Science with Python: NumPy, SciPy and Matplotlib

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for Earth Scientists:
27 & 29 Sept. 2011

Three collections of interrelated modules

SciPy

Mathematical algorithms and functions for science

NumPy

Deals with arrays of numbers

Matplotlib

Graphing and plotting tools

Much science in here: take a collection of numbers, do something to them and plot the results.

NumPy

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NumPy - provides `array` objects

Has size (number of elements).

Has shape (length of each dimension).

Has dtype (type of the data) and a type (ndarray).

Size, shape and data type are all fixed.

a =

10.0	15.7	12.2
14.2	77.3	-2.5
12.22	1.00E-03	77.2
12.0	2.0	111.23

(Actually, NumPy provides the ndarray class but this is a detail that can be ignored)

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Think of them like Fortran arrays.

(Actually, NumPy provides the ndarray class but this is a detail that can be ignored)

array

Create an empty array, fill it with zeros (or ones) or start from a list or a list of lists.

```
import numpy as np
a = np.array([10.0, 13.2, 4.3])
a.size # 3
a.shape # (3,)
a.dtype # ‘float64’
b = np.zeros((3,3))
c = np.ones((3,3))
```

Create arrays

array arithmetic

Most operators are overloaded, work element wise on arrays and return arrays.

```
import numpy as np
a = np.array([10.0, 10.0, 10.0])
b = np.array([1.0, 2.0, 3.0])
a + b # 11.0, 12.0, 13.0
a * b # 10.0, 20.0, 30.0
```

Add arrays

Functions for arrays

Most operators are overloaded, work element wise on arrays and return arrays.

```
import numpy as np
a = np.array([0.0, 30.0, 90.0])
b = np.radians(a)
c = np.sin(b)
# c is 0.0, 0.5, 1.0
```

Use numpy like math, but for arrays

Array indices

Work like list indices but you can have several of them separated by commas.

```
import numpy as np
a = np.array([[1.0, 2.0, 3.0],
              [4.0, 5.0, 6.0]])
a[0,0] # 1.0
a[0,2] # 3.0
a[1,0] # 4.0
a[1,2] # 6.0
```

Like lists

Array indices

Work like list indices but you can have several of them separated by commas.

```
import numpy as np
a = np.array([[1.0, 2.0, 3.0],
              [4.0, 5.0, 6.0]])
a[0,0:3] # 1.0, 2.0, 3.0
a[0:2,0] # 1.0, 4.0
a[1,:] # 4.0, 5.0, 6.0
a[0,0:3:2] # 1.0, 3.0
```

Colons - start:length:stride

Internally array data is just a chunk of memory

a =

.dtype = ubite .size = 9

.shape = (3,3) .data =

10010100	10010101	10010111
11010101	10010010	10111101
00011001	10011001	01011001

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a =

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Directly access compiled code: fast for array ops

Looks like a C or Fortran array

SciPy: a collection of useful modules

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Stats

The SciPy stats module provides simple and advanced statistics functions

```
import numpy as np
import scipy.stats as sps
a = np.array([23,33,25,34,20,21,22,21,20,23])
np.mean(a) # ~24.2
sps.gmean(a) # ~23.8
sps.hmean(a) # ~23.4
sps.mode(a) # 20
```

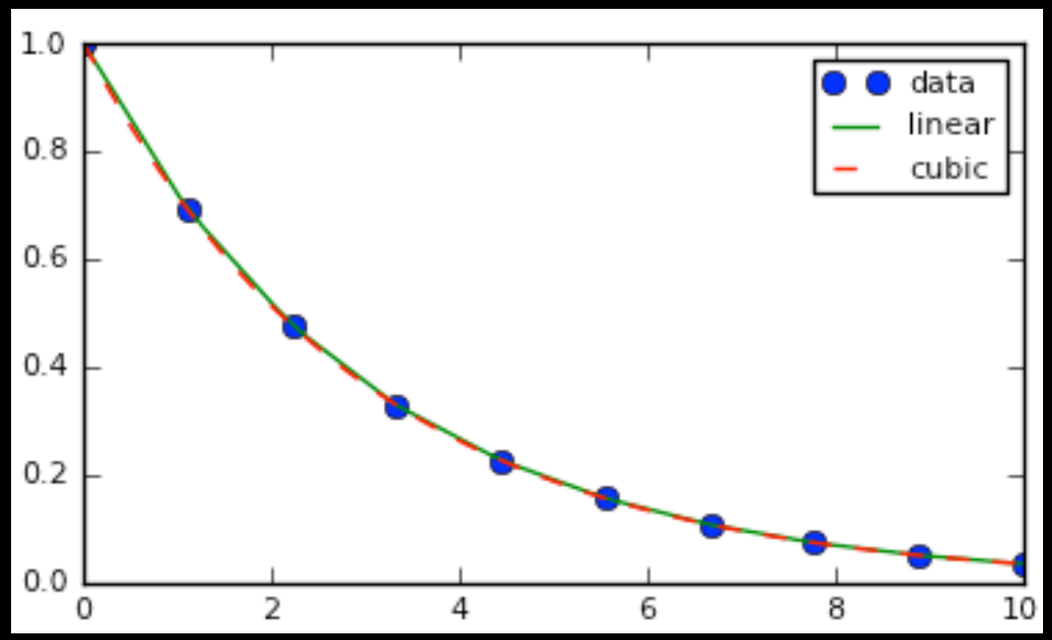
Lots more

Interpolate

The SciPy interpolate module has a large number of interpolation schemes

```
import numpy as np
import scipy.interpolate as spi

x = np.linspace(0, 10, 10)
y = np.exp(-x/3.0)
f = spi.interp1d(x, y)
f2 = spi.interp1d(x, y, kind='cubic')
```



Matplotlib

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Interpolate and plot

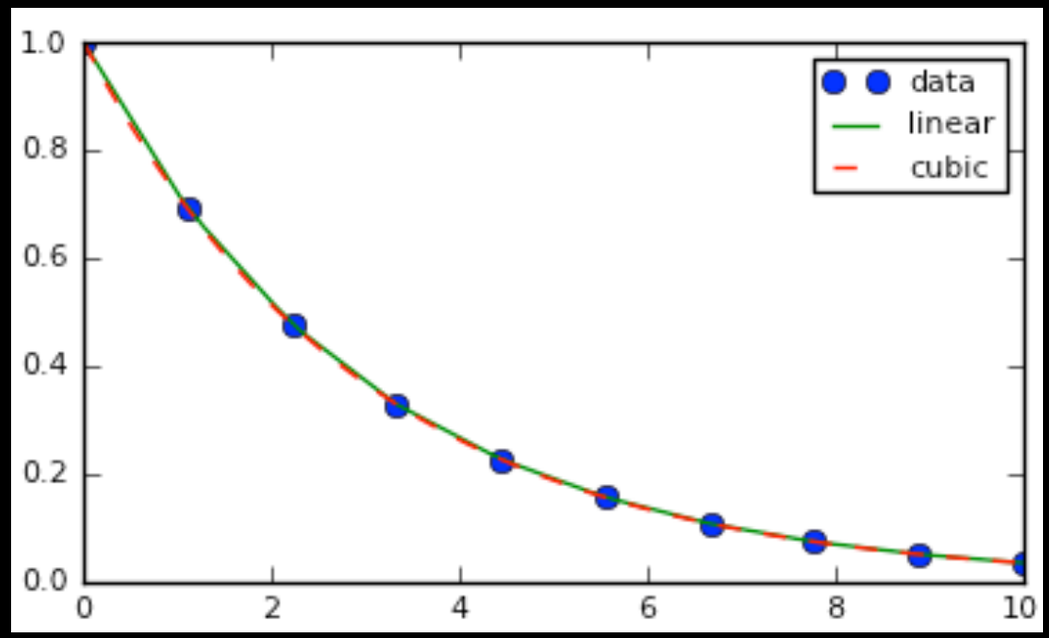
Matplotlib allows plotting of functions

```
import numpy as np
import scipy.interpolate as spi
import matplotlib.pyplot as plt

x = np.linspace(0, 10, 10)
y = np.exp(-x/3.0)
f = spi.interp1d(x, y)
f2 = spi.interp1d(x, y, kind='cubic')

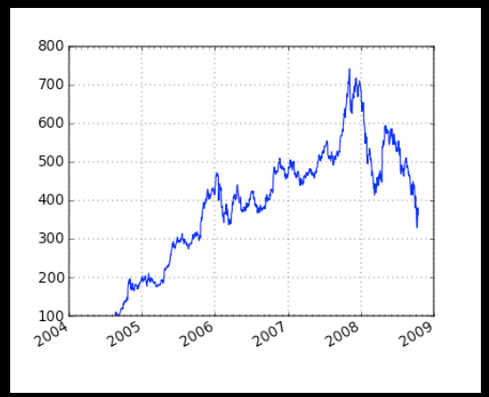
xnew = np.linspace(0, 10, 40)

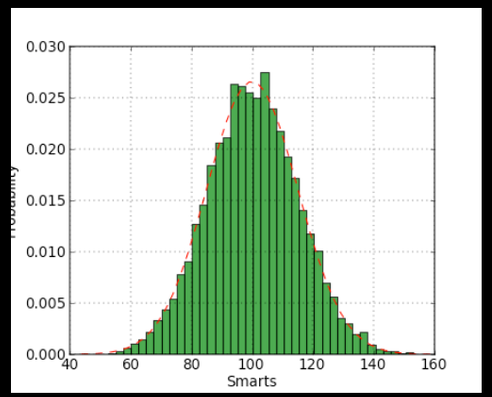
plt.plot(x,y,'o',xnew,f(xnew),
         '-', xnew, f2(xnew),'--')
plt.legend(['data', 'linear', 'cubic'],
          loc='best')
plt.show()
```

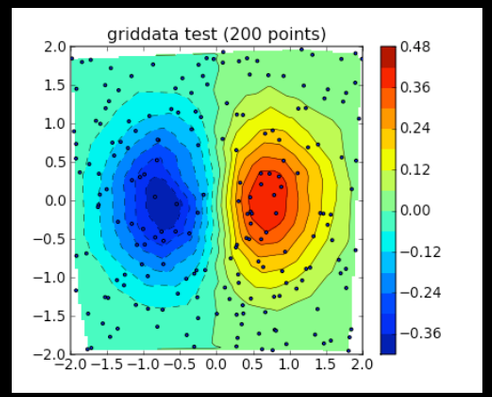


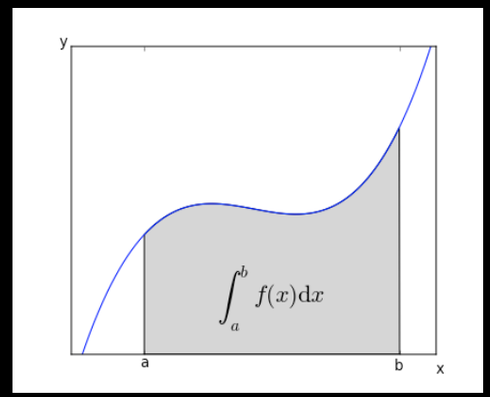
Matplotlib

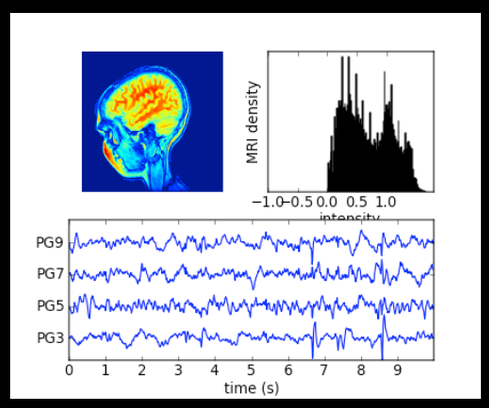
Many plot types: the gallery has lots of examples.
written in python very similar to Matlab and free.

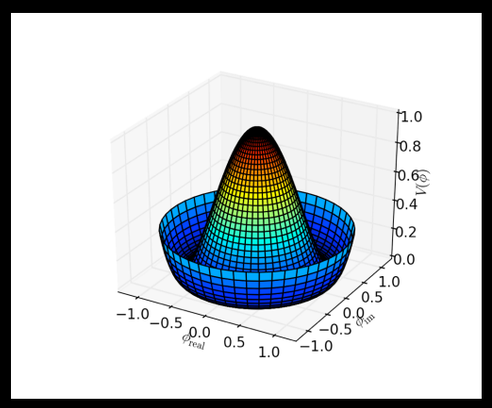


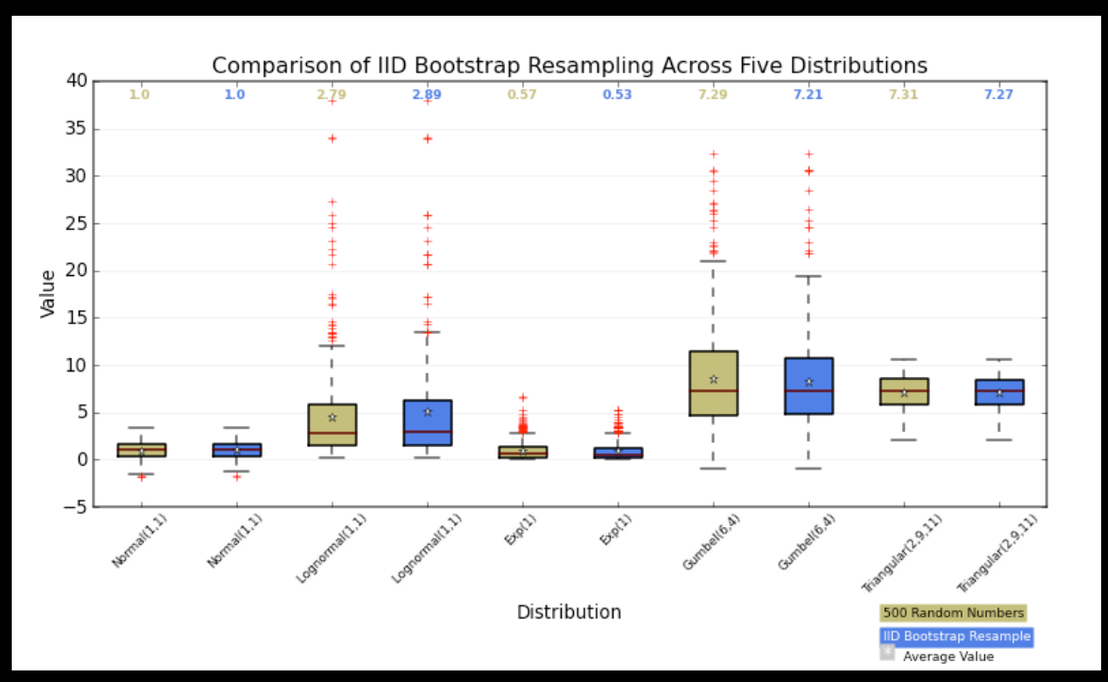












python

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Pyplot: a matplotlib state-machine

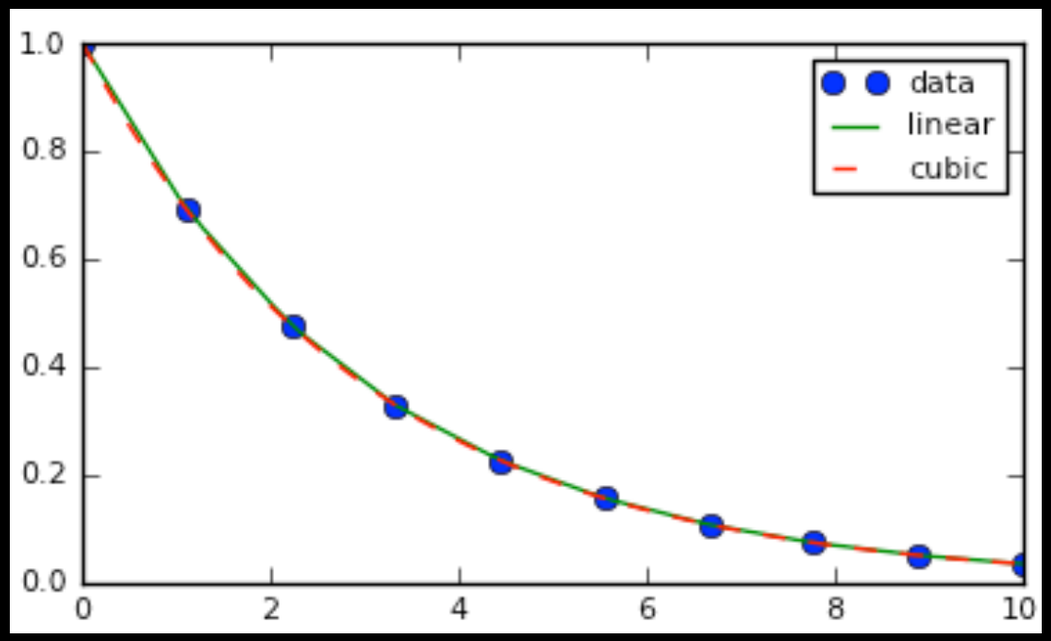
```
import numpy as np
import scipy.interpolate as spi
import matplotlib.pyplot as plt

x = np.linspace(0, 10, 10)
y = np.exp(-x/3.0)
f = spi.interp1d(x, y)
f2 = spi.interp1d(x, y, kind='cubic')

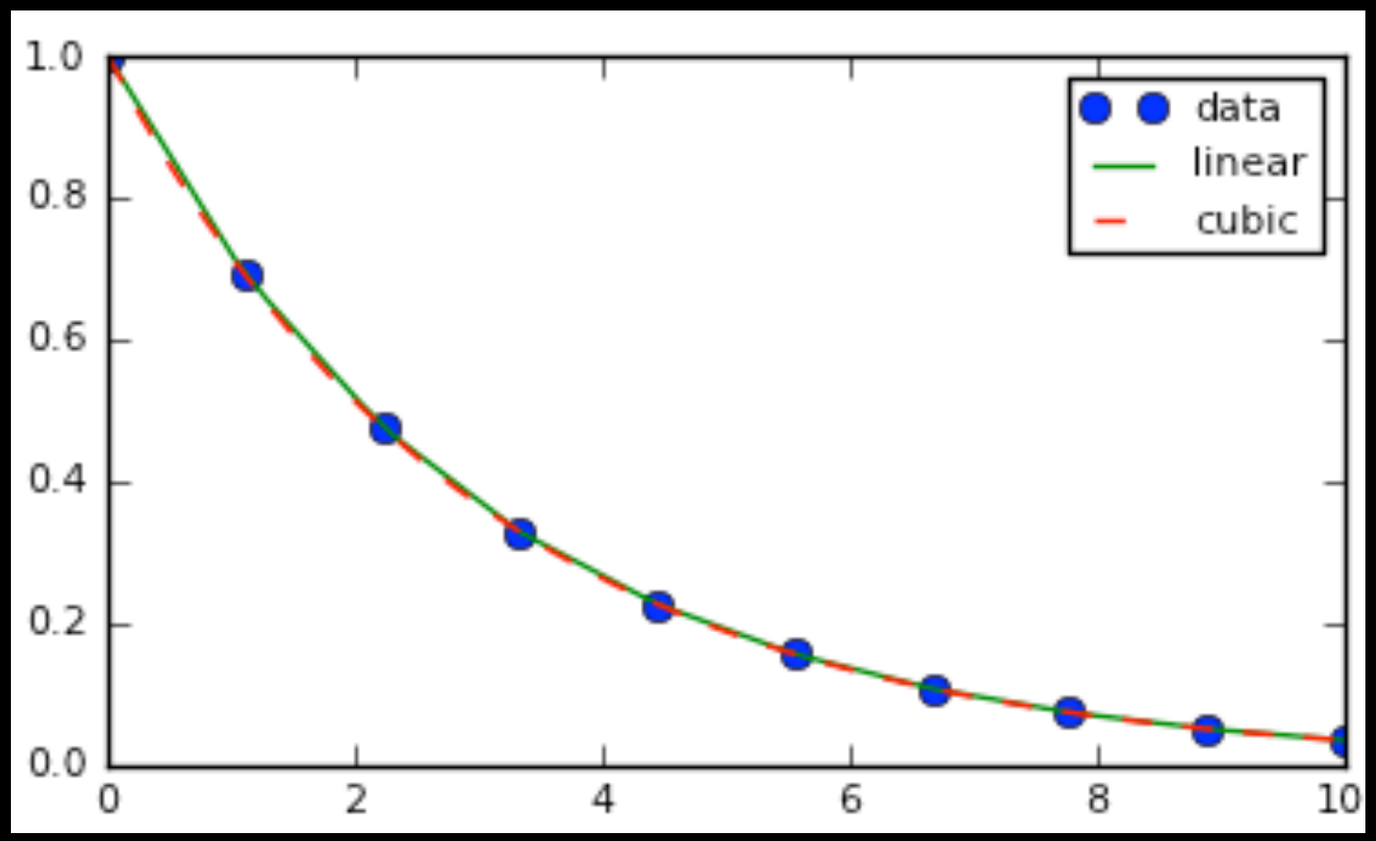
xnew = np.linspace(0, 10, 40)

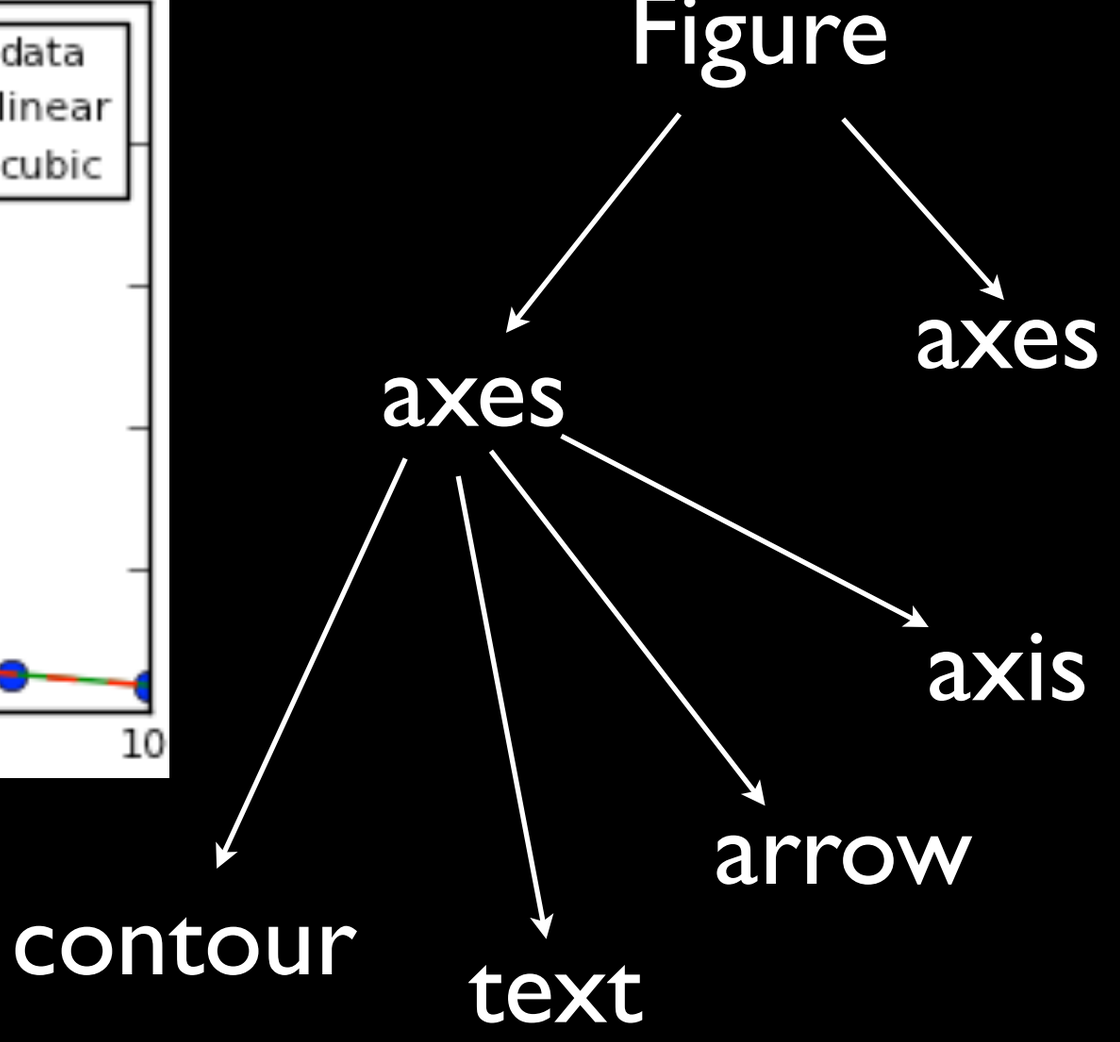
plt.plot(x,y,'o',xnew,f(xnew),
         '-', xnew, f2(xnew),'--')
plt.legend(['data', 'linear', 'cubic'],
          loc='best')
plt.show()
```

(1) Create a figure
(2) Modify figure
(3) More modifications
(4) Show figure



OO Matplotlib





python

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OO Matplotlib

```
import numpy as np
import scipy.interpolate as spi
import matplotlib.pyplot as plt

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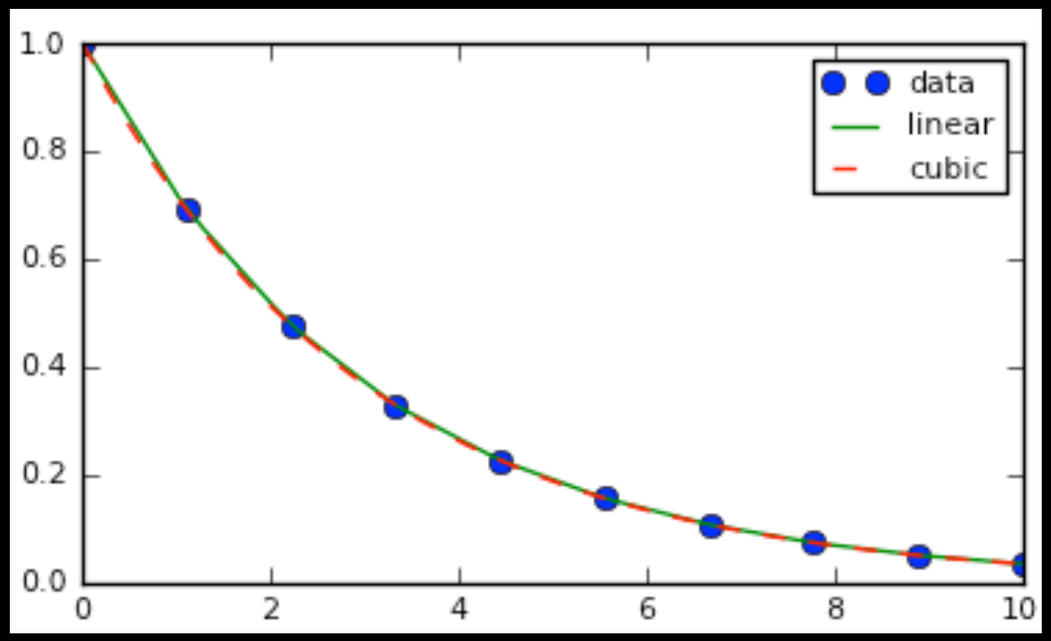
y = np.exp(-x/3.0)
f = spi.interp1d(x, y)
f2 = spi.interp1d(x, y, kind='cubic')

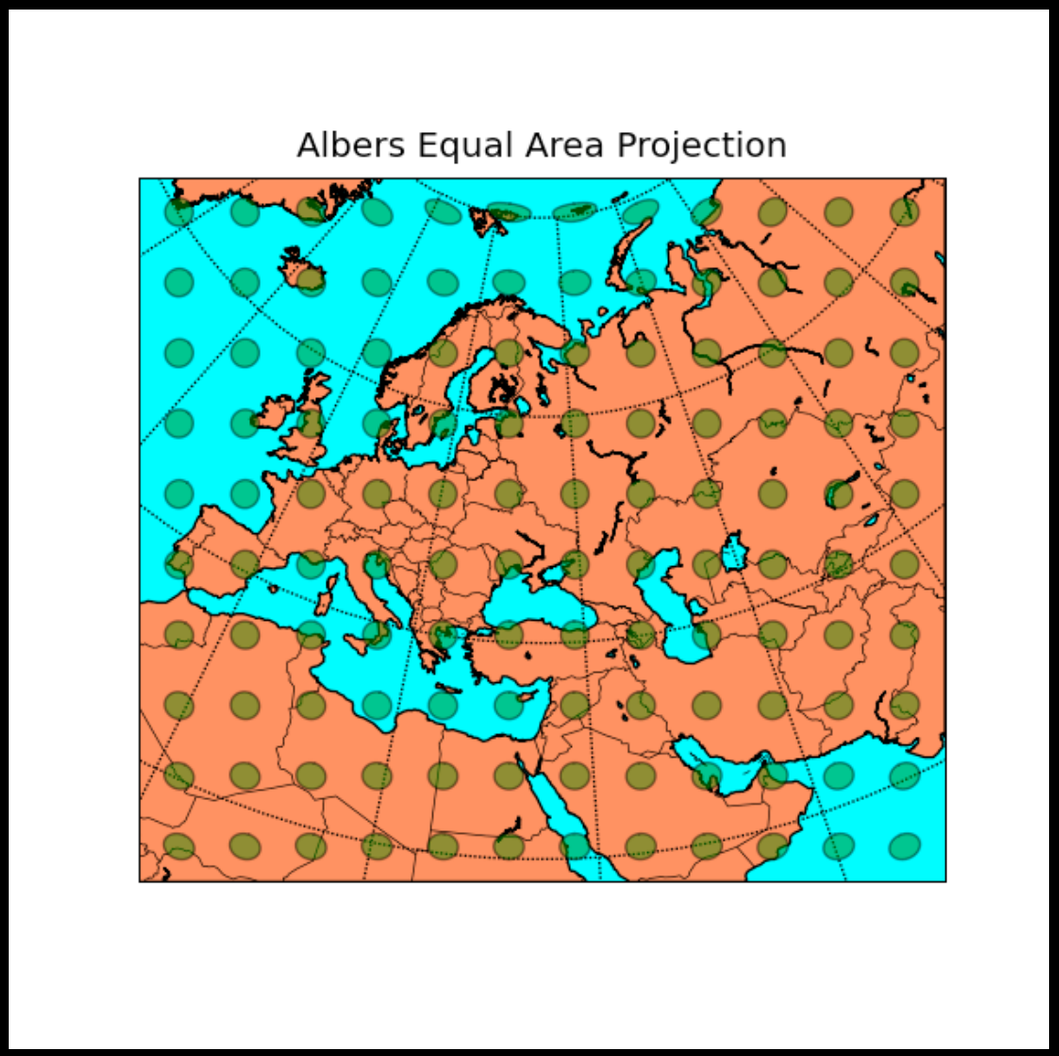
xnew = np.linspace(0, 10, 40)

fig = plt.figure()
ax = fig.add_subplot(111)
ax.plot(x,y,'o',xnew,f(xnew),
        '-', xnew, f2(xnew),'--')
ax.legend(['data', 'linear', 'cubic'],
          loc='best')
plt.show()
```

OO interface allows finer control over plot, permits embedding in graphical programs and makes it easer to reuse code.



Basemap

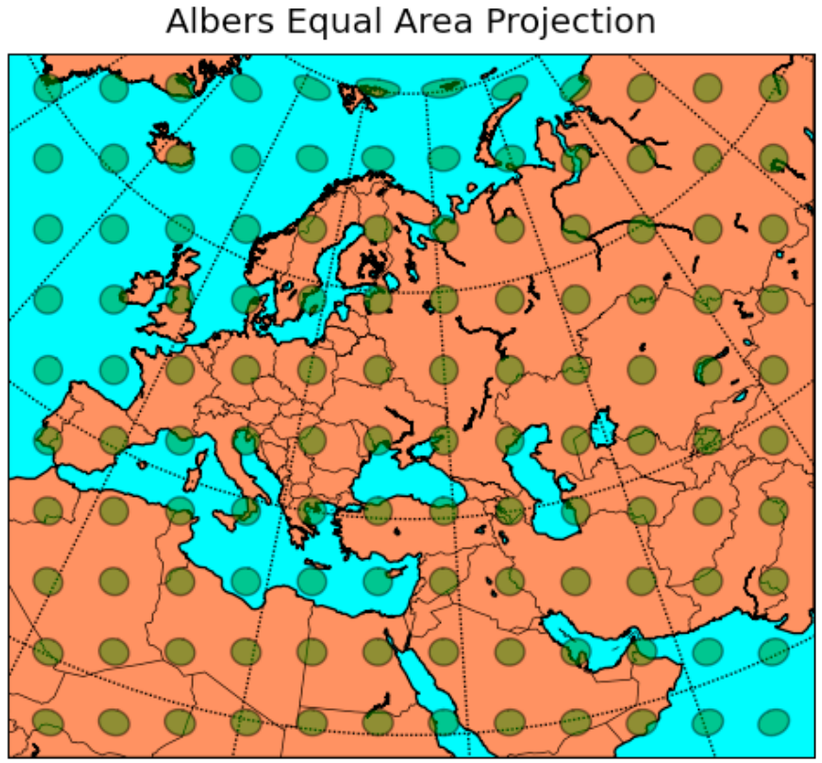


Uses the same database of coastlines, rivers and boundaries as GMT

Provides a way to warp between geographical coordinates and many different map projections

Use matplotlib to plot on basemap

Basemap



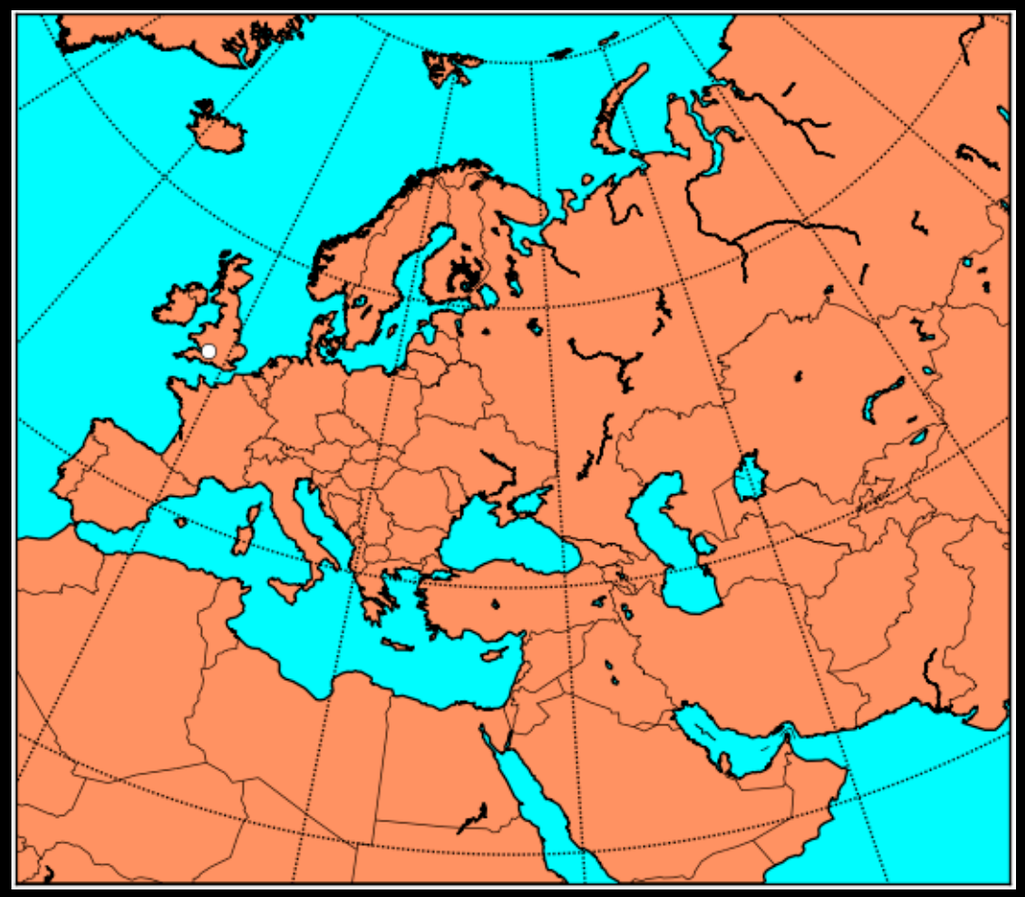

```
from mpl_toolkits.basemap import Basemap
import numpy as np
import matplotlib.pyplot as plt
m = Basemap(width=8000000,height=7000000,
    resolution='l',projection='aea',
    lat_1=40.,lat_2=60,lon_0=35,lat_0=50)
m.drawcoastlines()
m.drawcountries()
m.fillcontinents(color='coral',
                 lake_color='aqua')
# draw parallels and meridians.
m.drawparallels(np.arange(-80.,81.,20.))
m.drawmeridians(np.arange(-180.,181.,20.))
m.drawmapboundary(fill_color='aqua')

...

plt.title("Albers Equal Area Projection")
plt.savefig('aea.png')
```

m is a basemap instance

Basemap



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# draw parallels and meridians.
m.drawparallels(np.arange(-80.,81.,20.))
m.drawmeridians(np.arange(-180.,181.,20.))
m.drawmapboundary(fill_color='aqua')

x, y = m(-2.58, 51.54)
m.plot(x,y,'wo')

plt.title("Albers Equal Area Projection")
plt.savefig('aea.png')
```

Use m to convert from geographical to map coordinates

What I've not covered

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- NumPy array broadcasting
- Special NumPy arrays (masked, sparse, etc.)
- Many SciPy modules (linear algebra...)
- Huge numbers of Matplotlib plot types

http://matplotlib.sourceforge.net/gallery.html

- Exceptions
- Functional programming
- Decorators and aspect oriented programming
- Making Python modules with Fortran, C or Java
- Lots more of the standard library

http://docs.python.org/tutorial/

- Version control
- Unit tests
- Documentation
- Profiling
- Debugging

Whatever language you
happen to use