Introduction to Scientific Python

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Topics

- Numpy
- Scipy
- Matplotlib

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)
```

numpy.arange:
evenly spaced values within a given interval.

numpy.linspace:
evenly spaced numbers over a specified interval.

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
```

numpy.random.normal: Draw random samples from a normal (Gaussian) distribution

loc: mean
scale: standard deviation

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
```

numpy.reshape:
Gives a new shape to an array without changing its data.

Basic operations

- Arithmetic operators: elementwise application

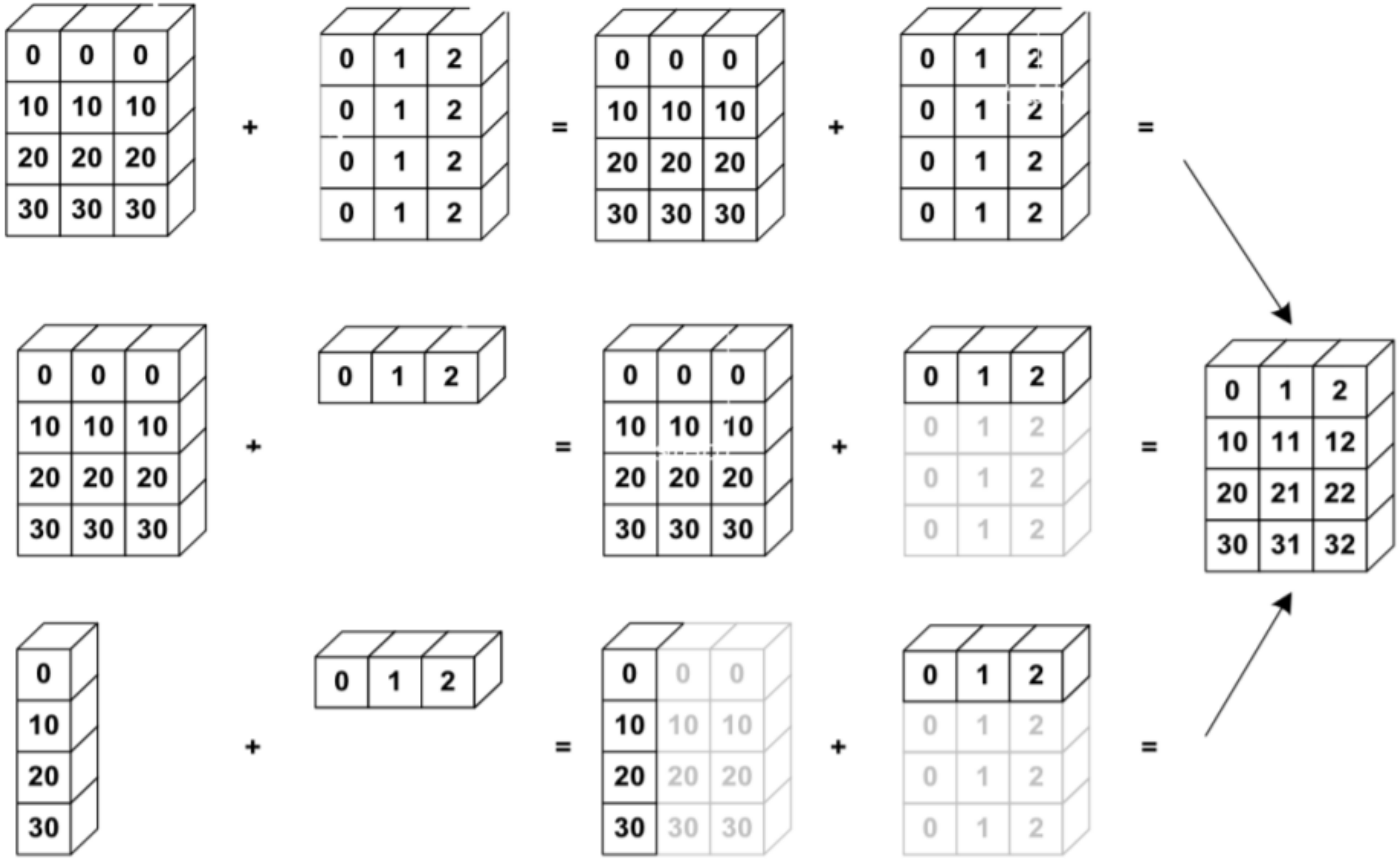
```
a = np.arange(4)
# array([0, 1, 2, 3])

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
  - They are of equal size
  - 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)
```

np.dot(a,b)

If f both *a* and *b* are 1-D arrays, it is inner product of vectors

If both *a* and *b* are 2-D arrays, it is matrix multiplication

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

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 $\arg\min_x \|Ax - b\|_2$
`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`

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

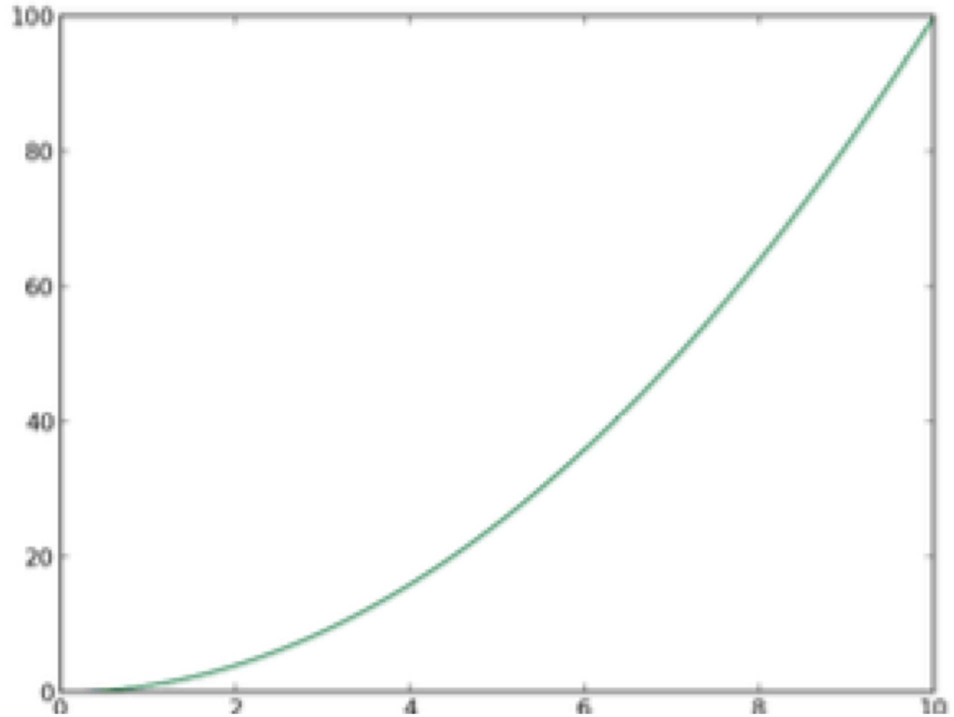
- Methods for loading and saving data
  - Matlab files
  - Matrix Market files (sparse matrices)
  - Wav files

What is Matplotlib?

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

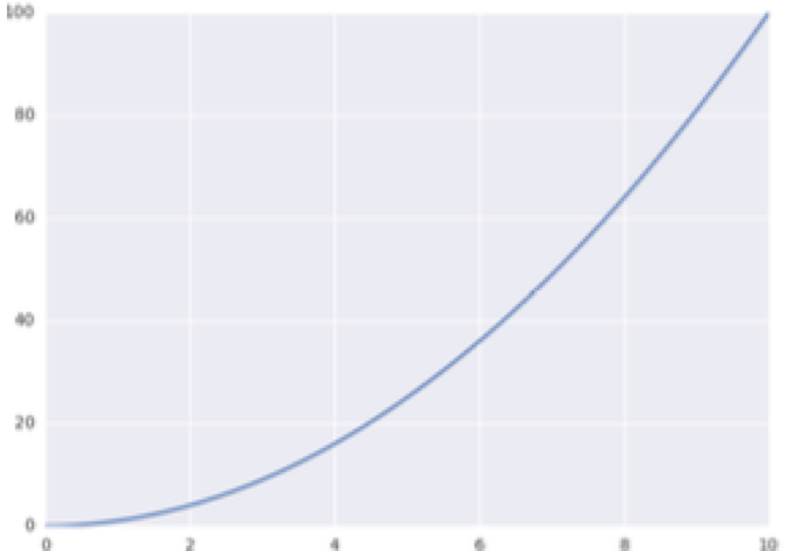
Scatter Plot

```
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()
```

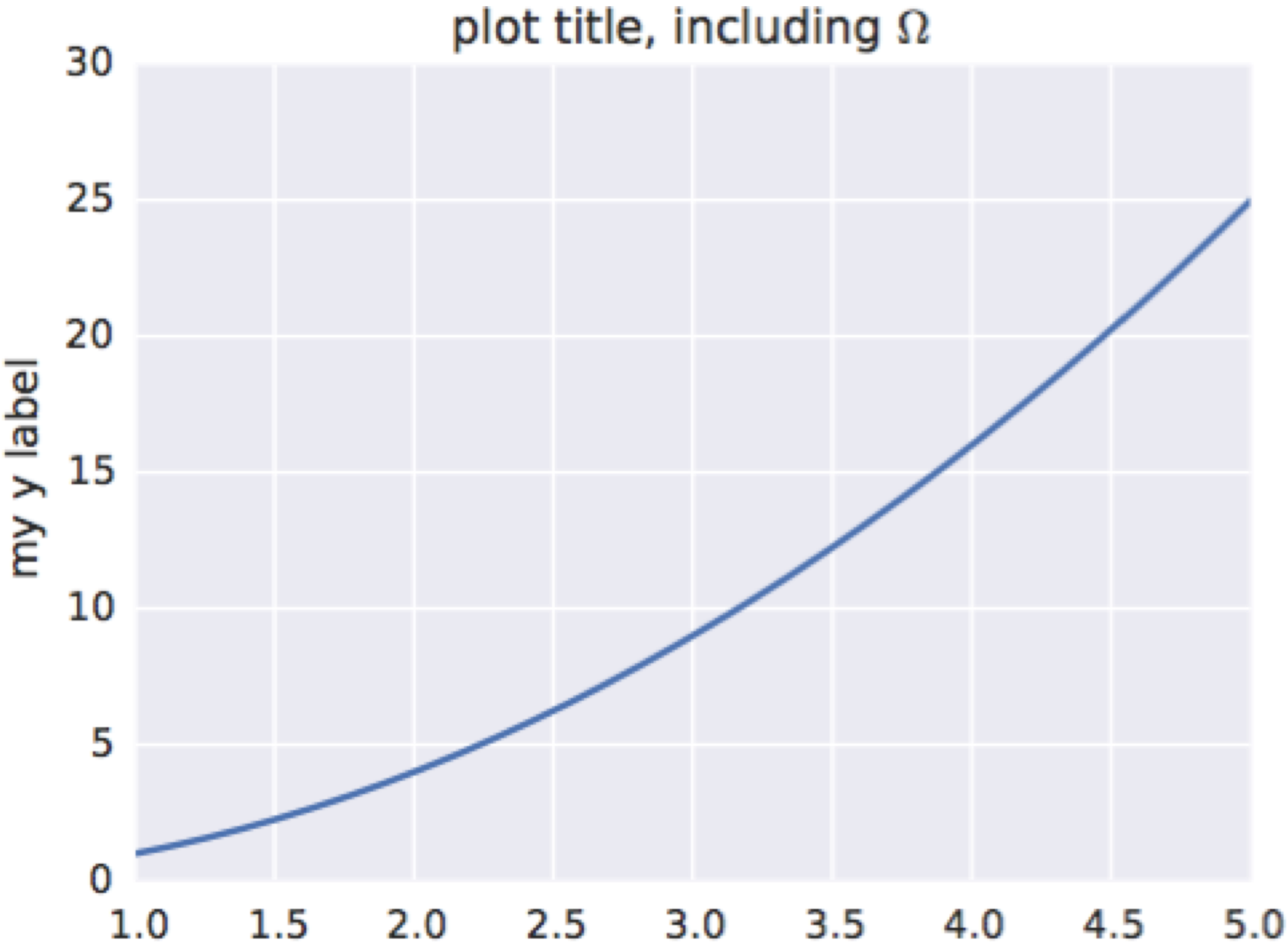


Scatter Plot

- 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

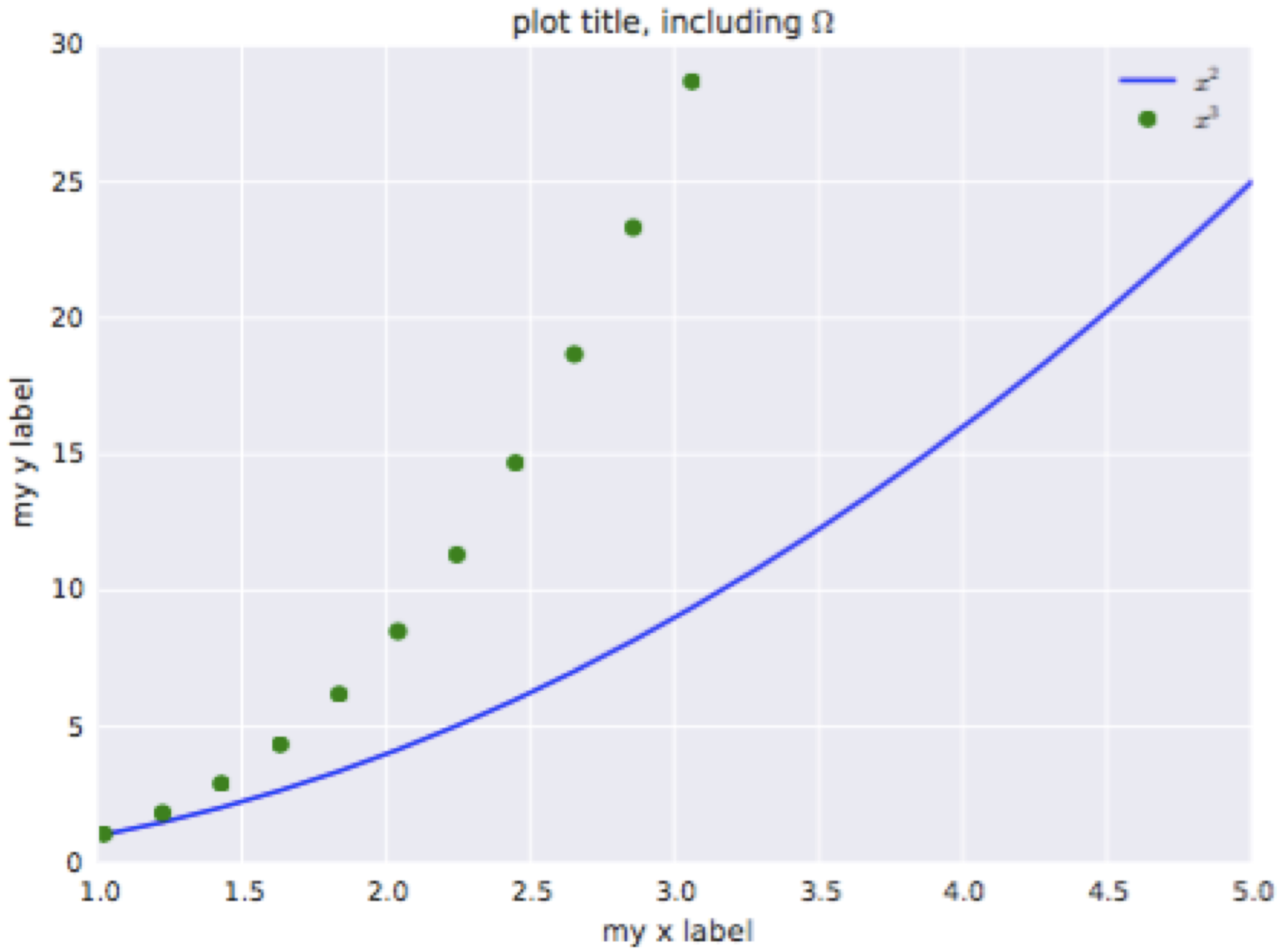


Scatter Plot

- 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')
```

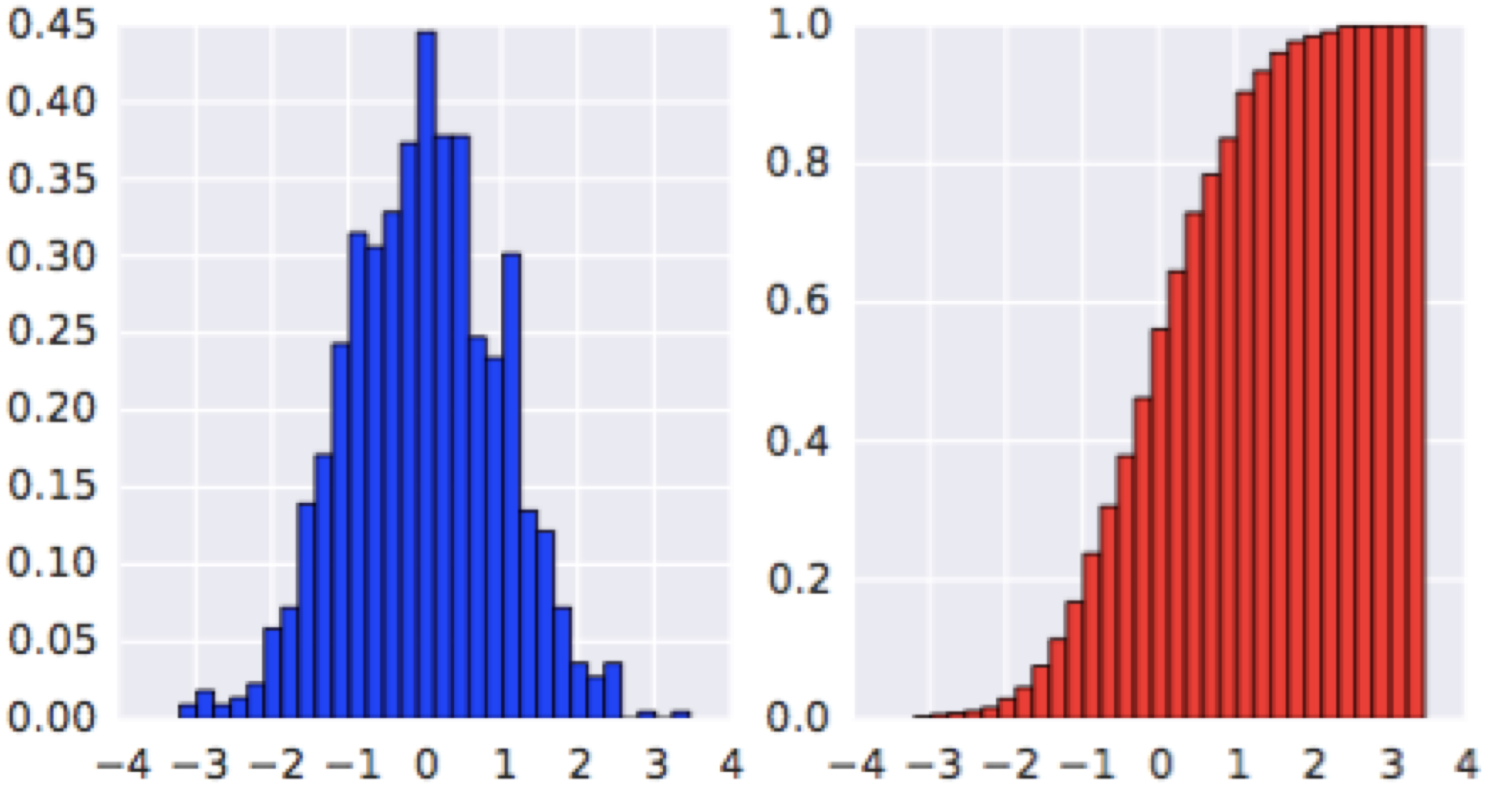
Scatter Plot



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

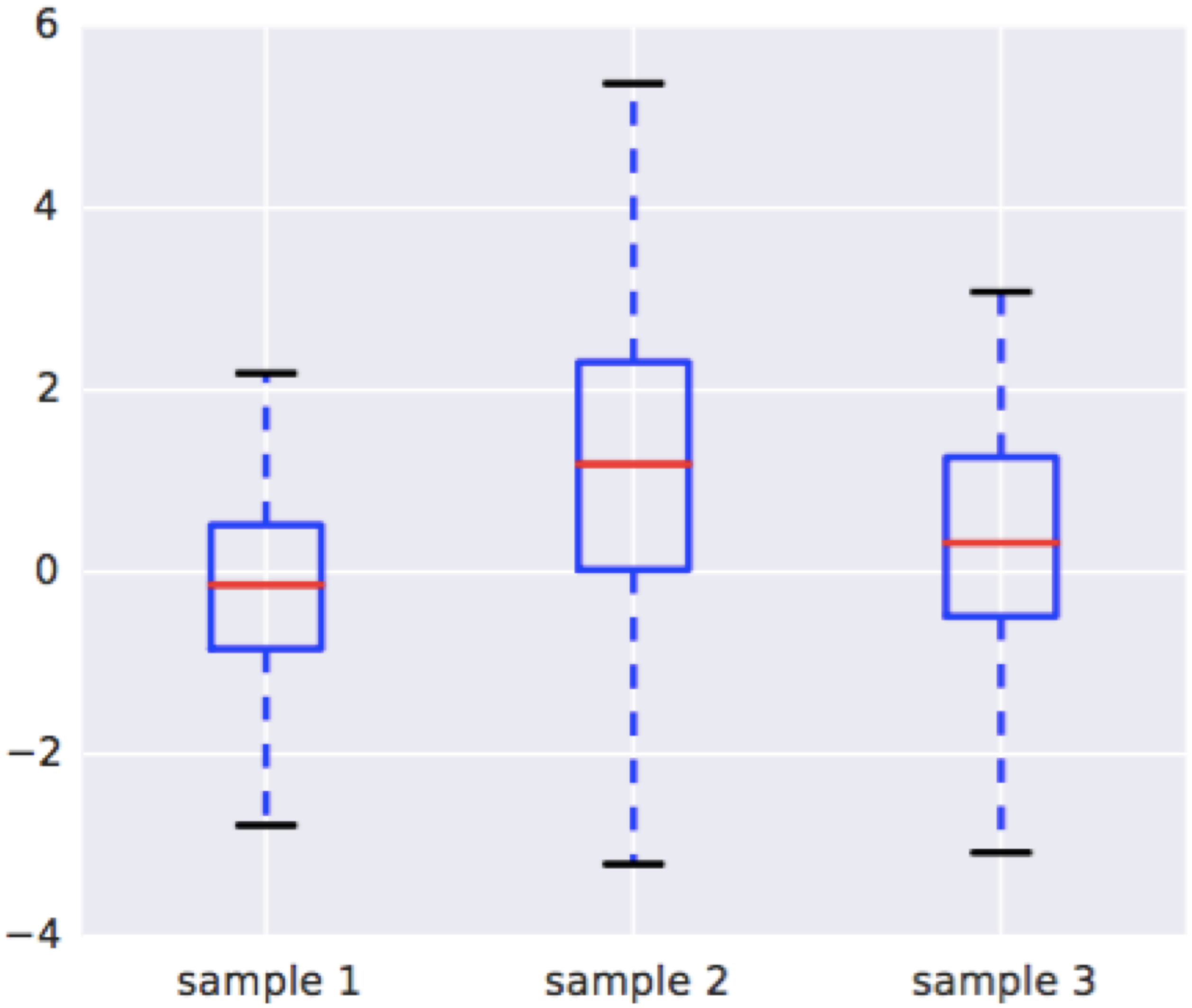
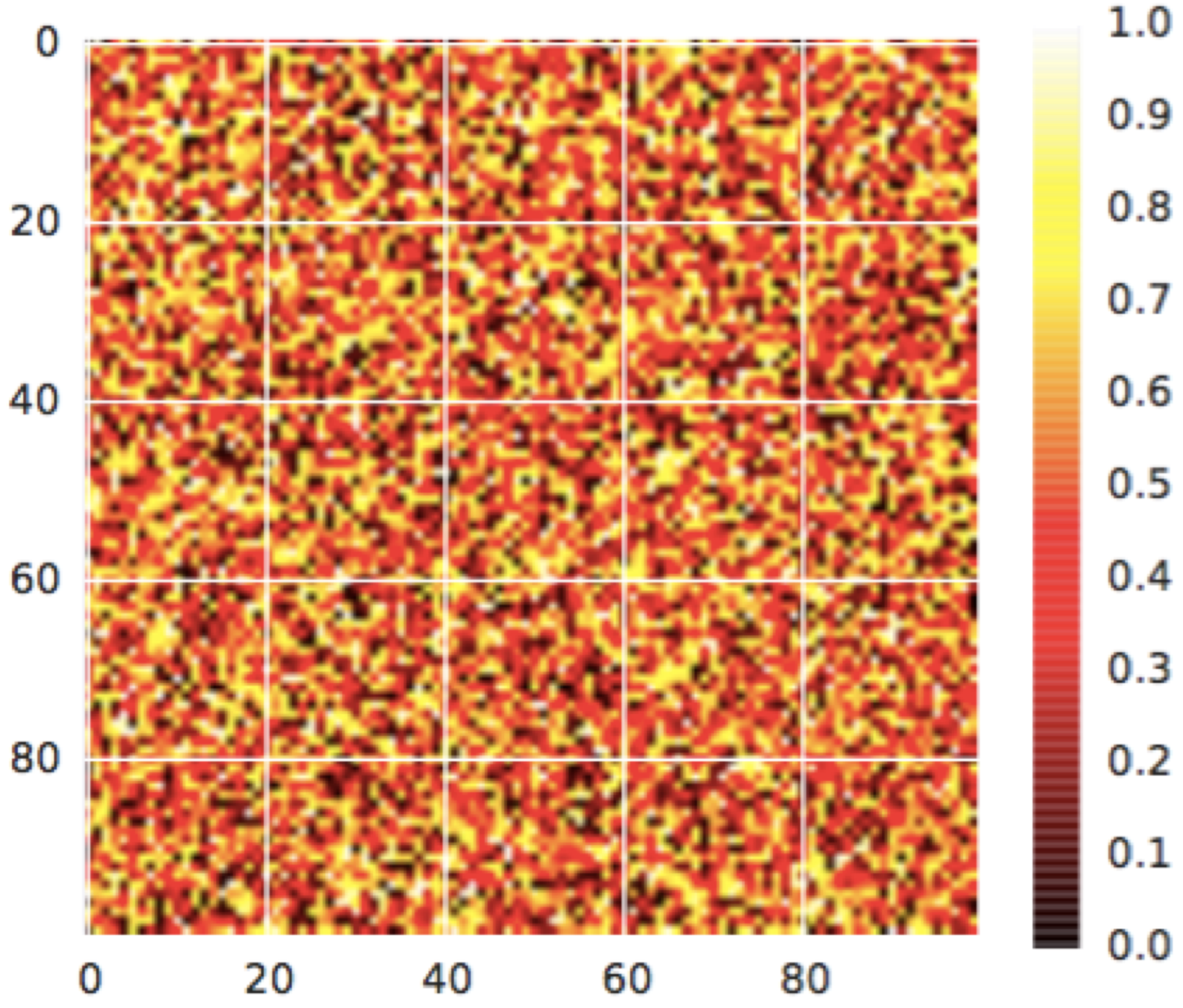


Image Plot

```
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