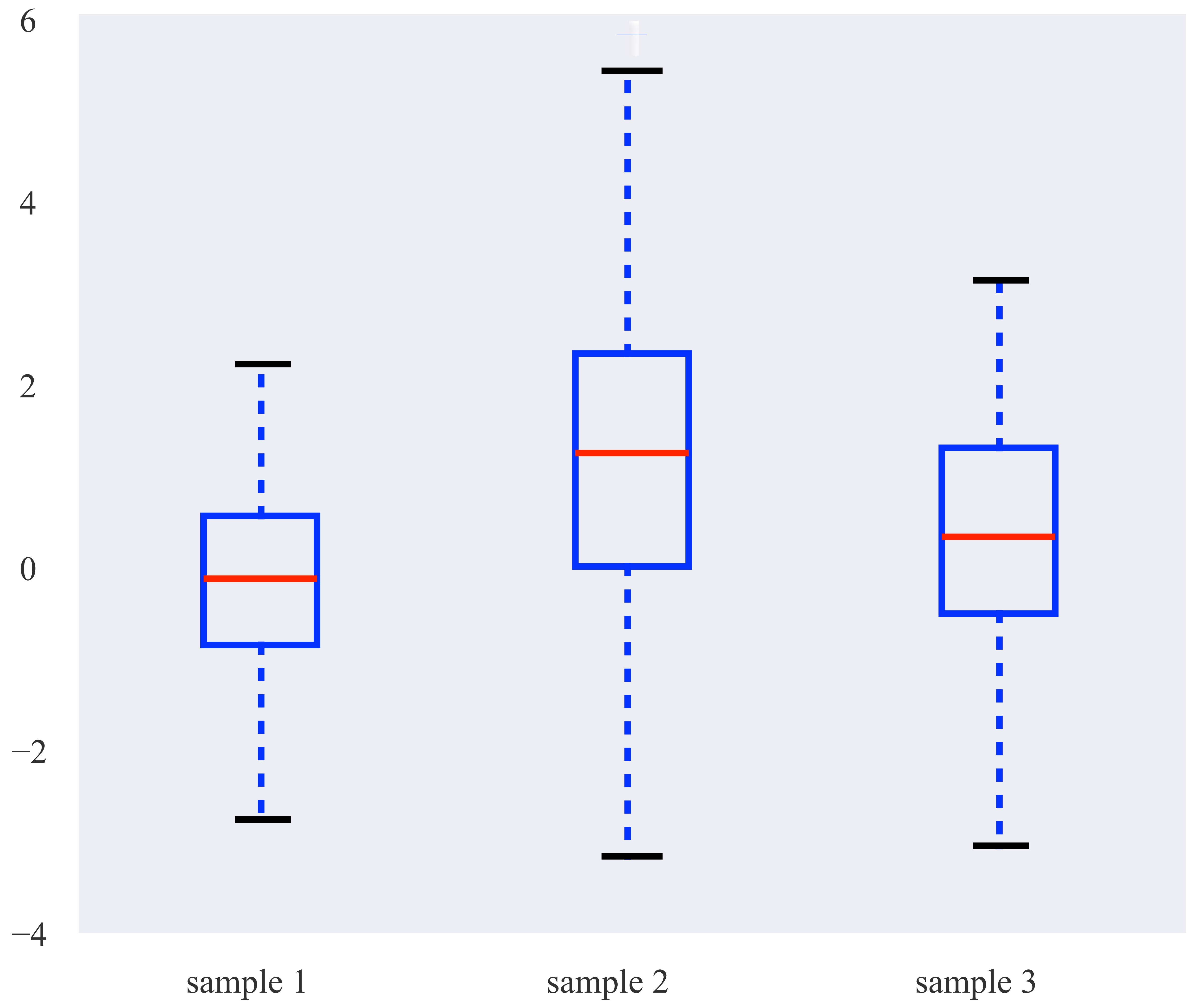
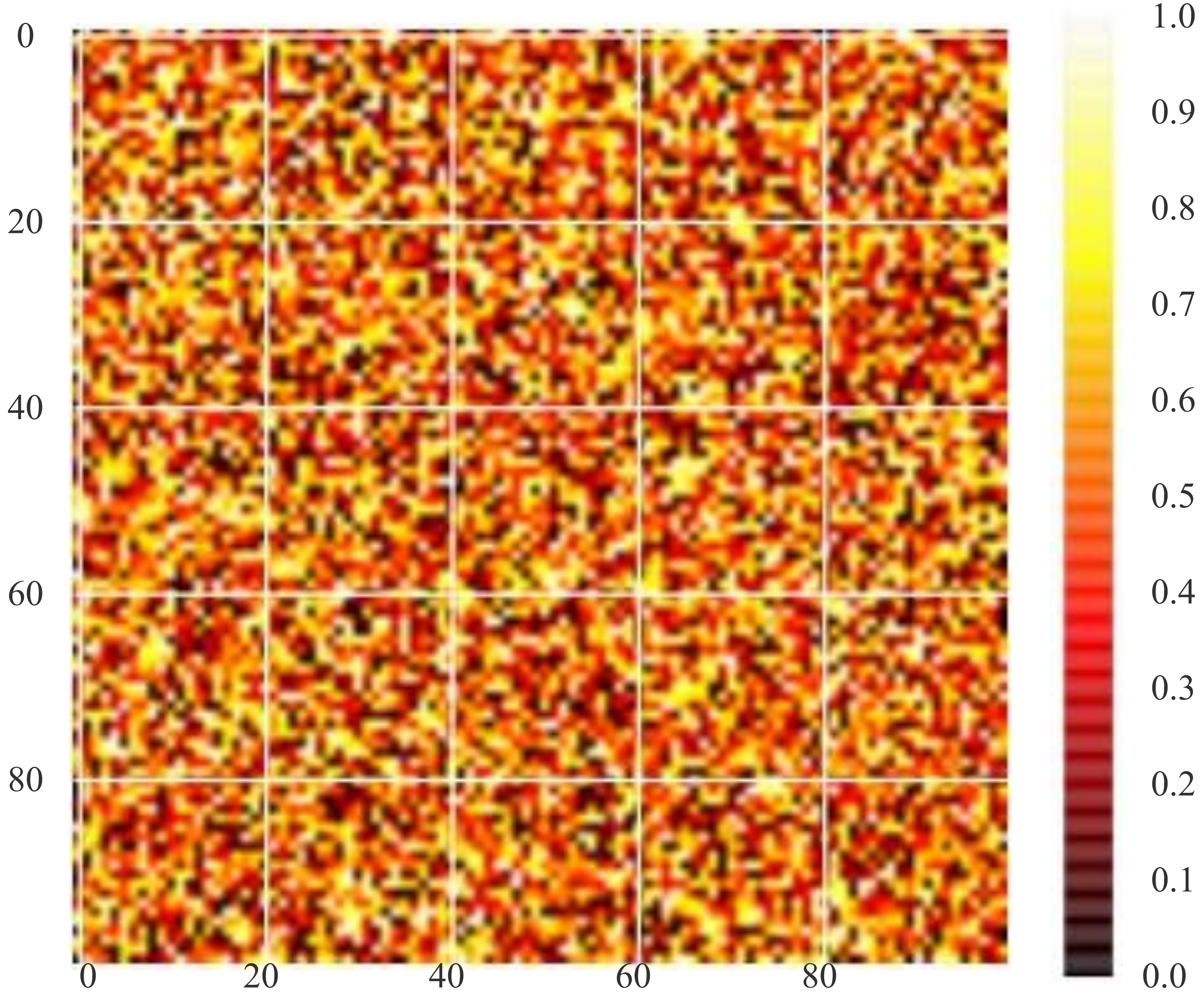


Image Plot

```
A = np.random.random((100, 100))

plt.imshow(A)
plt.hot()
plt.colorbar()

plt.savefig('imageplot.pdf')
```

Image Plot

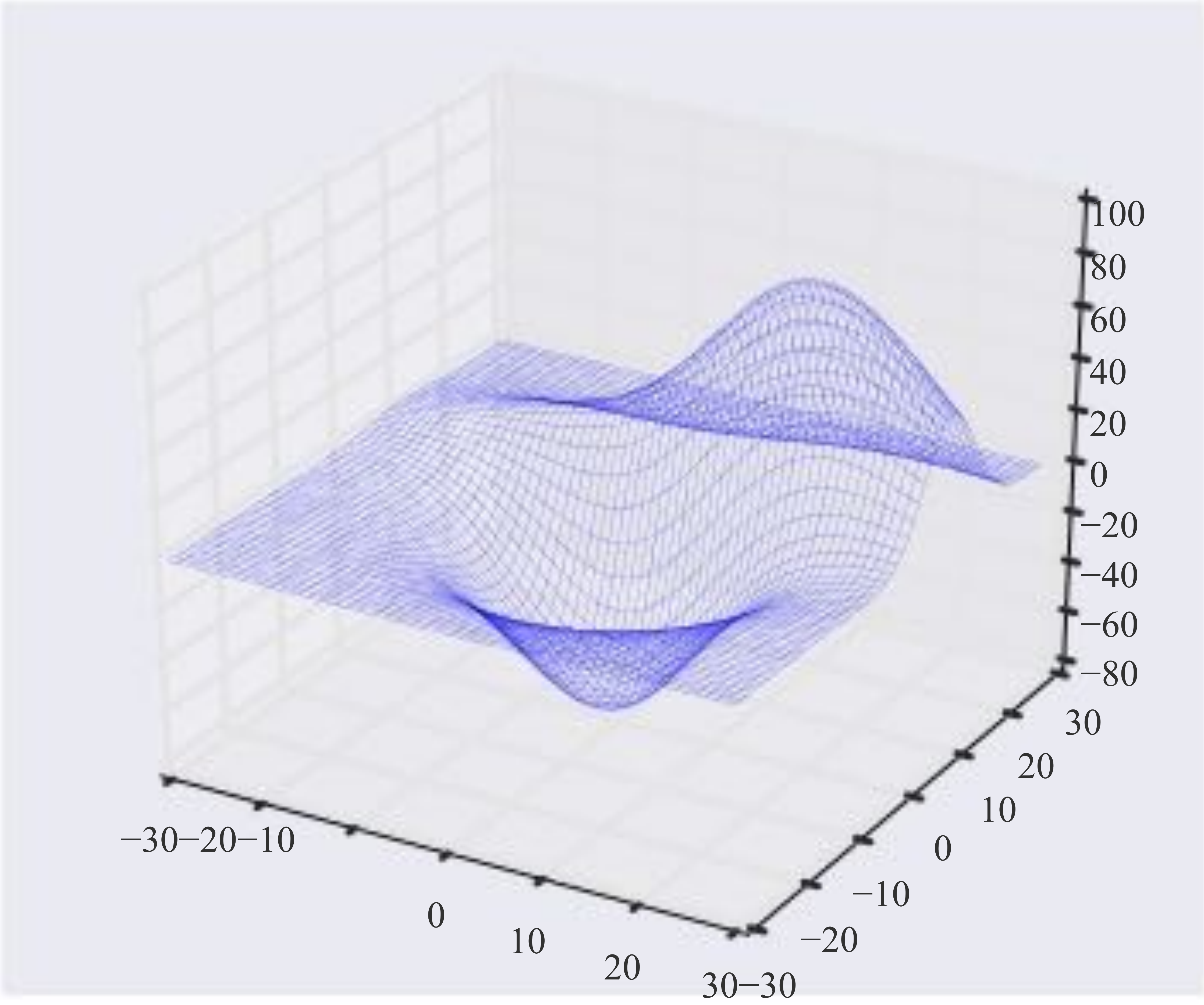


Wire Plot

matplotlib toolkits extend funtionality for other kinds of visualization

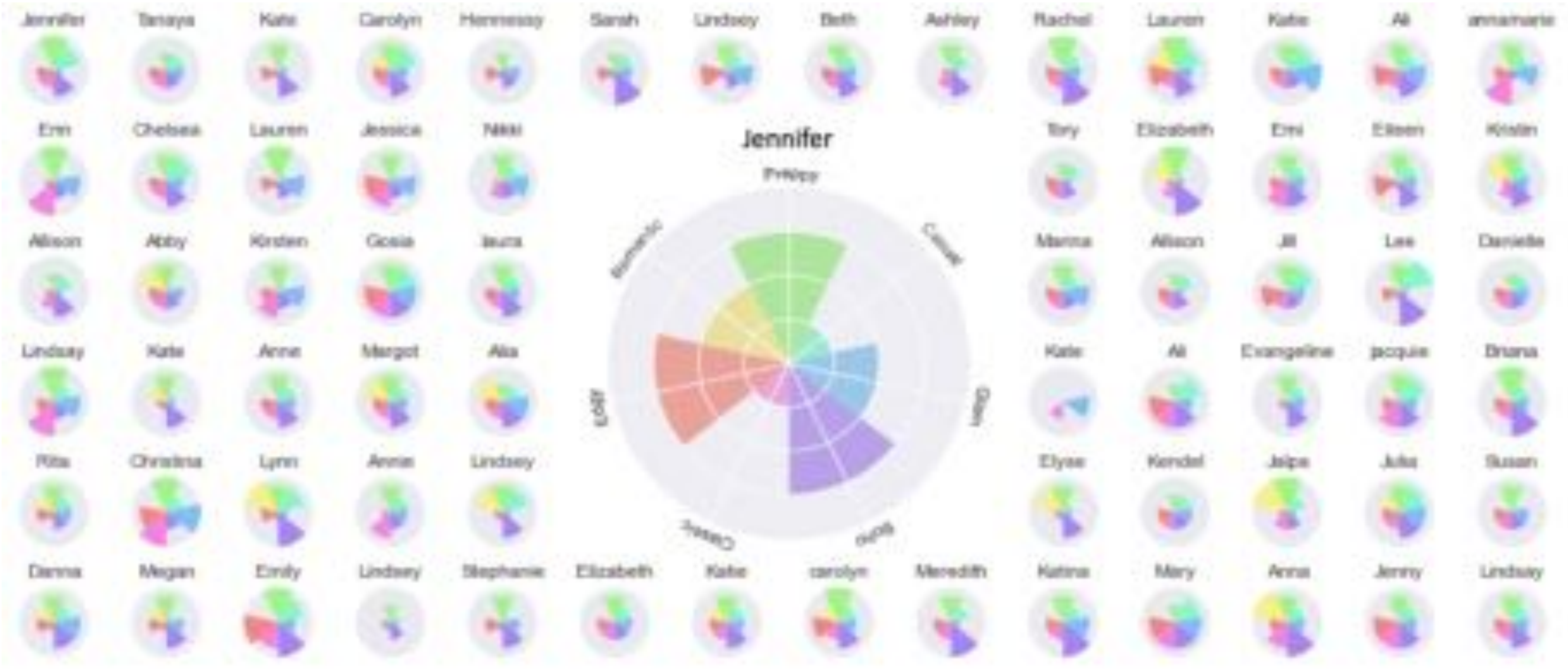
```
from mpl_toolkits.mplot3d import axes3d

ax = plt.subplot(111, projection='3d')
X, Y, Z = axes3d.get_test_data(0.1)
ax.plot_wireframe(X, Y, Z, linewidth=0.1)

plt.savefig('wire.pdf')
```

Wire Plot



Possibilities

A lot is possible, but not always easy to figure out how...



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