CME 193: Introduction to Scientific Python

Winter 2017

Lecture 5: Numpy, Scipy, and Matplotlib

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Contents

Congrats, we are halfway!

Up to now

- Covered the basics of Python
- Worked on a bunch of tough exercises

From now

- Cover specific topics
- Less exercises
- Time for project

Feedback

Thanks for the great feedback, very useful

And thanks for the great questions in and outside of class!

Remaining topics

- Numpy, Scipy, Matplotlib (today)
- pandas, scikitlearn (Thursday)
- Exception handling, unit testing, recursion
- Brief look at some more modules
  - Flask
  - Regex
  - ... (suggestions welcome)

Reminder

Homework 1 is due tonight at midnight

Office hours directly after class today

Homework 2/ Project

Option: Homework 2 or project

Homework 2 will be posted today

Email me project proposal ideas before Thurs lecture

Project ideas

- See course website, new Project tab
- Data science/ML projects - most important is that you have the data
- Think in terms of the two week timeline - be realistic

Project ideas

Final version of Python scripts and write-up: due one week after Lecture 8, on Thursday February 16.

The final version should include all source code and data, and be zipped. Make sure your code runs (whatever the input) smoothly.

Final write-up: an updated version of your proposal, explaining things that have changed and your results.

Contents

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

Numpy

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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]]
print A[0,0] # 1
print A[0,1:3] # [2 3]

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])
```

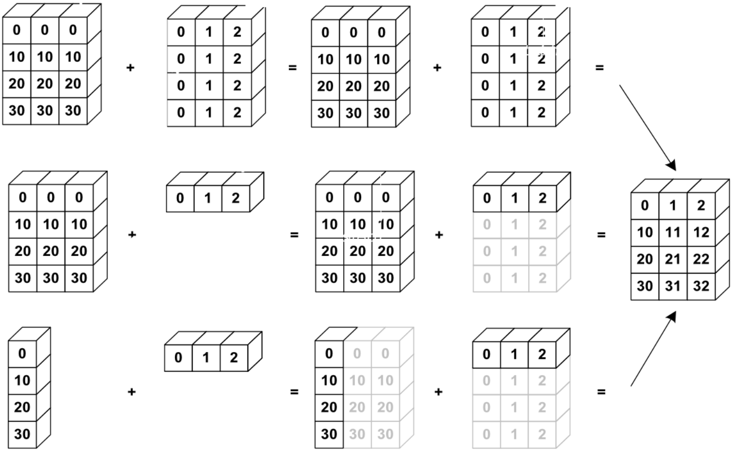
Also, we can use += and *=.

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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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

`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`

Exercise

Write a script that creates a random square matrix (A) with standard normal random variables and a random column vector (b) of the same size (also standard normal random variables).

Solve the system $Ax = b$.

Compute both the 2-norm and infinity norm of x as well as the Frobenius norm of A.

Hint see documentation for np.linalg.norm

Exercise

```python
import numpy as np

n = 200
A = np.random.randn(n,n)
b = np.random.randn(n,1)
x = np.linalg.solve(A,b)

print np.linalg.norm(x)
print np.linalg.norm(x, np.inf)
print np.linalg.norm(A, 'fro')
```

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

Example

```
from scipy import optimize

def f(x):
  return [x[0]  + 0.5 * (x[0] - x[1])**3 - 1.0,
      0.5 * (x[1] - x[0])**3 + x[1]]

x0 = [0, 0] # initial guess

sol = optimize.root(f, x0)

print sol.x
print sol.success
```

Exercise

Create a matrix (A) of random entries (your choice on distribution) with $m > n$ (more rows than columns).

Create a column vector $b \in \mathbb{R}^m$.

Find x that minimizes $\|Ax - b\|_2$. What is the norm of the residual?

Hint: use scipy.linalg.lstsq

Exercise

```python
import numpy as np
from scipy import linalg

n = 100
m = 200

A = np.random.randn(m,n)
b = np.random.randn(m,1)

x = linalg.lstsq(A, b)
print linalg.norm(np.dot(A,x[0])-b)
```

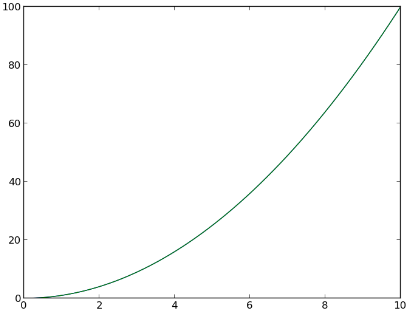
Contents

What is Matplotlib?

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

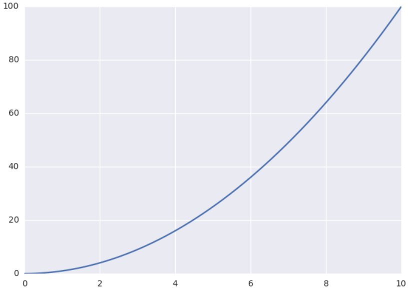
Scatter Plot

```
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

```python
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()
```



plt.show()

Calling `plt.show()` displays the figure objects to screen.

To create/display multiple figures, use `plt.figure()`, very similar to Matlab.

plt.figure()

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

x = np.linspace(0, 10, 1000)
y1 = np.power(x, 2)
y2 = np.power(x, 3)
f1 = plt.figure()
plt.plot(x, y1)
f2 = plt.figure()
plt.plot(x, y2)
plt.show()
```

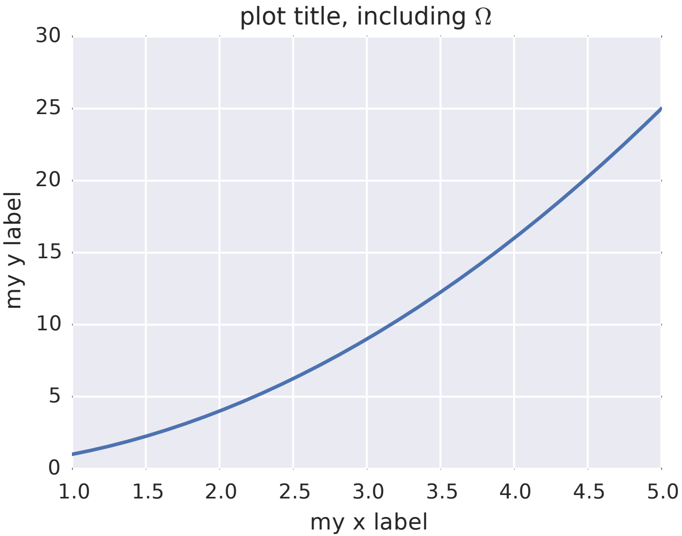
If we had not used separate figure calls, it would default to plotting both curves on same figure.

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

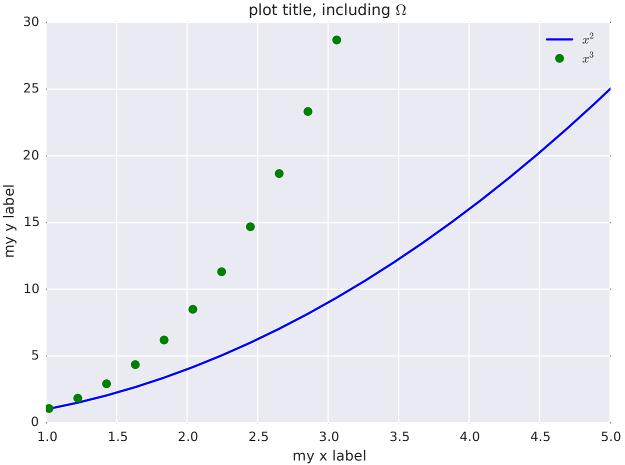


Scatter Plot

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')
```

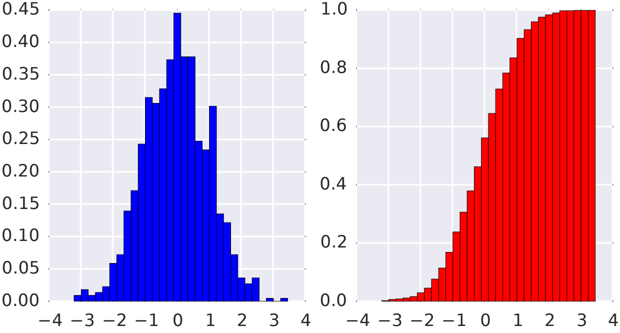
Scatter Plot



Histogram

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

data = np.random.randn(1000)

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

# histogram (pdf)
ax[0].hist(data, bins=30, normed=True, color='b')

# empirical cdf
ax[1].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

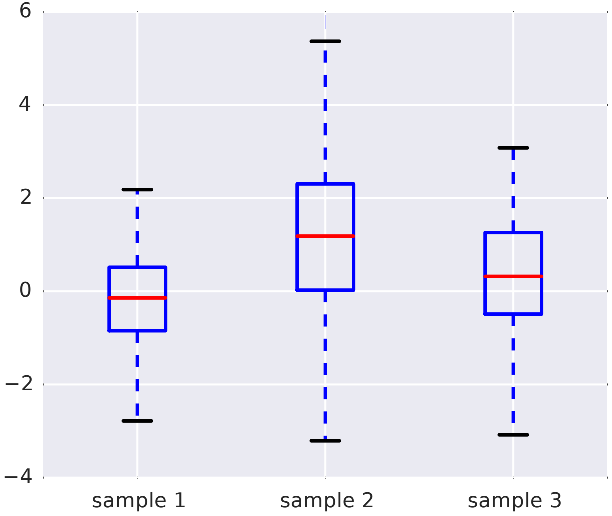
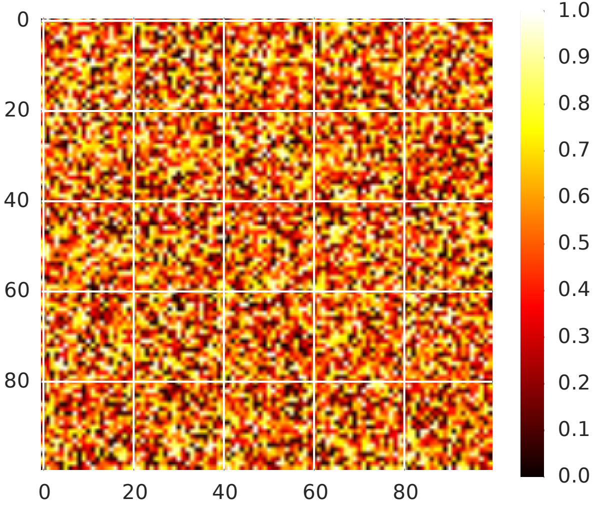


Image Plot

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

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

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

Image Plot

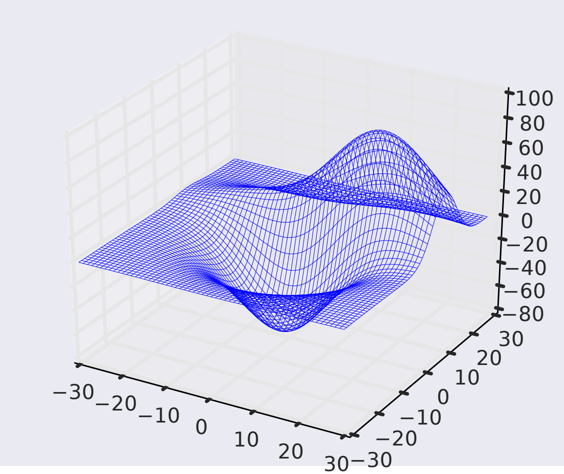


Wire Plot

matplotlib toolkits extend funtionality for other kinds of visualization

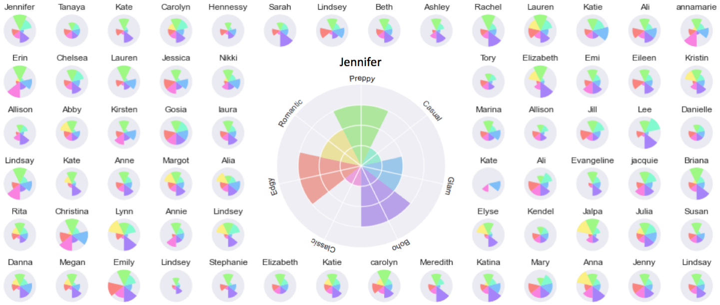
```
from mpl_toolkits.mplot3d import axes3d

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...



Exercise

Plot the following function on the interval $[-2, 2]$.

$$f(x) = sin(x)cos(x - \pi)e^{-x}$$

Exercise

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

def f(x):
  return np.sin(x)*np.cos(x-np.pi)*np.exp(-1.*x)

x = np.linspace(-2,2)
y = f(x)
plt.plot(x, y)
plt.show()
```