NumPy

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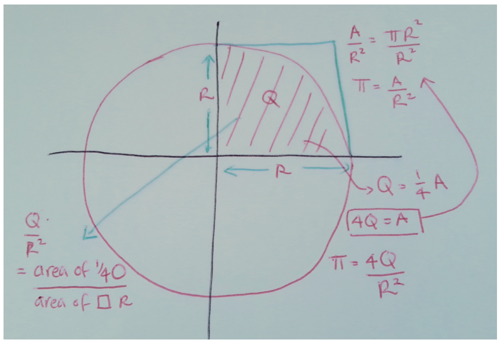
[NumPy] Introducing NumPy

- Core Python provides lists
  - Lists are slow for many numerical algorithms
- NumPy supports:
  - multidimensional arrays (ndarray) : faster and more space-efficient than lists
  - matrices and linear algebra operations
  - random number generation
  - Fourier transforms
  - polynomials
  - tools for integrating with Fortran/C (more about this later)
- NumPy provides fast precompiled functions for numerical routines
- https://www.numpy.org/

[NumPy] Calculating π

If we know the area A of square length R, and the area Q of the quarter circle with radius R, we can calculate π : $\frac{Q}{A} = \frac{\pi R^2}{4R^2}$, so

$$\pi = 4\frac{Q}{A}$$



We can use the *monte carlo* method to determine areas A and Q and approximate π as follows:

For N iterations

1. randomly generate the coordinates (x, y), where $0 \leq \,x,\, y
2. Calculate distance $r = x^2 + y^2$.check if (x, y) lies within radius of circle
3. Check if r lies within radius R of circle i.e. if $r \leq R$
4. if yes, add to count for approximating area of circle

The numerical approximation of π is then : 4 * (count/N)

In [ ]:
```python
# import module numpy as alias 'np'
import numpy as np
a = (np.arange(10000)).reshape([100,100])
```

In [ ]:
```python
a=[[1,2,3],[4,5,6]];
x=a[0][0]; y=a[1][0];
modsq = (x+y)**2; print modsq
```

In [ ]:
```python
stoptime = 5; numpoints = 25
t = [stoptime * float(i) / (numpoints - 1)
      for i in range(numpoints)]
type(t)

args=(t,);
type(args)
```

[NumPy] Calculating π II

In [ ]:
```
# calculate an approximation to pi
# will understand this code by the
# end of the session!
import numpy as np

# N : number of iterations
def calc_pi(N):
    x = np.random.ranf(N);
    y = np.random.ranf(N);
    r = np.sqrt(x*x + y*y);
    c=r[ r <= 1.0 ]
    return 4*float((c.size))/float(N)

# time the results
pts = 6; N = np.logspace(1,8,num=pts);
result = np.zeros(pts); count = 0;
for n in N:
    result = %timeit -o -n1 calc_pi(n)
    result[count] = result.best
    count += 1

# and save results to file
np.savetxt('calcpi_timings.txt', np.c_[N,results],
           fmt='%1.4e %1.6e');
```

[NumPy] Calculating π III

By the end of this session you will:

- be able to handle arrays (create, access, manipulate)
- understand vectorization
- know about random number generation
- be able to save and load data to and from text files
- be aware of performance subtleties
- be able to fully understand the source code for calculating pi!

[NumPy] Creating arrays I

In [ ]:
```
# import numpy as alias np
import numpy as np
```

In [ ]:
```
# create a scalar (zero dimensional array)
a = np.array( 42 ); a
```

[NumPy] Creating arrays II

In [17]:
```
# create a 1d array with a list
a = np.array( [-1,0,1] ); a
```

In [21]:
```
# use functions that create lists e.g. range()
a = np.array( range(-2,6,2) ); a
```

In [ ]:
```
# use arrays to create arrays
b = np.array( a ); b
```

In [ ]:
```
# use numpy functions to create arrays
# arange for arrays, range for lists!
a= np.arange( -2, 6, 2 ); a
```

[NumPy] Creating arrays III

In [ ]:
```
# between start, stop, sample step points
a = np.linspace(-10,10,5);
a;
```

In [ ]:
```
# Ex: can you guess these functions do?
b = np.zeros(3); print a
c = np.ones(3); print b
```

In [ ]:
```
# Ex++: try these and see what you get
h = np.hstack( (a, a, a) ); print h
o = np.ones_like(a); print  o
```

[NumPy] Array characteristics

In [ ]:
```
# array characteristics such as:
print a
#print a.ndim  # dimensions
#print a.shape # shape
#print a.size  # size
#print a.dtype # data type
```

In [ ]:
```
# can choose data type
a = np.array( [1,2,3], np.int16 ); a.dtype
```

In [ ]:
```
# Ex: query the characteristics of the arrays you have created
```

[NumPy] Multi-dimensional arrays I

In [ ]:
```
# multi-dimensional arrays e.g. 2d array or matrix
# e.g. list of lists
mat = np.array( [[1,2,3], [4,5,6]]);
print mat; print mat.size; mat.shape
```

In [ ]:
```
# can create 2d arrays with complex elements (e.g.1 + 2*i)
lst = [[1, 2, 3], [4,5,6]];
mat = np.array(lst, complex);
print mat; print mat.size; print mat.shape
```

In [ ]:
```
# join arrays along first axis (0)
d=np.r_[np.array([1,2,3]), 0, 0, [4,5,6]];
print d; d.shape
```

[NumPy] Multi-dimensional arrays II

In [ ]:
```
# join arrays along second axis (1)
d=np.c_[np.array([1,2,3]), [4,5,6]];
print d; d.shape
```

In [ ]:
```
# Ex: use r_, c_ with nd (n>1) arrays
```

In [ ]:
```
# Ex: can you guess the shape of these arrays?
h = np.array( [1,2,3,4,5,6] ); print h.shape
i = np.array( [[1,1],[2,2],[3,3],[4,4],[5,5],[6,6]] );
print i.shape
j = np.array( [[[1],[2],[3],[4],[5],[6]]] ); print j.shape
k = np.array( [[[[1],[2],[3],[4],[5],[6]]]] ); print k.shape
```

In [ ]:
```
i=np.array([[1, 2], [3, 4], [5, 6]]); j=[1,2,3,4,5,6]
k= np.array([[[1],[2],[3]], [[4],[5],[6]]]); k.shape
```

[NumPy] Reshaping arrays I

In [ ]:
```
# reshape 1d arrays into nd arrays original matrix unaffected
mat = np.arange(6); print mat
print mat.reshape( (3, 2) )
print mat; print mat.size;
print mat.shape
```

In [ ]:
```
mat = np.resize(mat, (1,mat.size));
mat.shape
```

In [ ]:
```
# can also use the shape, this modifies the original array
a = np.zeros(10);
print a
a.shape = (2,5)
print a; print a.shape;
```

[NumPy] Reshaping arrays II

In [ ]:
```
# use flatten() or ravel() to go from nd to 1d
# this creates a COPY of the original
mat = np.array([[1,2,3],[4,5,6]])
mat2 = mat.flatten()
print mat2; print mat2.size; mat2.shape
```

In [ ]:
```
# unlike shape, original matrix unaffected
print mat; print mat.size; mat.shape
```

In [ ]:
```
# Ex: split a martix? Change the cuts and axis values
# need help?: np.split?
cuts=2;
np.split(mat, cuts, axis=0)
```

[NumPy] More array functions I

In [ ]:
```
# use copyto to copy values
# to array
a = np.array( [-2,6,2] ); print a
b = np.ones(3); print b
np.copyto(b, a); print b
```

In [ ]:
```
# Ex: create some nd arrays from the methods we've seen
# query their characteristics, have a play
```

In [ ]:
```
# Ex++: can you guess what these functions do?
v = np.vstack( (arr2d, arr2d) ); print v; v.ndim;
c0 = np.concatenate( (arr2d, arr2d), axis=0); c0;
```

In [ ]:
```
# Ex++: can you guess what this will do?
c1 = np.concatenate(( mat, mat ), axis=1); print "c1:", c1;
```

[NumPy] More array functions II

In [ ]:
```
# Ex++: other functions to explore
#
# stack(arrays[, axis])
# tile(A, reps)
# repeat(a, repeats[, axis])
# unique(ar[, return_index, return_inverse, ...])
# trim_zeros(filt[, trim]), fill(scalar)
# xv, yv = meshgrid(x,y)
```

[NumPy] Accessing arrays I

In [ ]:
```
# basic indexing and slicing we know from lists
# a[start:stop:step] --> [start, stop every step)
a = np.arange(8); print a
print a[0:7:2]
print a[0::2]
```

In [ ]:
```
# negative indices are valid!
print a[2:-3:2]
```

[NumPy] Accessing arrays II

In [ ]:
```
# basic indexing of a 2d array :take care of each dimension
nd = np.arange(12).reshape((4,3)); print nd;
print nd[(2,2)];
print nd[2][2];
```

In [ ]:
```
# get corner elements 0,2,9,11
print nd[0:4:3, 0:3:2]
```

In [ ]:
```
# Ex: get elements 7,8,10,11 that make up the bottom right corner
nd = np.arange(12).reshape((4,3));
print nd; nd[2:4, 1:3]
```

[NumPy] Slices and copies I

In [ ]:
```
# slices are views (like references)
# on array, can change elements
nd[2:4, 1:3] = -1; nd
```

In [ ]:
```
# assign slice to a variable to prevent this
s = nd[2:4, 1:3]; print nd;
s = -1; nd
```

In [ ]:
```
# slicing creates a 'view' on array
# so can change original array
b = a[0::2]; b[0:2]=-1
a
```

[NumPy] Slices and copies II

In [ ]:
```
# simple assignment creates references,
nd = np.arange(12).reshape((4,3))
md = nd
md[3] = 1000
print nd
```

In [ ]:
```
# can avoid this by using copy()
nd = np.arange(12).reshape((4,3))
md = nd.copy()
md[3]=999
print nd
```

[NumPy] Fancy indexing I

In [24]:
```
# advanced or fancy indexing lets you do more
p = np.array([[ 0,  1,  2],[ 3,  4,  5],[ 6,  7,  8],[ 9, 10, 11]]);
print p
```

In [ ]:
```
rows = [0,0,3,3]; cols = [0,2,0,2];
print p[rows,cols]
```

In [30]:
```
# Ex: what will this slice look like?
m = np.array([[0,-1,4,20,99],[-3,-5,6,7,-10]]);
print m[[0,1,1,1],[1,0,1,4]];
```

[NumPy] Fancy indexing II

In [ ]:
```
# can use conditionals in indexing
# m = np.array([[0,-1,4,20,99],[-3,-5,6,7,-10]]);
m[ m < 0 ]
```

In [ ]:
```
# Ex: can you guess what this does? query: np.sum?
y = np.array([[0, 1], [1, 1], [2, 2]]);
rowsum = y.sum(1);
y[rowsum <= 2, :]
```

In [ ]:
```
# Ex: and this?
a = np.arange(10);
mask = np.ones(len(a), dtype=bool);
mask[[0,2,4]] = False; print mask
result = a[mask]; result
```

In [ ]:
```
# Ex: r=np.array([[0,1,2],[3,4,5]]);
xp = np.array([[[1,11],[2,22],[3,33]], [[4,44],[5,55],[6,66]]]);
xp[slice(1),slice(1,3,None),slice(1)]; xp[:1,1:3:,:1];
print xp[[1,1,1],[1,2,1],[0,1,0]]
```

[NumPy] Manipulating arrays

In [50]:
```
# add an element with insert
a = np.arange(6).reshape([2,3]); print a
np.append(a,np.ones([2,3]),axis=0)
```

In [49]:
```
# inserting an array of elements
np.insert(a, 1, -10, axis=0)
```

In [ ]:
```
# can use delete, or a boolean mask, to delete array elements
a = np.arange(10)
np.delete(a, [0,2,4], axis=0)
```

[NumPy] Vectorization I

In [53]:
```
# vectorization allows element-wise operations (no for loop!)
a = np.arange(10).reshape([2,5]); b = np.arange(10).reshape([2,5]);
```

In [55]:
```
-0.1*a
```

In [61]:
```
a*b
```

In [62]:
```
a/(b+1)  #.astype(float)
```

[NumPy] Random number generation

In [70]:
```
# random floats
a = np.random.ranf(10); a
```

In [ ]:
```
# create random 2d int array
a = np.random.randint(0,high=5,size=25).reshape(5,5);
print a;
```

In [ ]:
```
# generate sample from normal distribution
# (mean=0, standard deviation=1)
s = np.random.standard_normal((5,5)); s;
```

In [ ]:
```
# Ex: what other ways are there to generate random numbers?
# What other distributions can you sample?
```

[NumPy] File IO

In [ ]:
```
# easy way to save data to text file
pts=5; x=np.arange(pts); y=np.random.random(pts);
```

In [ ]:
```
# format specifiers: d = int, f = float, e = exponential
np.savetxt('savedata.txt', np.c_[x,y],header='DATA', footer='END',
           fmt='%d %1.4f')
```

In [ ]:
```
!cat savedata.txt
#p=np.loadtxt('savedata.txt')
```

In [ ]:
```
# much more flexibility with genfromtext
p = np.genfromtxt('savedata.txt', skip_header=2,skip_footer=1); p
```

In [ ]:
```
# Ex++: what do numpy.save, numpy.load do ?
```

[NumPy] Polynomials

Can represent polynomials with the numpy class Polynomial from numpy.polynomial.polynomial.

Polynomial([a, b, c, d, e]) is equivalent to $p(x) = a + b\,x + c\,x^2 + d\,x^3 + e\,x^4$.
For example:

- Polynomial([1,2,3]) is equivalent to $p(x) = 1 + 2\,x + 3\,x^2$
- Polynomial([0,1,0,2,0,3]) is equivalent to $p(x) = x + 2\,x^3 + 3\,x^5$

Can carry out arithmetic operations on polynomials, as well integrate and differentiate them.

Can also use the *polynomial* package to find a least-squares fit to data.

[NumPy] Polynomials : calculating π I

The Taylor series expansion for the trigonometric function $\arctan(y)$ is :

$$\arctan(y) = y - \frac{y^3}{3} + \frac{y^5}{5} - \frac{y^7}{7} + \dots$$

Now, $\arctan(1) = \frac{\pi}{4}$, so

$$\pi = 4\left(- \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \dots \right)$$

We can represent the series expansion using a numpy Polynomial, with coefficients:
$p(x)$ = [0, 1, 0, -1/3, 0, 1/5, 0, -1/7,...], and use it to approximate π.

[NumPy] Polynomials : calculating π II

In [72]:
```
# calculate pi using polynomials
# import Polynomial class
from numpy.polynomial import Polynomial as poly;
num = 100000;
denominator = np.arange(num);

denominator[3::4] *=-1 # every other odd coefficient is -ve
numerator = np.ones(denominator.size);

# avoid dividing by zero, drop first element denominator
almost=numerator[1:]/denominator[1:];

# make even coefficients zero
almost[1::2] = 0

# add back zero coefficient
coeffs = np.r_[0,almost];

p=poly(coeffs); 4*p(1) # pi approximation
```

[NumPy] Performance

Python has a convenient timing function called 'timeit'.

Can use this to measure the execution time of small code snippets.

To use timeit function, either import module timeit and use timeit.timeit or use the magic command `%timeit`:

By default, `timeit` loops over your code 3 times and outputs the best time. It also tells you how many iterations it ran the code per loop. You can specify the number of loops and the number of iterations per loop:

- %timeit -n<iterations_per_loops> -r<number_of_loops> <code_snippet>
- %timeit? for more information

https://docs.python.org/2/library/timeit.html

[NumPy] Performance II

Here are some timeit experiments for you to run.

In [ ]:
```
# accessing a 2d array
nd = np.arange(100).reshape((10,10))

# accessing element of 2d array
%timeit -n10000000 -r3 nd[5][5]
%timeit -n10000000 -r3 nd[(5,5)]
```

In [ ]:
```
# Ex: multiplying two vectors
x=np.arange(10E7)
%timeit -n1 -r10 x*x
%timeit -n1 -r10 x**2

# Ex++: from the linear algebra package
%timeit -n1 -r10 np.dot(x,x)
```

[NumPy] Performance III

In [ ]:
```
import numpy as np
# Ex: range functions and iterating
# in  for loops
size = int(1E6)

%timeit for x in range(size): x ** 2

# faster than range for very large arrays
%timeit for x in xrange(size): x ** 2

%timeit for x in np.arange(size): x ** 2

%timeit np.arange(size) ** 2
```

In [ ]:
```
# Ex: look over the two ways of calculating pi.
# Make sure you understand the code.
# Time each method, which is faster?
```

[NumPy] Summary

- Numpy introduces multi-dimensional arrays to Python
- It also provides fast numerical routines convenient for scientific computation
- Next up: Matplotlib