

Introduction to High Performance Scientific Computing

Autumn, 2016

Lecture 6

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27 October, 2016

Python notes

Getting comfortable with python:

- Have command of *all* of the material in lecture 3 slides and numpy section of lecture 5 slides (use lab 2 and lab 3 exercises for self-assessment)
- Understand structure and purpose of functions (lecture 4 slides)
- Understand *mysqrt.py* (provided in lecture5 directory of course repo)
- Today's material: plotting, SVD, solving initial value problems
- Further help: list of supplementary material on course webpage, office hours

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Importing modules

- In scripts, use:

```
In [1]: import numpy as np
```

```
In [2]: np.linspace(0.0,1,3)
```

```
Out[2]: array([ 0. ,  0.5,  1. ])
```

- This way, users know which packages are needed and which specific functions are being used

- If only using one or two functions, can use:

```
In [3]: from numpy import linspace
```

```
In [4]: linspace(0.0,1,3)
```

```
Out[4]: array([ 0. ,  0.5,  1. ])
```

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Importing modules

- Can also import all functions at once:

```
In [6]: from numpy import *
```

```
In [7]: linspace(0.0,1,3)
```

```
Out [7]: array([ 0. ,  0.5,  1. ])
```

- **Ok at terminal, but not in scripts! Makes it difficult to see where and how the module is being used.**

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Importing modules

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```
In [6]: from numpy import *
```

```
In [7]: linspace(0.0,1,3)
```

```
Out [7]: array([ 0. ,  0.5,  1. ])
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- **Ok at terminal, but not in scripts! Makes it difficult to see where and how the module is being used.**
- When launching ipython with `ipython --pylab`, the `pylab` flag means terminal is launched with:
 - In [1]: from numpy import *
 - In [2]: from matplotlib import *

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Importing modules

- Can also import all functions at once:

```
In [6]: from numpy import *
```

```
In [7]: linspace(0.0,1,3)
```

```
Out [7]: array([ 0. ,  0.5,  1. ])
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- **Ok at terminal, but not in scripts! Makes it difficult to see where and how the module is being used.**
- When launching ipython with `ipython --pylab`, the `pylab` flag means terminal is launched with:
 - In [1]: from numpy import *
 - In [2]: from matplotlib import *
- The `%pylab` command in ipython notebook does the same thing.

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2d plots

- Matplotlib package provides Matlab-like plotting
- Usually included in scripts as: `import matplotlib.pyplot as plt`
- Will look at illustrative example here and provide supplementary ipython notebook

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2d plots: simple example

- Create and plot 2 simple functions

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

#Create some arrays to be plotted
Nx = 100
Ny = 200
x = np.linspace(0.0, np.pi, Nx)
y = np.linspace(-np.pi, np.pi, Ny)

f = np.sin(x)
g = np.cos(y)
```

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2d plots: simple example

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x = np.linspace(0.0, np.pi, Nx)
y = np.linspace(-np.pi, np.pi, Ny)

f = np.sin(x)
g = np.cos(y)

#Create plot
plt.figure() #make new figure

plt.plot(x, f, 'b-', label='sin') #blue line
plt.plot(y, g, 'r--', label='cos') #red dashed line
```

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2d plots: simple example

- Create and plot 2 simple functions

```
#Create plot
plt.figure() #make new figure

plt.plot(x,f,'b-',label='sin') #blue line
plt.plot(y,g,'r--',label='cos') #red dashed line

#add axis labels,legend, and figure title
plt.xlabel('time')
plt.ylabel('f(t),g(t)')
plt.legend(loc='best')
plt.title('Illustrative figure prepared by Prasun Ray')
```

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2d plots: simple example

- Create and plot 2 simple functions

```
#Create plot
plt.figure() #make new figure

plt.plot(x,f,'b-',label='sin') #blue line
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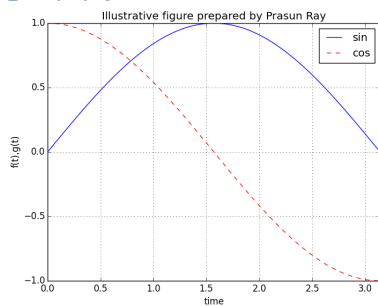
#adjust x-axis limits, turn on grid, display and save figure
plt.xlim(0,np.pi)
plt.grid()
plt.show()

plt.savefig('plot_example.png')
```

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2d plots: simple example

- Create and plot 2 simple functions
- *plot_example.png:*



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2d plots

- Use `loglog`, `semilogx`, `semilogy` for logarithmic axes
- `contour` for functions of two variables
- `hold(True)` or `hold(False)` to overlay curves on single figure (or not)
- Example code in repo: `plot_example.py`
- See online tutorial for further info: http://matplotlib.org/users/pyplot_tutorial.html
- Also look at: <http://matplotlib.org/gallery.html> (includes complex figures + code that generates them)

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scipy overview

- `scipy` is a module which contains a wide variety of scientific tools
- A few useful submodules:
 - `scipy.special`
 - `scipy.integrate`
 - `scipy.optimize`
 - `scipy.fftpack`
 - `scipy.signal`
- Try tab completion: `scipy. <tab>`
`import scipy. <tab>`

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A scipy example

- Use `odeint` from `scipy.integrate` module to solve:

$$\frac{d^2 y}{dt^2} + \omega^2 y = 0$$

- First, rewrite as two 1st-order ODEs:

$$\frac{dy_1}{dt} = y_2$$

$$\frac{dy_2}{dt} = -\omega^2 y_1$$

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A scipy example

$$\frac{dy_1}{dt} = y_2$$

$$\frac{dy_2}{dt} = -\omega^2 y_1$$

- **Basic idea:** discretize time, $t = 0, dt, \dots, N \cdot dt$, and starting from $y(0)$ march forward in time and compute $y(dt), \dots, y(N \cdot dt)$
- `odeint` chooses the stepsize, dt , so that error tolerances are satisfied
- Need to specify:
 - Initial condition
 - Timespan for integration
 - A Python function which provides RHS of the ODE to `odeint`
- Look at `ode_example.py`

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Singular Value Decomposition

SVD is a powerful tool for data analysis and optimization

- Widely used for extracting "important" components of multidimensional data, reducing number of dimensions: Principal Component Analysis
- Provides information on maximum growth of linear ODEs
- Can be used for simple data compression

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Singular Value Decomposition

Overview, any $M \times N$ matrix, A , can be decomposed as:

$$A = USV^T$$

U is a $M \times M$ matrix whose columns are the eigenvectors of AA^T

V is a $N \times N$ matrix whose columns are the eigenvectors of $A^T A$

S is a $M \times N$ matrix with $\min(M, N)$ entries on its diagonal

- These entries are real, non-negative, ordered

$$S_{11} \geq S_{22} \geq S_{33} \geq \dots \geq 0$$

- Called singular values, square root of eigenvalues of AA^T , $A^T A$

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Singular Value Decomposition

Overview, *any* $M \times N$ matrix, A , can be decomposed as:

$$A = USV^T$$

Importance of SVD stems (primarily) from importance of AA^T and $A^T A$

Can be used to find maximum of $|Ax|^2 = x^T A^T A x$

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Singular Value Decomposition

Overview, *any* $M \times N$ matrix, A , can be decomposed as:

$$A = USV^T$$

Importance of SVD stems (primarily) from importance of AA^T and $A^T A$

Can be used to find maximum of $|Ax|^2 = x^T A^T A x$

SVD of measurements can be used to analyze covariance matrix AA^T :

$$A = \begin{bmatrix} a_1 & a_2 & \dots & a_n \\ b_1 & b_2 & \dots & b_n \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} \quad \frac{1}{n} \sum_{j=1}^n a_j = 0$$

Principal component analysis (PCA)

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Singular Value Decomposition

Can rewrite SVD as:

$$A = u_1 S_{11} v_1^T + u_2 S_{22} v_2^T + u_3 S_{33} v_3^T + \dots$$

Here, u_i is i^{th} eigenvector of AA^T

and v_i is i^{th} eigenvector of $A^T A$

- These eigenvectors have length=1, so the singular values indicate importance of each term in sum
- Can discard terms with small S_{ii} values
- Then only need to save the first "K" eigenvectors and singular values
- Can reconstruct partial sum from these stored quantities, choose K based on: how quickly S_{ii} terms decrease, and desired memory savings

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Singular Value Decomposition

SVD in Python:

- `np.linalg.svd`
- `scipy.linalg.svd`
- `scipy.sparse.linalg.svds`
- `scipy.linalg` routines will be at least as fast as `np.linalg`, depending on installation, could be faster
- `sparse.linalg.svds` slower than others, but uses *much* less memory.
-- Very important for large matrices (and datasets)

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Beyond Scipy and Numpy

Pandas: Powerful module for data analysis

Scikit-learn: Machine learning

And much more... look around online!

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Homework 2

- Will be posted late afternoon today
- Using python for image processing
- Numerically solve system of ODEs modeling spread of infectious diseases
- Today's office hour (in MLC): 4-5 pm instead of 5-6 pm

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