MAS212 Scientific Computing and Simulation

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Important info

- Class test in Week 2 lab class (Wed 10am / Fri 11am).
- The test will appear on home page:
  `http://sam-dolan.staff.shef.ac.uk/mas212`
- Submission deadline Sun midnight (13th Oct):
  `https://somas-uploads.shef.ac.uk/mas212`

Today's lecture

- Scientific computing modules:
  - **numpy**
  - `matplotlib`
  - `scipy`
- Arrays: data types, creation, slicing, views, vectorization, ufuncs, broadcasting, etc.
- Linear algebra
- Functions
- Objects and classes
- Standard modules: `math`, `cmath`, `random`, `os`, `datetime`

Modules for scientific computing

- `numpy` : efficient arrays, broadcasting and linear algebra.
  `http://www.numpy.org/`
- `matplotlib` : 2D plotting and animation
  `http://matplotlib.org/`
- `scipy` : for common tasks in scientific computing.
  `http://docs.scipy.org/doc/scipy-dev/reference/`

numpy

- How to create new arrays
- *N*-dimensional arrays
- Array manipulation: slicing, views, etc.
- Universal functions, **vectorization** and **broadcasting**
- Linear algebra (matrix multiplication etc)
- Other capabilities: random numbers, Fourier transforms

numpy

Convention:

Import the module as follows:

```
>>> import numpy as np
```

Arrays in numpy

What is an array?

In essence, an array consists of:

- a block of memory – the raw data
- an indexing scheme – how to locate elements
- a data type – how to interpret the raw data

`ndarray` : the N-dimensional array in `numpy`

An `ndarray` is a (usually fixed-size) multidimensional container of items of the same type and size. The number of dimensions and items in an array is defined by its shape, which is a tuple of N positive integers that specify the sizes of each dimension. The type of items in the array is specified by a separate data-type object (dtype), one of which is associated with each ndarray.

`http://docs.scipy.org/doc/numpy/reference/arrays.ndarray.html`

numpy

There are many ways to make a new 1D array:

- from a list : `np.array([1,2,3])`
- `arange` : evenly-spaced with step size
- `linspace` : evenly-spaced with number of points
- `zeros` : array set to zeros
- `ones` : array set to 1s
- `empty` : an uninitialized array

```
>>> np.array([1,2,3])
array([1, 2, 3])
>>> np.arange(0, 3, 1)
array([0, 1, 2])
>>> np.arange(0, 3, 0.5)
array([ 0. ,  0.5,  1. ,  1.5,  2. ,  2.5])
>>> np.linspace(0, 3, 5)
array([ 0.  ,  0.75,  1.5 ,  2.25,  3.  ])
>>> np.zeros(6)
array([ 0.,  0.,  0.,  0.,  0.,  0.])
>>> np.ones(6)
array([ 1.,  1.,  1.,  1.,  1.,  1.])
>>> 2*np.ones(6)   # array of twos
array([ 2.,  2.,  2.,  2.,  2.,  2.])
>>> np.empty(2)
array([  6.91667204e-310,   6.91667204e-310])
```

- Arrays are **homogeneous**: All elements in an array must be of the same **data type** (`dtype`).
- Each element is of a fixed size in memory.
- numpy supports a range of data types, including:

int8	A byte (-128 to 127)
uint8	An unsigned integer (0 to 255)
...	
int64	A 64-bit integer (-9223372036854775808 to 9223372036854775807)
float64	A double precision float: sign bit, 11 bits exponent, 52 bits mantissa.
complex128	A complex number, represented by two 64-bit floats (real and imaginary components).

- Examples :

```
>>> a = np.linspace(0, 5, 11)
>>> b = np.arange(0, 11)
>>> print(a, b)
[ 0.   0.5  1.   1.5  2.   2.5  3.   3.5  4.   4.5  5. ]
[ 0  1  2  3  4  5  6  7  8  9 10]
>>> a.dtype   # data type of array
dtype('float64')
>>> b.dtype
dtype('int64')
>>> a.shape
(11,)
>>> a.ndim  # number of dimensions
1
>>> a.size
11
```

Special values: `nan` and `inf`

- `nan` = not a number
- `inf` = infinity.

```
>>> a = np.arange(4)
>>> a / 0
array([ nan,  inf,  inf,  inf])
```

Making a 2D array

- From a list-of-lists.
- By reshaping 1D arrays.
- By broadcasting 1D arrays.

```
>>> np.array([[1,2], [3,4]])  # from a list-of-lists
array([[1, 2],
       [3, 4]])
>>> np.arange(4).reshape(2,2)  # by reshaping
array([[0, 1],
       [2, 3]])
>>> np.array([[1,2]]) * np.array([[3],[4]])  # by broadcasting
array([[3, 6],
       [4, 8]])
```

Re-shaping an array

```
>>> a = np.arange(12)
>>> a
array([ 0,  1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11])
>>> a.reshape(3,4)  # 3 rows, 4 columns
array([[ 0,  1,  2,  3],
       [ 4,  5,  6,  7],
       [ 8,  9, 10, 11]])
>>> a.reshape(2,2,3)   # a 3D array
array([[[ 0,  1,  2],
        [ 3,  4,  5]],

       [[ 6,  7,  8],
        [ 9, 10, 11]]])
```

Indexing and Slicing

- It is straightforward to access a single element of the array:

```
>>> a = np.arange(6).reshape(2,3)  # create a 2x3 array
>>> print(a)
[[0 1 2]
 [3 4 5]]
>>> a[1,2]  # get element in the 2nd row, 3rd column
5
>>> a[1,2] = -1  # modify this element
>>> print(a)
[[ 0  1  2]
 [ 3  4 -1]]
```

Indexing and Slicing

- Using **slicing**, one can access subarrays :

```
>>> a = np.arange(12).reshape(3,4)  # create a 3x4 array
>>> print(a)
[[ 0  1  2  3]
 [ 4  5  6  7]
 [ 8  9 10 11]]
>>> print(a[0,:]) # the 1st row
[0 1 2 3]
>>> print(a[:, 1]) # the 2nd column
[1 5 9]
>>> print(a[::-1, :])  # reverse the order of the rows
[[ 8  9 10 11]
 [ 4  5  6  7]
 [ 0  1  2  3]]
```

Views

- Slices of arrays are **not** new arrays.
  They are **views** on the original array.
- Example:

```
>>> a = np.arange(12).reshape(3,4)
>>> b = a[0, :]  #  the first row
>>> b[2] = 99    #  By changing an element of b  ...
>>> print(a)     # ... we are changing the data in a
[[ 0  1 99  3]
 [ 4  5  6  7]
 [ 8  9 10 11]]
```

Universal functions (ufuncs)

- A `ufunc` is a function that operates on whole arrays in an element-by-element fashion.
- Examples:

```
>>> a = np.linspace(0, 2*np.pi, 7)
>>> np.sin(a)  # sin is an example of a ufunc
array([  0.00000000e+00,   8.66025404e-01,   8.66025404e-01,
         1.22464680e-16,  -8.66025404e-01,  -8.66025404e-01,
        -2.44929360e-16])
>>> # multiplication, addition and raising-to-the power are also ufunc
>>> 3*a + a**2
array([  0.        ,   4.23821536,  10.66967615,  19.29438236,
        30.11233399,  43.12353105,  58.32797353])
```

Universal functions (ufuncs)

- Standard `ufuncs` are typically implemented in compiled C code
- $\Rightarrow$ they are **fast**
- Example: multiplying by 2

```
>>> # Using list comprehension:
>>> a = range(1000)
>>> %timeit [2*n for n in a]
10000 loops, best of 3: 65.3 \mu s per loop
>>> # Using an array with multiplication ufunc
>>> a = np.arange(1000)
>>> %timeit 2*a
1000000 loops, best of 3: 1.59 \mu s per loop
```

- i.e. the latter is approximately 40 times faster

Vectorization

- **Vectorization**: the practice of replacing `for` loops with array expressions . . .
- . . . so that batch operations are implemented efficiently.

Vectorization: Exercise

Exercise

- Generate 1000 random numbers from the standard uniform distribution $[0, 1)$
- Compute the variance of your sample using:
  1. `for` loops and lists
  2. arrays and vectorization
- Compare the efficiencies of the implementations.

$$\mathrm{var}(x) = \left\langle x^2 \right\rangle - \langle x \rangle^2$$

Implementation #1 (with loops)

```
import random as rnd
def attempt1(n=1000):
    l = []
    for i in range(n):    # Build a list of random numbers
        l.append(rnd.random())
    xsum = 0; x2sum = 0;
    for i in range(n):
        xsum += l[i]
        x2sum += l[i]**2
    xmean = xsum / n
    x2mean = x2sum / n
    return x2mean - xmean**2
```

Implementation #2 (vectorized)

```
import numpy as np
def attempt2(n=1000):
    r = np.random.random(n)
    xmean = r.sum() / n
    x2mean = (r**2).sum() / n
    return x2mean - xmean**2
```

Comparing efficiencies

```
>>> %timeit attempt1()
1000 loops, best of 3: 372 us per loop
>>> %timeit attempt2()
100000 loops, best of 3: 17.8 us per loop
```

- The vectorized version is $\sim$ 20 times faster.

Broadcasting

What is broadcasting?

- An efficient way of combining two arrays of different shapes during arithmetic operations.
- The smaller array is ‘broadcast’ across the larger array
- The loops are carried out in C rather than Python
  $\Rightarrow$ **fast!**

Broadcasting

Example: Arrays of same size

- If the arrays are the same size, they are combined element-by-element:

```
>>> a = np.array([1,2,3])
>>> b = np.array([4,5,6])
>>> a * b
array([ 4, 10, 18])
>>> a + b
array([5, 7, 9])
>>> a - b
array([-3, -3, -3])
>>> a**b
array([  1,  32, 729])
```

Broadcasting

Example: Scalar $\times$ vector

```
>>> a = np.array([1,2,3])
>>> b = 2
>>> a*b
array([2, 4, 6])
```

Broadcasting

A more interesting example

```
>>> x = np.arange(4)
>>> xx = x.reshape(4, 1)
>>> y = np.arange(5)
>>> print(x.shape, xx.shape, y.shape)
(4,) (4, 1) (5,)
>>> x + y
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: operands could not be broadcast together with shapes (4,)
>>> xx + y
array([[0, 1, 2, 3, 4],
       [1, 2, 3, 4, 5],
       [2, 3, 4, 5, 6],
       [3, 4, 5, 6, 7]])
```

Broadcasting

Broadcasting rules for combining two arrays:

- Their shapes are compared, starting with last dimension
- Two dimensions are compatible iff:
  - They are the same, or
  - One or both of them is 1.
- If dimensions are not compatible, an error is thrown
- **Note:** the arrays do not need to have same number of dimensions
- Example:

```
A      (4d array):  8 x 1 x 6 x 1
B      (3d array):      7 x 1 x 5
A*B    (4d array):  8 x 7 x 6 x 5
```

- More info: `http://docs.scipy.org/doc/numpy/user/basics.broadcasting.html`

Broadcasting

Warning!

Broadcasting is not the same as matrix multiplication!
For example,

```
>>> A = np.arange(4).reshape(2,2)
>>> b = np.arange(1,3).reshape(2,1)
>>> print(A)
[[0 1]
 [2 3]]
>>> print(b)
[[1]
 [2]]
>>> A * b   # Warning : not matrix multiplication
array([[0, 1],
       [4, 6]])
```

Broadcasting

Matrix multiplication

For matrix multiplication, use `np.dot()` or first convert arrays to matrices :

```
>>> np.dot(A, b)
array([[2],
       [8]])
>>> np.mat(A) * np.mat(b)
matrix([[2],
        [8]])
```

Linear algebra with `numpy.linalg`

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

- Matrix & vector multiplication with `np.dot` function
- The dot product $\mathbf{a} \cdot \mathbf{b}$:

```
>>> a = np.array([1, 2])
>>> b = np.array([3, 4])
>>> np.dot(a,b)   # dot product
11
```

- Matrix multiplication:

```
>>> A = np.array([[1,2], [3,4]])
>>> b = np.array([5,6])
>>> np.dot(A, b)   # matrix-by-vector
array([17, 39])
>>> np.dot(A, A)   # matrix-by-matrix
array([[ 7, 10],
       [15, 22]])
```

Linear algebra with `numpy.linalg`

- Matrix determinant & inverse

```
>>> import numpy.linalg as la
>>> A = np.array([[1,2], [3,4]])
>>> la.det(A)
-2.0000000000000004
>>> la.inv(A)
array([[-2. ,  1. ],
       [ 1.5, -0.5]])
>>> np.dot(A, la.inv(A))
array([[  1.00000000e+00,   0.00000000e+00],
       [  8.88178420e-16,   1.00000000e+00]])
```

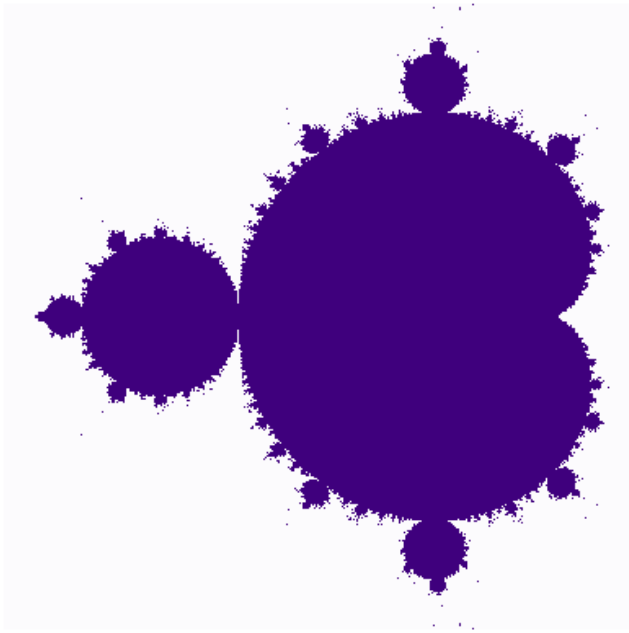
Exercise

Find out how to:

- Find eigenvalues and eigenvectors
- Solve a set of linear equations.

Challenge: the Mandelbrot set

- Use `numpy` arrays, with universal functions/vectorization and broadcasting, to make an image of the Mandelbrot set.



- The Mandelbrot set is the set of complex numbers c for which the function $f_c(z) = z^2 + c$ does not diverge when iterated from $z = 0$.

Challenge: the Mandelbrot set (code)

```
# Python code to plot the Mandelbrot set, using
# numpy arrays, broadcasting, vectorization and universal functions.

import numpy as np
import matplotlib.pyplot as plt

# Part (a).
xmin = -1.5; xmax = 0.5; ymin = -1; ymax = 1.0; # the domain
npts = 501;  # number of points on each axis
xs = np.linspace(xmin,xmax,npts)  # real parts
ys = np.linspace(ymin,ymax,npts, dtype=np.complex128)*1j  # imag parts
 # Now make a 2D array by broadcasting two 1D arrays
cs = xs.reshape((1,npts)) + ys.reshape((npts,1))
```

Challenge: the Mandelbrot set (code)

```
# Part (b)
zs = np.zeros((npts,npts), dtype=np.complex128)

# Part (c).
nits = 100
for i in range(nits):
    zs = zs**2 + cs   # using a ufunc

# Part (d).
maxval = 100.0
mandelbrot = np.abs(zs) < maxval

# Part (e)
fig = plt.imshow(mandelbrot, cmap='Purples', origin='lower')
plt.axis('off')
plt.savefig("mandelbrot.png")
```

Functions

- A function is like a 'black box' that takes one or more inputs (**arguments** or **parameters**) and produces one output.
- (Since the output may be a container type (e.g. `list`), it can actually produce several outputs).
- New functions are defined with the `def` and `return` keywords. Example:

```
>>> def square(i):
...     return i**2
...
>>> square(7)  # try the function
49
>>> square(7.0)
49.0
```

- Try passing a `list` or `str` data type to `square` – what happens?
- More info: `https://docs.python.org/release/1.5.1p1/tut/functions.html`

An example function: Fibonacci sequence

- Let's try a function to compute the Fibonacci sequence from the recurrence relation $f_{k+1} = f_k + f_{k-1}$:

```
>>> def fibonacci(n=10):
...     """Computes a list of the first n Fibonacci numbers."""
...     l = [0, 1]
...     for i in range(n-1):
...             l.append(l[-1] + l[-2])
...     return l
...
```

- Example output

```
>>> fibonacci(10)
[0, 1, 1, 2, 3, 5, 8, 13, 21, 34, 55]
```

An example function: Fibonacci sequence

- The ratio of successive terms should tend towards the Golden Ratio $(\sqrt{5}+1)/2$. Let's check this:

```
>>> l = fibonacci(100)
>>> l[-1] / float(l[-2])  # an approximation to the Golden Ratio
1.618033988749895
>>> (5**0.5 + 1)/2.0  # the true Golden Ratio
1.618033988749895
```

Functions: optional parameters

- Functions can have *optional* named parameters. Example:

```
>>> def raisepower(a, power=2):
...     # Note that 'power' is assigned a default value of 2
...     return a**power
...
>>> raisepower(3)
9
>>> raisepower(2, power=3)
8
>>> raisepower(2, 0.5)
1.4142135623730951
```

- The function may be called *without* specifying optional parameters, or,
- optional parameters may be set by name, or in order.

Functions: docstrings

- At the start of a function, you may write a (multiline) **docstring** to explain what the function does:

```
>>> def raisepower(a, power=2):
...     """This is a docstring.
...     This function raises the first parameter to
...     the power of the second parameter."""
...     return a**power
...
>>> help(raisepower)
```

- Now the docstring should appear in the 'help' for the function.
- In `ipython`, there is enhanced help. Try entering `?raisepower`.

Functions

- In Python, functions are allowed to modify their parameters. Example:

```
>>> def addanimal(a):
...     a.append("aardvark")
...
>>> l = ["horse"]
>>> addanimal(l)
>>> l
['horse', 'aardvark']
```

Functions

- **Q.** Are Python arguments passed **by value** or **by reference**?
- **A.** By value, but the value is a reference to an object . . .
- . . . and so if the object is **mutable**, it may be changed by the function.

Functions: scope

- A function can define, use and modify **local variables** . . .
- . . . and can use **global variables** defined elsewhere.
- When the function ends, all local variables fall out of scope.

- If there are local and global variables with the same name, Python will use the local variable.
- **LEGB**: Python checks Local then Enclosing (nested) then Global then Built-in scope.

```
>>> def fn():
...     a = 4
>>> a = "hello"  # global variable with the same name
>>> fn()
>>> a  # the global variable was not changed
'hello'
```

Functions: scope

- To allow a function to modify a global variable, use the `global` keyword:

```
def fn1():
    x += 1
def fn2():
    global x
    x += 1
```

```
>>> x = 3
>>> fn1()
UnboundLocalError: local variable 'x' referenced before assignmen
>>> fn2()
>>> x
4
```

- (Or, pass the global variable as an argument).

Simple file Input/Ouput

- Open a file for writing:

```
>>> f = open('dickens.txt', 'w')
```

- `f` is a an object with attributes:

```
>>> f.name
'dickens.txt'
>>> f.closed
False
```

Simple file I/O

- Write a line of text:

```
>>> s = """
... It was the best of times,
... it was the worst of times.
... """
>>> f.write(s)
```

- Close the file

```
>>> f.close()
>>> f.closed
True
```

Simple file I/O

- Open the file to read the contents:

```
>>> f = open('dickens.txt', 'r')
>>> s = f.read()  # Read into a string
>>> f.close()
>>> print(s)

It was the best of times,
it was the worst of times.
```

- https://docs.python.org/3/tutorial/inputoutput.html

os module

Example:

```
>>> import os
>>> os.getcwd()  # current directory
'/Code/ipython_notebooks'
>>> os.mkdir('temp')   # Make a new directory
>>> os.chdir('temp')   # Move to that directory
>>> os.chdir('..')    # Move back again
>>> os.rmdir('temp')   # Remove the directory
```

https://docs.python.org/3/library/os.html

Objects

- Python is object-orientated
- An **object** is created ('instantiated') from a blueprint called a **class**.
- The class defines the object's *attributes* and *methods*.
- Methods are functions defined by the class
- Syntax: `<object>.<method>(<arguments)`
- Everything in Python 3 is an object (numbers, lists, arrays, etc.)

Objects: an example

```
>>> z = 1 + 2j   # Python instantiates a new 'complex' object
>>> type(z)
<class 'complex'>
>>> z.imag    # This is an attribute
2.0
>>> z.conjugate()  # This is a method
(1-2j)
```

Standard modules: `math`

- The `math` module provides basic mathematical constants and functions.
- `https://docs.python.org/3/library/math.html#module-math`

Constants

`pi` = 3.141 ...

`e` = 2.718 ...

Basic functions

`exp(x)` $= e^x$, `log(x)` $= \ln(x)$, `sqrt(x)` $= \sqrt{x}$, ...

Trigonometric & hyperbolic functions

- Functions: `cos` `sin` `tan` `cosh` `sinh` `tanh`
- Inverses: `acos` `asin` `atan` `acosh` `asinh` `atanh`

Namespace dangers

- In Python it is very easy to accidently supercede functions or variables.
- **Example:** suppose we wished to sum the numbers 1 to 10

```
>>> sum = 0   # set a counter variable to zero
>>> for i in range(11):
...     sum += i
...
>>> print(sum)
55
```

- This looks fine, **but** . . . by choosing the variable name `sum`, we have accidently **superceded** the in-built function called `sum` (**!**)

Namespace dangers

- If we try using `sum` as a function after the previous code:

```
>>> sum(range(11))
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: 'int' object is not callable
```

- A confusing error message indeed!
- This is a quirk of Python we have to live with

Good practice

Avoid `from module import *` statements.

- **Good:** `import math` then later `print(math.pi)`
- **Bad:** `from math import *` then later `print(pi)`

The cmath module

- The cmath module provides functions for complex arithmetic.
- Use cmath instead of math module, if appropriate
- https://docs.python.org/3/library/cmath.html#module-cmath
- 1j is unit imaginary

Example: check that

$$\exp(\ln(2) + i\pi/2) = e^{\ln 2} e^{i\pi/2} = 2i$$

```
>>> import cmath
>>> z = cmath.log(2.0) + 1j * cmath.pi / 2.0
>>> cmath.exp(z)
(1.2246467991473532e-16+2j)
```

`random` module

Random number generation

- `seed()` : initialize the random number generator
- `random()` : float in range 0 to 1
- `randint(1,10)` : integer in range 1 . . . 10
- `shuffle(l)` : in-place shuffle of a list `l`
- `gauss(m, s)` : random float drawn from a Gaussian distribution with mean `m` and standard deviation `s`.

random module

Example: Generating and shuffling a random string of letters

```
>>> import random
>>> letters = [chr(random.randint(65,90)) for k in range(10)]
>>> for k in range(5):
...     random.shuffle(letters)
...     print("".join(letters))
...
EHUMMFWSDJ
DSMUEHFJWM
HMJSEDWMUF
SFMJWUHMDE
MUMJHWFSDE
```

datetime module

```
>>> import datetime
>>> today = datetime.datetime.today()  # get time and date now
>>> today
datetime.datetime(2014, 10, 7, 14, 4, 10, 47725)
>>> today.weekday()  # 0 = Monday, 6 = Sunday
1
```

https://docs.python.org/3/library/datetime.html