An introduction to scientific programming with

python™

Session 2:

Numerical Python and plotting

Session 2

In this session:

- Session 1 exercise solutions
- Proper numerical arrays
- Plotting with matplotlib
- Other plotting options
- Exercises

Any questions?

- shout and wave (now)
- tweet @thebamf (now)
- email steven.bamford@nottingham.ac.uk (later)

Exercises 1

1) Start your python interpreter and check the version.
2) Use python as a calculator (use variables and the math module).
3) Look at help for the math module.
4) Create a list of five numbers on the range (0, 10) and check the identity $\cosh^2(x) - \sinh^2(x) = 1$ holds true for them, using (a) a for loop, and (b) a list comprehension.
5) Write a function f(x, n), where x is a list of numbers and n is a single number, which returns a list of the indices of x where the value is exactly divisible by n. Check it works!
6) Put the above function in a script, with documentation. Import and test it.
7) Adapt your previous solution to take a filename instead of a list, and read the numbers to be tested from that file, considering one line at a time.
8) Adapt your solution to use a class with an attribute n and a method that returns which elements of a provided list are divisible by n.

Jupyter (IPython) notebooks

- Mathematica/Maple-style notebooks
- Store code and output together in one file
- Blend interactive prompt and scripts
- Good for demonstrations / trying things out
- Keep reproducable record of interactive analyses

  - To start, in terminal:

    ```
    jupyter notebook
    ```
  - Opens notebook interface in web browser
  - If you put them online (especially on GitHub) can easily display with nbviewer.ipython.org
  - `jupyter nbconvert` can be used to convert to python/html/slides, etc.

Session 1 exercise solutions

[link to online notebook]

Numerical Python

- So far…
  - core Python language and libraries
- Extra features required:
  - fast, multidimensional arrays
  - plotting tools
  - libraries of fast, reliable scientific functions *(next session)*

Arrays – Numerical Python (Numpy)

- Lists ok for storing small amounts of one-dimensional data

```
>>> a = [1,3,5,7,9]
>>> print(a[2:4])
[5, 7]
>>> b = [[1, 3, 5, 7, 9], [2, 4, 6, 8, 10]]
>>> print(b[0])
[1, 3, 5, 7, 9]
>>> print(b[1][2:4])
[6, 8]
```

- But, can't use directly with arithmetical operators (+, -, *, /, …)
- Need efficient arrays with arithmetic and better multidimensional tools
- **Numpy**

```
>>> import numpy
>>> import numpy as np  # common abbreviation
```

- Similar to lists, but much more capable, except *fixed size and type!*

Numpy – array creation and use

```
>>> import numpy
>>> l = [[1, 2, 3], [3, 6, 9], [2, 4, 6]]  # create a list
>>> a = numpy.array(l)  # convert a list to an array
>>> print(a)
[[1 2 3]
 [3 6 9]
 [2 4 6]]
>>> a.shape
(3, 3)
>>> print(a.dtype)  # get type of an array
int32
>>> print(a[0])  # this is just like a list of lists
[1 2 3]
>>> print(a[1, 2])  # arrays can be given comma separated indices
9
>>> print(a[1, 1:3])  # and slices
[6 9]
>>> print(a[:,1])
[2 6 4]
```

Numpy – array creation and use

```
>>> a[1, 2] = 7
>>> print(a)
[[1 2 3]
 [3 6 7]
 [2 4 6]]
>>> a[:, 0] = [0, 9, 8]
>>> print(a)
[[0 2 3]
 [9 6 7]
 [8 4 6]]

>>> b = numpy.zeros(5)
>>> print(b)
[ 0.  0.  0.  0.  0.]
>>> b.dtype
dtype('float64')
>>> n = 1000
>>> my_int_array = numpy.zeros(n, dtype=numpy.int)
>>> my_int_array.dtype
dtype('int32')
```

Numpy – array creation and use

```
>>> c = numpy.ones(4)
>>> print(c)
[ 1.  1.  1.  1. ]

>>> d = numpy.arange(5)  # just like range()
>>> print(d)
[0 1 2 3 4]

>>> d[1] = 9.7
>>> print(d)  # arrays keep their type even if elements changed
[0 9 2 3 4]
>>> print(d*0.4)  # operations create a new array, with new type
[ 0.   3.6  0.8  1.2  1.6]

>>> d = numpy.arange(5, dtype=numpy.float)
>>> print(d)
[ 0.  1.  2.  3.  4.]

>>> numpy.arange(3, 7, 0.5)  # arbitrary start, stop and step
array([ 3. , 3.5, 4. , 4.5, 5. , 5.5, 6. , 6.5])
```

Numpy – array creation and use

```
>>> a = numpy.arange(4.0)
>>> b = a * 23.4
>>> c = b/(a+1)
>>> c += 10
>>> print c
[ 10.    21.7   25.6   27.55]

>>> arr = numpy.arange(100, 200)
>>> select = [5, 25, 50, 75, -5]
>>> print(arr[select])  # can use integer lists as indices
[105, 125, 150, 175, 195]

>>> arr = numpy.arange(10, 20)
>>> div_by_3 = arr%3 == 0  # comparison produces boolean array
>>> print(div_by_3)
[ False False  True False False  True False False  True False]
>>> print(arr[div_by_3])  # can use boolean lists as indices
[12 15 18]
```

Numpy – array creation and use

```
>>> b = arr[1:].reshape((3,3))        # now 2d 3x3 array
>>> print b
[[11 12 13]
 [14 15 16]
 [17 18 19]]

>>> b_2 = b%2 == 0
>>> b_3 = b%3 == 0
>>> b_2_3 = b_2 & b_3                 # boolean operators
>>> print b_2_3                       # also logical_and(b_2, b_3)
[[False  True False]
 [False False False]
 [False  True False]]

>>> print b[b_2_3]                    # select array elements
[12 18]                               # with boolean arrays
>>> i_2_3 = b_2_3.nonzero()
>>> print i_2_3
(array([0, 2]), array([1, 1]))
>>> print b[i_2_3]                    # or index arrays
[12 18]
```

Numpy – array methods

```
>>> arr.sum()
145
>>> arr.mean()
14.5
>>> arr.std()
2.8722813232690143
>>> arr.max()
19
>>> arr.min()
10
>>> div_by_3.all()
False
>>> div_by_3.any()
True
>>> div_by_3.sum()
3
>>> div_by_3.nonzero()        # note singleton tuple returned
(array([2, 5, 8]),)           # for consistency with N-dim case
```

Numpy – array methods – sorting

```
>>> arr = numpy.array([4.5, 2.3, 6.7, 1.2, 1.8, 5.5])
>>> arr.sort()  # acts on array itself
>>> print(arr)
[ 1.2  1.8  2.3  4.5  5.5  6.7]

>>> x = numpy.array([4.5, 2.3, 6.7, 1.2, 1.8, 5.5])
>>> y = numpy.array([1.5, 2.3, 4.7, 6.2, 7.8, 8.5])
>>> numpy.sort(x)
array([ 1.2,  1.8,  2.3,  4.5,  5.5,  6.7])
>>> print(x)
[ 4.5  2.3  6.7  1.2  1.8  5.5]
>>> s = x.argsort()
>>> s
array([3, 4, 1, 0, 5, 2])
>>> x[s]
array([ 1.2,  1.8,  2.3,  4.5,  5.5,  6.7])
>>> y[s]
array([ 6.2,  7.8,  2.3,  1.5,  8.5,  4.7])
```

Numpy – array functions

Most array methods have equivalent functions

```
>>> arr.sum()             # array method
45
>>> numpy.sum(arr)        # array function
45
```

Ufuncs provide many element-by-element math, trig., etc. operations

- e.g., add(x1, x2), absolute(x), log10(x), sin(x), logical_and(x1, x2)

```
>>> arr.sum()
45
>>> numpy.sum(arr)
45
```

numpy.mat creates matrices (with corresponding matrix operations)

See http://numpy.scipy.org

Numpy – array functions

Most array methods have equivalent functions

```
>>> arr.sum()             # array method
45
>>> numpy.sum(arr)        # array function
45
```

Array functions often return a result, leaving original array unchanged

Array methods often perform the operation in-place

```
>>> a = numpy.array([23, 7, 80])
>>> s = numpy.sort(a)                  # returns sorted array
>>> print a, s                         # original unaltered
[23  7 80] [ 7 23 80]
>>> a.sort()                           # nothing returned
>>> print a                            # operation applied in-place
[ 7 23 80]
```

Numpy – array functions

Many array functions (and methods) can take an *axis*, with the operation only applied along that one direction in the array

```
>>> print a
[[19 18 17]
 [16 15 14]
 [13 12 11]]

>>> a.sum()
135

>>> a.sum(axis=0)
array([48, 45, 42])

>>> a.sum(axis=1)
array([54, 45, 36])
```

```
>>> numpy.sort(a)
array([[17, 18, 19],
       [14, 15, 16],
       [11, 12, 13]])

>>> numpy.sort(a, axis=0)
array([[13, 12, 11],
       [16, 15, 14],
       [19, 18, 17]])

>>> numpy.sort(a, axis=1)
array([[17, 18, 19],
       [14, 15, 16],
       [11, 12, 13]])
```

Defaults are to operate on the whole array (axis=None) for accumulative operations and on the highest dimension (axis=−1) otherwise.

Numpy – random numbers

High quality (pseudo-) random number generator
with many common distributions

```
>>> numpy.random.seed(12345)  # or default seed taken from clock
>>> numpy.random.uniform()
0.9296160928171479

>>> numpy.random.uniform(-1, 1, 3)
array([-0.36724889, -0.63216238, -0.59087944])

>>> r = numpy.random.normal(loc=3.0, scale=1.3, size=100)
>>> r.mean(), r.std()
(3.1664506480570371, 1.2754634208344433)

>>> p = numpy.random.poisson(123, size=(1024,1024))
>>> p.shape
(1024, 1024)
>>> p.mean(), p.std()**2
(123.0230646133422, 122.99512022056578)
```

Numpy – recarray

- Arrays usually have homogeneous type, but different type arrays can be combined – best way is as a recarray
- Used by Astropy Tables, PyTables (see Sessions 4 and 5)

```
>>> x = numpy.arange(0,100)
>>> y = numpy.sqrt(x)
>>> z = y.astype(numpy.int)
>>> r = numpy.rec.array((x,y,z), names=('x', 'y', 'z'))
>>> r.x
array([   0,    1,    2, ..., 9997, 9998, 9999])
>>> r.y
array([  0.        ,   1.        ,   1.41421356, ...,  99.98499887,
        99.9899995 ,  99.99499987])
>>> r.z
array([ 0,  1,  1, ..., 99, 99, 99])
```

Numpy – loading and saving data

- Custom binary format:
  - save
  - load
- Text format:
  - savetxt
  - loadtxt
  - genfromtxt
  - recfromcsv

```
$ head mydata
     0       0.000000      0
     1       1.000000      1
     2       1.414214      1
     3       1.732051      1
     4       2.000000      2
     5       2.236068      2
     6       2.449490      2
     7       2.645751      2
     8       2.828427      2
     9       3.000000      3
```

```
>>> numpy.savetxt('mydata', r, fmt=”%6i %12.6f %6i”) # save to file

>>> data = numpy.genfromtxt('mydata')  # reads a 2d array

>>> data = numpy.recfromtxt('myfile.txt', names=('x', 'y', 'z'))
```

- Not very portable, not self-describing
- FITS and HDF5 covered in Sessions 4 and 5

Numpy – using arrays wisely

- Array operations are implemented in C or Fortran
- Optimised algorithms - i.e. fast!
- Python loops (i.e. for i in a:…) are much slower
- Prefer array operations over loops, especially when speed important
- Also produces shorter code, often much more readable

- If you're working with large datasets, watch out for swapping…

Numpy – saving memory

- Numpy arrays reside entirely in memory
- Save memory by using lower precision where possible

```
>>> d = numpy.arange(100000000, dtype=numpy.int32)  # default int64
>>> d = numpy.arange(1e8, dtype=numpy.float32)    # default float64
```

- Save memory by performing operations in place where possible

```
>>> a = numpy.arange(100000000)  # 1e8 * 64 / 8 / 1e6 ~ 800Mb
>>> b = numpy.random.normal(0, 1000, 100000000)  # also ~ 800 Mb
>>> a = a + b  # requires additional 800Mb memory (maybe swap)
>>> a += b     # in-place: no more memory required and faster
>>> a = numpy.sqrt(a)      # requires extra 800Mb memory
>>> numpy.sqrt(a, out=a)   # in-place: no more memory required
```

- Use sparse arrays (provided by SciPy, see Session 3)
- Use a solution which keeps data on disk (memmap, PyTables)
- Change your algorithm

Plotting – matplotlib

- User friendly, but powerful, plotting capabilities for python
- http://matplotlib.org/

- Once installed, to use type:

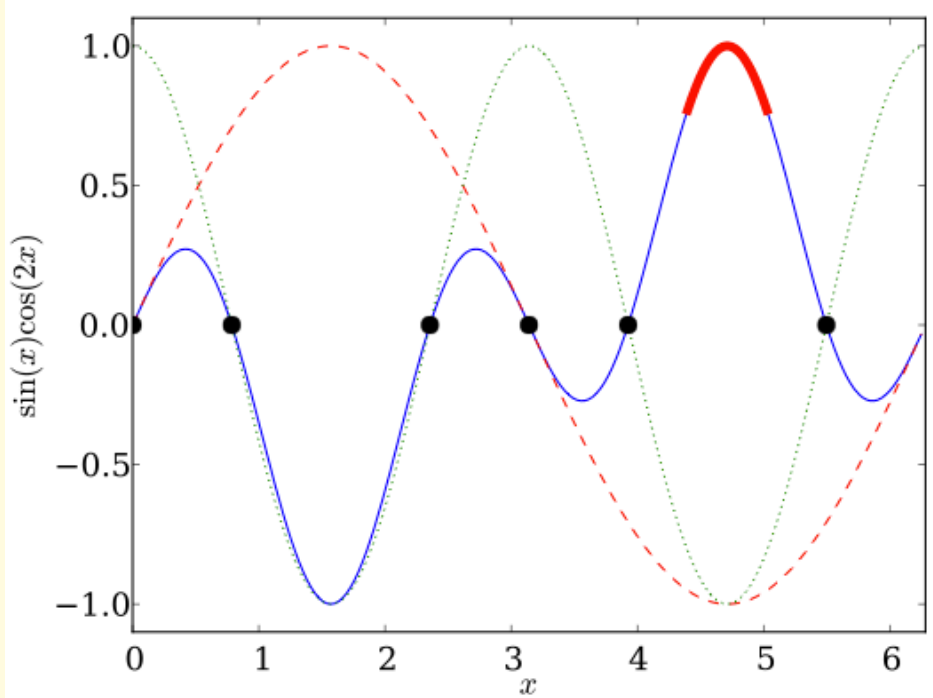
```
>>> import pylab                             # handy for interactive use
>>> import matplotlib.pyplot as plt  # better for in scripts
```

- Settings can be customised by editing ~/.matplotlib/matplotlibrc
  - Set *backend* and default font, colours, layout, etc.
- Helpful website
  - many examples

```
>>> pyplot.ion()  # turn on interactive mode!
```

Plotting – matplotlib

```
>>> from numpy import sin, cos, pi
>>> x = numpy.arange(0, 2*pi, pi/100)
>>> y = sin(x)*cos(2*x)
>>> pyplot.plot(x, y)
>>> pyplot.plot(x, sin(x), '--r')
>>> pyplot.plot(x, cos(2*x),
                linestyle='dotted',
                color='green')
>>> thresh = y > 0.75
>>> pyplot.plot(x[thresh], y[thresh],
...             'r', linewidth=5)
>>> zeros = numpy.abs(y) < pi/200
>>> pyplot.plot(x[zeros], y[zeros],
                'ok', markersize=10)
>>> pyplot.xlabel(r'$x$')
>>> pyplot.ylabel(r'$\sin(x)\cos(2x)$')
>>> pyplot.axis([0, 2*pi, -1.1, 1.1])
>>> pyplot.savefig('wiggles.pdf')
```



Plotting – matplotlib

- Plots can be altered in an object oriented manner

For example,

```
>>> fig = pyplot.figure(1)
>>> ax = fig.axes[0]
>>> ax.xaxis.labelpad = 10
>>> pyplot.draw()
>>> l = ax.lines[2]
>>> l.set_linewidth(3)
>>> pyplot.draw()
>>> ax.xaxis.set_ticks((0, pi/2, pi, 3*pi/2, 2*pi))
>>> pyplot.draw()
>>> ax.xaxis.set_ticklabels(('0', r'$\frac{1}{2}\pi$', r'$\pi$',
                             r'$\frac{3}{2}\pi$', r'$2\pi$'))
>>> pyplot.draw()
>>> pyplot.subplots_adjust(bottom=0.25)
```

```
Shorthand to get current axes
>>> ax = pyplot.gca()
```

Plotting – matplotlib

Some useful functions:

- figure – create a new figure, or get an existing figure object
- plot – add line or points
- hist / hist2d – create a 1D/2D histogram
- imshow / contour – plot an array as an image / contours
- axis – set axis limits
- subplot – set to draw on subset of the canvas
- subplots – create new figure with a grid of subplots
- subplots_adjust – adjust the canvas margins

Some functions update the plot, others don't (for efficiency)
To update the plot display:

- draw() – draw plot and continue
- show() – blocks interpreter until window closed

- close(), close('all') – close figure windows

Matplotlib/Ipython notebook scatter plot example

[link to online notebook]

Plotting – interactive notebook plots

- There are some tools for producing interactive plots in a web browser (via JavaScript), and hence in IPython notebooks
- matplotlib
  - %matplotlib inline – inserts image of plot in notebook
  - %matplotlib notebook – inserts interactive plot in notebook
- mpld3
  - use matplotlib commands (e.g. some existing plotting code)
  - generate HTML with mpld3 – automatically get pan and zoom
  - optionally add interactivity (tooltips, highlighting, selections, …)
- bokeh, plotly, …
  - similar functionality, but different (non-matplotlib) interface

Plotting – alternative interfaces

- Large variety of different approaches

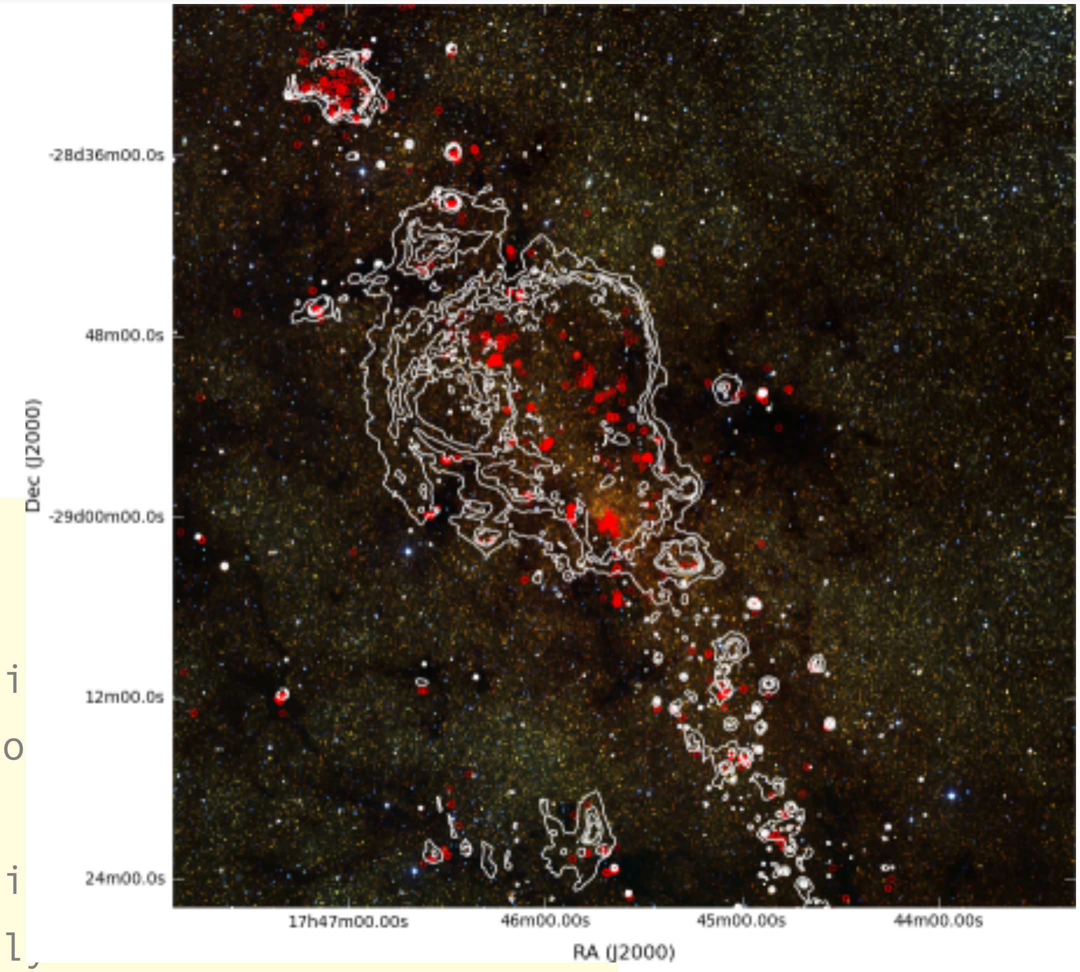
- seaborn, pandas – easy, sophisticated statistical plots
- plotnine – grammar of graphics (ggplot2) interface
- bokeh, plotly – web targetted
- datashader, yt – for large datasets of points, densities
- altair, vega – declarative visualisation

- Making sense of the deluge:
  - https://www.youtube.com/watch?v=FytuB8nFHPQ

Plotting – astronomical data

- AplPy: plotting library for astronomical images
- Based on matplotlib
- http://aplpy.github.com/

```
import aplpy
import numpy
gc = aplpy.FITSFigure('fits/2MASS_k.fi
gc.show_rgb('graphics/2MASS_arcsinh_co
gc.set_tick_labels_font(size='small')
gc.show_contour('fits/mips_24micron.fi
data = numpy.loadtxt('data/yso_wcs_onl
ra,dec = data[:,0],data[:,1]
gc.show_markers(ra,dec,layer='scatter_set_1',edgecolor='red',
    facecolor='none',marker='o',s=10,alpha=0.5)
gc.save('tutorial.png')
```



Also WCSAxes from astropy

Coursework

- A Python program relevant to your research
  - put course material into practice
  - opportunity to become familiar with Python
  - get feedback on your coding
  - requirement to qualify for credits

- Your program should…
  - be written as an importable module (.py file) or Jupyter notebook (.ipynb)
  - do something meaningful: analyse real data or perform a simulation
  - use at least two user functions
  - use at least one of the modules introduced in Sessions 3 – 5
  - produce at least one informative plot
  - comprise >~ 50 lines of actual code (excluding comments and imports)

Coursework

- Submit as source code (.py/.ipynb file) and pdf/png files of the output plot(s)
  - Email me (steven.bamford@nottingham.ac.uk) with subject "MPAGS coursework"
  - Link to a GitHub repository, etc. or attach code
    - if private add me (bamford) as a collaborator
    - make sure any requirements are clear

  - Three stages:
    - One (optional)
      - README describing what you intend your code to do
      - Rough outline of the code (classes, functions, snippets, comments, pseudocode)
      - If submitted by **10 Nov**, I will provide feedback
    - Two (optional)
      - Roughly working version of your code, although may be incomplete, have bugs, although try to make it reasonable and easy to understand!
      - If submitted by **24 Nov**, I will provide feedback
    - Three (for MPAGS credits)
      - Full (ideally) working version of your code (doesn't have to be amazing!)
      - **15 Dec deadline**

Exercises 2

1) Create an array x = [-3.00, -2.99, -2.98, …, 2.98, 2.99, 3.00]

2) Create a corresponding array for the Gaussian function $y = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$

3) Check the result is unit normalised: $\sum_i y_i \; \delta x = 1$

4) For convenience, put x and y together in a recarray and save to a file

5) Create a sample of one hundred Gaussian random numbers

6) Plot your Gaussian curve, x versus y, with axis labels

7) Add a histogram of the random numbers to your plot

8) Over-plot another histogram for a different sample and prettify
(try histtype='stepfilled' and 'step', and transparency, e.g., alpha=0.5)