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

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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

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])
```

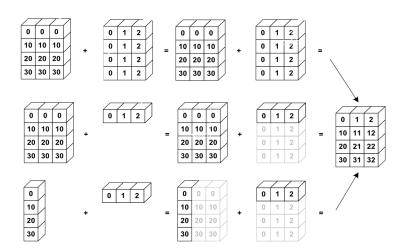
Also, we can use += and *=.

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

Matrix operations

First, define some matrices:

Matrix operations

```
np.dot(A, B)
# array([[ 2., 2., 2.],
  [2., 2., 2.],
        Γ 2.. 2.. 2.11)
np.dot(B, A)
# array([[ 3., 3.],
  [3., 3.11)
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 1)
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 zero: First dimension has 'priority', so beware of unexpected results

Try it

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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 $\arg\min_{x} \|Ax - b\|_2$

eig(A) Eigenvalue decomposition

 $\verb"eig(A) \qquad \qquad \textit{Eigenvalue decomposition for symmetric or hermitian}$

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 (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

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Contents

- Second part of course
- Numpy
- Scipy
- Matplotlib
- Exercises

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

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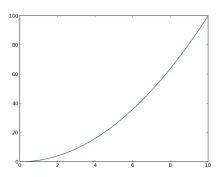
What is Matplotlib?

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

Scatter Plot

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

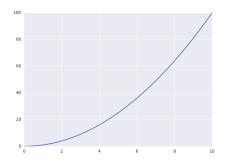
x = np.linspace(0, 10, 1000)
y = np.power(x, 2)
plt.plot(x, y)
plt.show()
```



Seaborn makes plot pretty

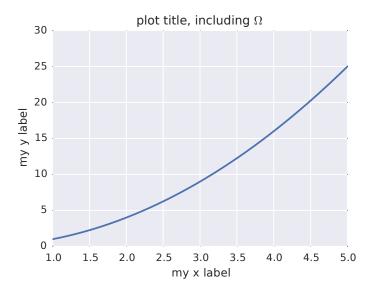
```
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

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



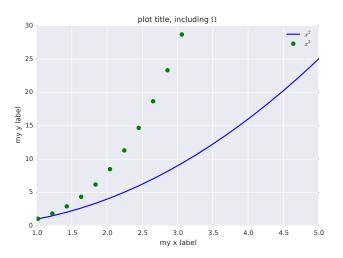
Adding titles and labels

```
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')
```



Adding multiple lines and a legend

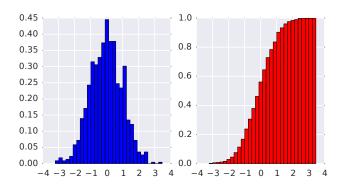
```
x = np.linspace(0, 10, 50)
y1 = np.power(x, 2)
v2 = np.power(x, 3)
plt.plot(x, y1, 'b-', label='$x^2$')
plt.plot(x, y2, 'go', label='$x^3$')
plt.xlim((1, 5))
plt.ylim((0, 30))
plt.xlabel('my x label')
plt.ylabel('my y label')
plt.title('plot title, including $\Omega$')
plt.legend()
plt.savefig('line_plot_plus2.pdf')
```



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



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

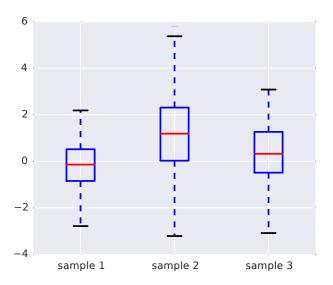
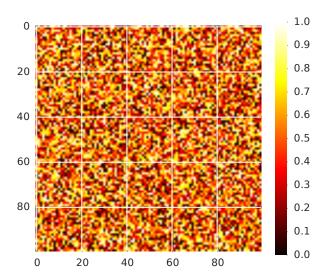


Image Plot

```
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

