LECTURE 5: NUMPY AND MATPLOTLIB

Introduction to Scientific Python, CME 193

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Download exercises from:

`web.stanford.edu/~ermartin/Teaching/CME193-Winter15`

Eileen Martin

Some slides are from Sven Schmit's Fall '14 slides

Overview

- Numpy: basic objects, methods, functions
- Numpy: linear algebra
- Numpy: random
- Matplotlib: 2D plots
- Matplotlib: 3D plots
- Scipy vs Numpy
- Discuss assignment 4

Numpy

- Fundamental package for working with N-dimensional array objects (vector, matrix, tensor, …)

- corn has version 1.9.1, documentation:

  http://docs.scipy.org/doc/numpy/index.html

- Numpy arrays are a fundamental data type for some other packages to use
- Numpy has many specialized modules and functions:

numpy.linalg (Linear algebra)	numpy.random (Random sampling)
numpy.fft (Discrete Fourier transform)	sorting/searching/counting
math functions	numpy.testing (unit test support)

Declaring a Numpy array

Each Numpy array has some attributes:

shape (a tuple of the size in each dimension), dtype (data type of entries), size (total # of entries), ndim (# of dimensions), T (transpose)

Use these attributes to insert print statements into declaration.py to figure out each object's type, dimensions and entry data type:

```
import numpy as np

x0 = np.array([True,True,False])
x1 = np.array([2,1,4], np.int32)
x2 = np.array([[2,0,4],[3,2,7]])
x3 = np.empty([3,2])
x4 = np.empty_like(x2)
x5 = np.zeros(4, np.complex64)
x6 = np.arange(1,9,2.0)
x7 = np.diag([1, 2, 4])
x8 = np.linspace(0,np.pi,10)
```

http://docs.scipy.org/doc/numpy/reference/routines.array-creation.html

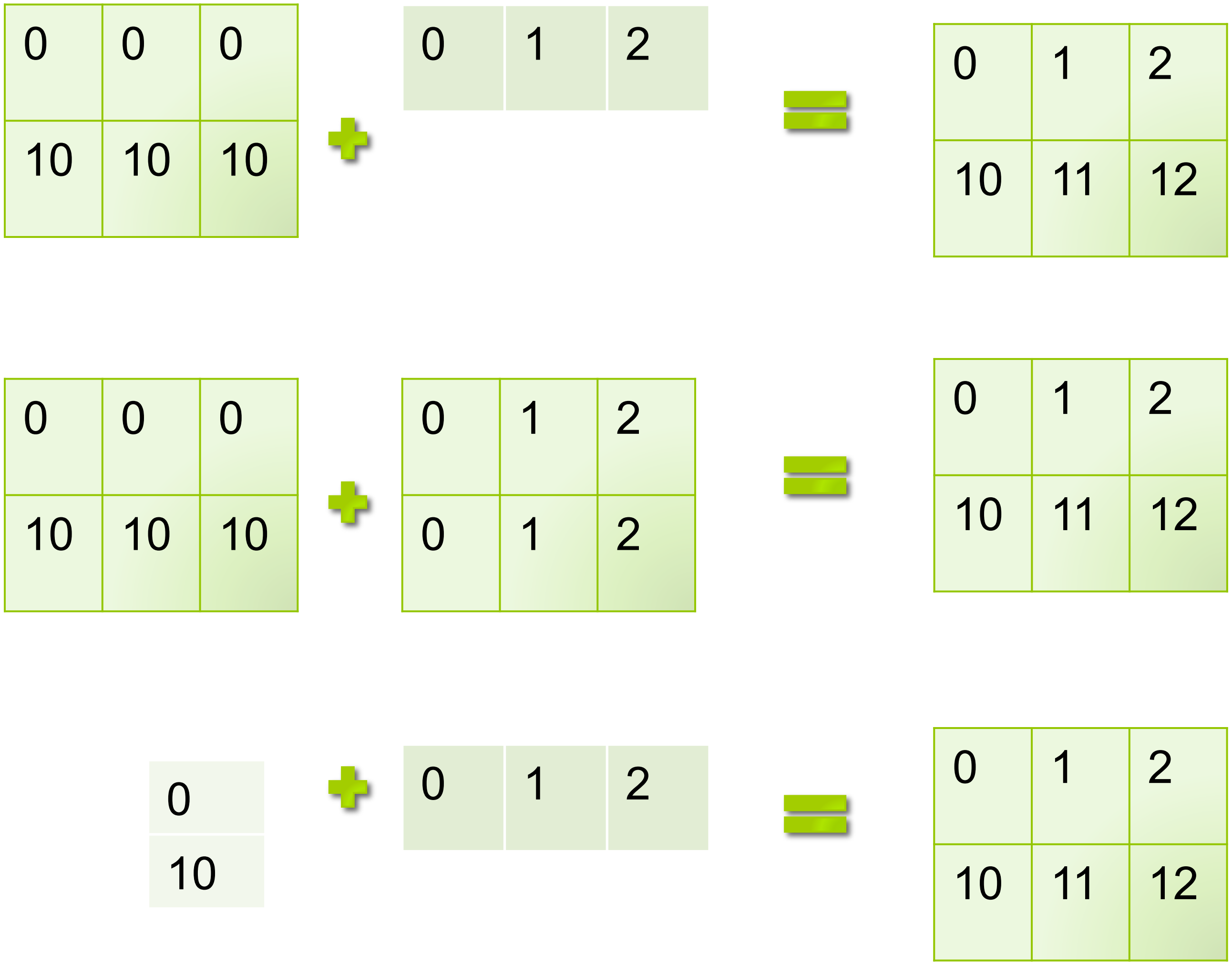
What can you do?

- Add two arrays
- Add all entries in one array
- Multiply two arrays (1D, 2D)
- Take the exponential of each element in an array
- Multiply an array by a scalar
- Get the minimum element of an array
- Print a few elements of an array
- Print a single column or row of an array
- Multiply two arrays via matrix multiplication

Solutions will be posted on website after class

Array broadcasting:

Automatically make copies of arrays to fill in length 1 dimensions



$$\begin{bmatrix}0 & 0 & 0\\10 & 10 & 10\end{bmatrix} + \begin{bmatrix}0 & 1 & 2\end{bmatrix} = \begin{bmatrix}0 & 1 & 2\\10 & 11 & 12\end{bmatrix}$$

$$\begin{bmatrix}0 & 0 & 0\\10 & 10 & 10\end{bmatrix} + \begin{bmatrix}0 & 1 & 2\\0 & 1 & 2\end{bmatrix} = \begin{bmatrix}0 & 1 & 2\\10 & 11 & 12\end{bmatrix}$$

$$\begin{bmatrix}0\\10\end{bmatrix} + \begin{bmatrix}0 & 1 & 2\end{bmatrix} = \begin{bmatrix}0 & 1 & 2\\10 & 11 & 12\end{bmatrix}$$

Iterating over an array

- Iteration over all elements of array:

```
for element in A.flat
```

- Iteration over multidimensional arrays is done on slices in the first dimension:

```
for row in A
```

- Alternatively, could access entries through indices:

```
for i in range(A.shape[0]):
   for j in range(A.shape[1]):
```

Reshaping an array

- Use `reshape` to modify the dimensions of an array while leaving the total number of elements the same

```
A = np.arange(8)
A.reshape(2,4)
# gives [[0,1,2,3],[4,5,6,7]]
```

- Use `resize` to remove elements or append 0's in place (size can change under some circumstances*)

```
A.resize(2,3)
```

- Use `resize` to return a copy with removed elements or repeated copies

```
b = resize(a,(2,4))
```

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Numpy: Linear Algebra

- The numpy.linalg module has many matrix/vector manipulation algorithms

(a subset of these is in the table)

name	explanation
dot(a,b)	dot product of two arrays
kron(a,b)	Kronecker product
linalg.norm(x)	matrix or vector norm
linalg.cond(x)	condition number
linalg.solve(A,b)	solve linear system Ax=b
linalg.inv(A)	inverse of A
linalg.pinv(A)	pseudo-inverse of A
linalg.eig(A)	eigenvalues/vectors of square A
linalg.eigvals(A)	eigenvalues of general A
trace(A)	trace (diagonal sum)
linalg.svd(A)	singular value decomposition

http://docs.scipy.org/doc/numpy/reference/routines.linalg.html

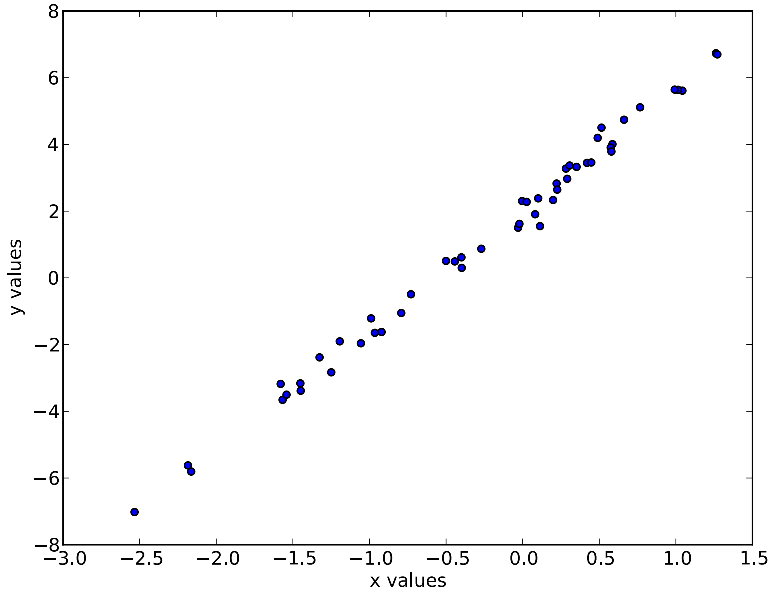
Linear algebra exercise: least squares

- In leastSquares.py, you are given a bunch of noisy data points and you want to fit them with a line:

$$ax_i + b = y_i$$

- This can be written in matrix format

$$\begin{pmatrix} x_0 & 1 \\ x_1 & 1 \\ \dots & 1 \\ x_{n-1} & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ \dots \\ y_{n-1} \end{pmatrix}$$



- Solve for (a,b) so that

$$\min_{a,b} \|X \begin{pmatrix} a \\ b \end{pmatrix} - y\|_2^2$$

- Hint: Try using linalg.solve(X,y), linalg.pinv(X), or linalg.lstsq(X,y)

http://docs.scipy.org/doc/numpy/reference/routines.linalg.html

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Numpy: Random

- In the linear regression exercise, those ‘measurements’ were actually generated by numpy.random

```
x = np.random.randn(50)    # draw 50 numbers from the standard normal dist.
y = 3.5*x+2+np.random.randn(50)*0.3  # apply a linear transform and add noise
```

- If you run this, you’ll get different numbers each time, so you might want to use `np.random.seed(someObject)` to reproduce a random experiment

http://docs.scipy.org/doc/numpy/reference/routines.random.html

Numpy: Random

- The numpy.random module has many distributions you can draw from (a very small subset of these is in the table)

name	explanation
rand(n0,n1,…)	ndarray of random values from uniform [0,1]
randn(n0,n1,…)	random standard normal
randint(lo, [hi, size])	random integers [lo, hi)
shuffle(seq)	shuffle sequence randomly
choice(seq,[size,replace,p])	sample k items from a 1D array with or without replacement
chisquare(df,[size])	sample from Chi-squared distribution with df degrees of freedom
exponential([scale,size])	sample from exponential distribution

http://docs.scipy.org/doc/numpy/reference/routines.random.html

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Matplotlib: 2D plots

- Matplotlib is the 2D Python plotting library
- We'll mostly use `matplotlib.pyplot`
- There are tons of options, so consult the documentation:
  http://matplotlib.org/users/beginner.html
- matplotlib.pyplot can do many types of visualizations including:
  - Histograms, bar charts (using hist)
  - Error bars on plots, box plots (using boxplot, errorbar)
  - Scatterplots (using scatter)
  - Line plots (using plot)
  - Contour maps (using contour or tricontour)
  - Images (matrix to image) (using imshow)
  - Stream plots which show derivatives at many locations (streamplot)
  - Pie charts, polar charts (using pie, polar)

Matplotlib: First example

- Run the code in sin.py
- How do we show two curves on the same plot?

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

# array of evenly spaces points from 0 to pi
x = np.linspace(0,np.pi,100)
# calculate the sine of each of those points
y = np.sin(x)
# create a plot of the sine curve
plt.plot(x,y)
# actually show that plot
plt.show()
```

More examples: http://matplotlib.org/gallery.html
Documentation: http://matplotlib.org/api/pyplot_api.html

Back to the linear regression example

- Uncomment lines 28-32 and run the code to produce a scatter plot

- At the end of the code create a plot that overlays the scatter plot with a line plot showing your fit: ax+b = y

- As an extra challenge, try to color the markers of the data points to reflect their distance from the line

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Matplotlib: 3D plots

- To do 3D plotting, we'll use `mpl_toolkits.mplot3d` Axes3D class
- Documentation:

http://matplotlib.org/mpl_toolkits/mplot3d/tutorial.html#mplot3d-tutorial

- Can do:
  - Line plots (use plot)
  - Scatter plots (use scatter)
  - Wireframe plots (use plot_wireframe)
  - Surface plots (use plot_surface)
  - Contours (use contour)
  - Bar charts (use bar)

3D Plots: First example

- Run the code in sin3D.py

```
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D

# arrays of evenly spaces points from 0 to pi
x = np.linspace(0,np.pi,40)
y = np.linspace(0,np.pi*2,80)
x,y = np.meshgrid(x,y)
# calculate the product of sines for each point
z = np.sin(x)*np.sin(y)
# create a plot of the sine product
ax = plt.subplot(111, projection=‘3d’)
ax.plot_surface(x,y,z)
# actually show that plot
plt.show()
```

More examples: http://matplotlib.org/gallery.html
Documentation: http://matplotlib.org/mpl_toolkits/mplot3d/

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Scipy vs. Numpy

- Scipy is a library that can work with Numpy arrays, but can achieve better performance and has some more specialized libraries
  - linear algebra (scipy.linalg uses BLAS/LAPACK)
  - statistics (scipy.stats has hypothesis tests, correlation analysis)
  - optimization (scipy.optimize has multiple solvers, gradient checks, simulated annealing)
  - sparse matrices (scipy.sparse supports sparse linear algebra, graph analysis, multiple sparse matrix formats)
  - signal processing (scipy.signal has convolutions, wavelets, splines, filters)

http://docs.scipy.org/doc/scipy/reference/

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Assignment 4 discussion

- Your questions on assignment 4?

- Tips for assignment 5:
  - **Online documentation is your friend.** Don’t hesitate to use it!
  - Stuck? test smaller, simpler statements in interactive mode
  - Build test cases to verify correctness of your code (not every unit test has to fit into the unittest module framework
  - Talk to each other. Use the CourseWork Forums.
  - Come to office hrs. Mon. 9:30-10:30, Wed. 3:15-4:15