Scientific Programming Practical 9

Introduction

Numpy

Numpy is a fundamental library for high performance scientific computations. It provides fast and memory efficient data structures like ndarray with broadcasting capabilities, standard mathematical functions that can be applied on the arrays avoiding loops, linear algebra functions, I/O methods and it is well integrated with programming languages like C.

import numpy as np

Numpy ndarray is an N-dimensional array object designed to contain **homogeneous** data (i.e. all data must have the same type)

np.array

(list of lists)

They have two information: a **shape**

and a dtype

np.ndarray.shape returns a tuple with the dimensions

np.ndarray.dtype returns the type of the **homgeneous** data

```
import numpy as np
Aint = np.array([[1,2,3], [4,5,6]])
Afloat = np.array([[1.1,2,3], [4.2,5,6], [1,2,3]])
print(Aint)
print(type(Aint))
print(Aint.shape)
print(Aint.dtype)
print("")
print(Afloat)
print(type(Afloat))
print(Afloat.shape)
print(Afloat.dtype)
[[1 2 3]
 [4 5 6]]
<class 'numpy.ndarray'>
(2, 3)
int64
[[1.1 2. 3.]
 [4.2 5. 6.]
 [1. 2. 3.]]
<class 'numpy.ndarray'>
(3, 3)
float64
```

Numpy ndarray is an **N-dimensional** array object designed to contain **homogeneous data** (i.e. all data must have the same type)

np.ndarray.ndim returns dimensionalty

```
Original lists:
[0.0, 1.0, 1.4142135623730951, 1.7320508075688772, 2.0]
[0.0, 1.0, 1.2599210498948732, 1.4422495703074083, 1.5874010519681994]
Numpy ndarray:
                        1.41421356 1.73205081 2.
[ 0. 1.
The shape: (5,)
The dimensionality: 1
The type: float64
The 2D array:
[[ 0.
                          1.41421356 1.73205081 2.
[ 0.
                          1.25992105 1.44224957 1.5874010511
The shape: (2, 5)
The dimensionality: 2
The type: float64
```

```
import numpy as np
import math
mysqrt = [math.sqrt(x) for x in range(0,5)]
mycrt = [x**(1/3) \text{ for } x \text{ in } range(0,5)]
print("Original lists:")
print(mysqrt)
print(mycrt)
print("")
npData = np.array(mysqrt)
print("Numpy ndarray:")
print(npData)
print("")
print("The shape:", npData.shape)
print("The dimensionality:", npData.ndim)
print("The type:", npData.dtype)
print("")
twoDarray = np.array([mysqrt, mycrt])
print("The 2D array:")
print(twoDarray)
print("")
print("The shape:", twoDarray.shape)
print("The dimensionality:", twoDarray.ndim)
print("The type:", twoDarray.dtype)
```

Zeros, ones and diagonals...

dimensions are either a number or a tuple

```
1. Array: np.zeros(N) or matrix: np.zeros((N,M))
```

```
2. Array: np.ones(N) or matrix: np.ones((N,M))
```

3. Matrix: np.eye(N)

np.diag(values): creates a diagonal matrix with values on the diagonal

```
Zero array (1x3)
                    import numpy as np
[ 0. 0. 0.]
                    zeros = np.zeros(3)
Zero matrix (4x3)
                    zMat = np.zeros((4,3))
[[ 0. 0. 0.]
                    ones = np.ones(3)
   0. 0. 0.1
                    oMat = np.ones((3,2))
   0. 0. 0.]
                    diag = np.eve(4)
 [ 0. 0. 0.]]
                    rng = np.arange(5) #5 excluded!
                    print("Zero array (1x3)")
Ones array (1x3)
                    print(zeros)
[ 1. 1. 1.]
                    print("")
                    D = zMat.shape
Ones matrix (3x2)
                    print("Zero matrix ({}x{})".format(D[0],D[1]))
[[ 1. 1.]
                    print(zMat)
 [ 1. 1.]
                    print("")
 [ 1. 1.]]
                    print("Ones array (1x3)")
                    print(ones)
Diagonal matrix
                    print("")
[[ 1. 0. 0. 0.]
                    print("Ones matrix (3x2)")
  0. 1. 0. 0.]
                    print(oMat)
  0. 0. 1. 0.]
                    print("")
       0.
                    print("Diagonal matrix")
                    print(diag)
Range 0-4
                    print("")
[0 1 2 3 4]
                    print("Range 0-4")
A diagonal matrix:
                    print(rng)
[[0 0 0 0 0]]
                    print("A diagonal matrix:")
 [0 1 0 0 0]
                    dm = np.diag(rng)
 [0 0 2 0 0]
                    print(dm)
 [0 0 0 3 0]
                    print("Its shape:")
 [0 0 0 0 4]]
                    print(dm.shape)
It's shape:
(5, 5)
```

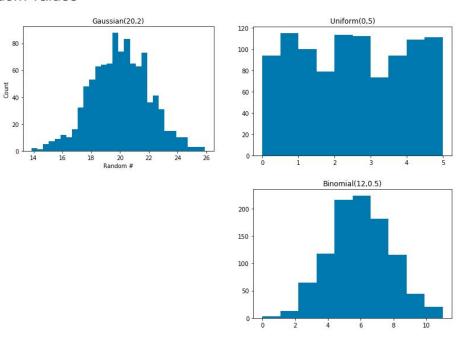
Zeros, ones and diagonals...

Numpy has its own range method that is called np.arange(N). Evenly spaced values in a range can be obtained also with np.linspace(S,E, num=N, endpoint=True/False) to obtain N linearly spaced values from S to E (included, unless endpoint = False is specified).

```
rng = np.arange(7)
print("Range 0-6")
print(rna)
myRange = np.linspace(-5, 2.5, num = 6)
print("6 linearly spaced elements in [-5 - 2.5]:")
print(myRange)
myRange = np.linspace(0,21,num = 7, endpoint=False)
print("7 linearly spaced elements in [0 - 21):")
print(myRange)
Range 0-6
[0 1 2 3 4 5 6]
6 linearly spaced elements in [-5 - 2.5]:
[-5. -3.5 -2. -0.5 1. 2.5]
7 linearly spaced elements in [0 - 21):
[ 0. 3. 6. 9. 12. 15. 18.]
```

Create a random array of 1000 values drawn from: 1. a gaussian distribution with $\sigma=20$ and $\mu=2$ 2. a uniform distribution from 0 to 5 3. a binomial distribution with p=0.5 and n=12

Random values



```
import numpy as np
import matplotlib.pvplot as plt
%matplotlib inline
#get the gaussian random array
q = np.random.normal(20, 2, 1000)
#a uniform random array with vals in [0,5]
u = np.random.uniform(0,5, 1000)
#get the binomial random array
b = np.random.binomial(12, 0.5, 1000)
plt.hist(q, bins = 30)
plt.title("Gaussian(20,2)")
plt.xlabel("Random #")
plt.ylabel("Count")
plt.show()
plt.hist(u, bins = 10)
plt.title("Uniform(0,5)")
plt.xlabel("Random #")
plt.ylabel("Count")
plt.show()
plt.hist(b, bins = 10)
plt.title("Binomial(12,0.5)")
plt.xlabel("Random #")
plt.ylabel("Count")
plt.show()
```

Distributions: https://docs.scipy.org/doc/numpy-1.16.0/reference/routines.random.html#distributions

random seed

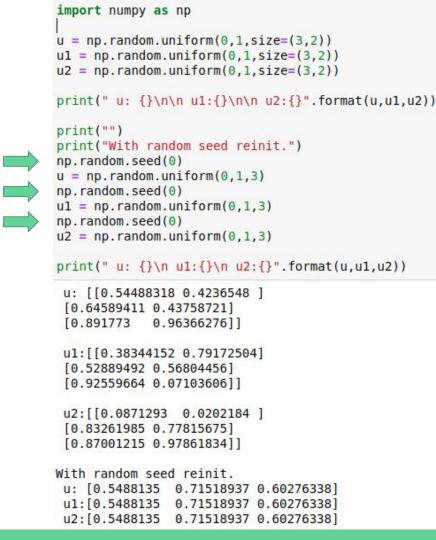
seed of PRSG

is reinitialized to

the same value!

Random values...

... are they really random?



Numpy ← → Pandas

```
{'two': 2, 'three': 3, 'one': 1, 'four': 4}
<class 'pandas.core.series.Series'>
<class 'numpy.ndarray'>
Numpy matrix
[0 0 0 0 0 0]
 [0 1 0 0 0 0]
 [0 0 2 0 0 0]
 [0 0 0 3 0 0]
 [0 0 0 0 4 0]
 [0 0 0 0 0 5]]
Pandas DataFrame
Reindexed DataFrame
      b2
```

```
import pandas as pd
import numpy as np
myDict = {"one" : 1, "two" : 2, "three" : 3, "four" : 4}
mySeries = pd.Series(myDict)
print(myDict)
print("")
print(type(mySeries))
print("")
print(type(mySeries.values))
print("")
myMat = np.diag(np.arange(6))
myDF = pd.DataFrame(myMat)
print("Numpy matrix")
print(myMat)
print("")
print("Pandas DataFrame")
print(myDF)
print("")
print("Reindexed DataFrame")
myDF = pd.DataFrame(myMat, index = list("ABCDEF"),
                    columns = ['a1', 'b2', 'c3', 'd4', 'e5', 'f6'])
print(myDF)
```

Reshaping

```
ndarrays can be reshaped...
```

np.ndarray.reshape(tuple): <u>returns a reshaped ndarray</u> according to the **integer dimensions** in the tuple

np.ndarray.ravel() : flattens the matrix down to a 1D array

```
import numpy as np
myA = np.arange(12)
print("The array:")
print(myA)
print("")
myB = myA.reshape((2,6))
print("Reshaped (2x6):")
print(myB)
print("")
myC = myA.reshape((3,4))
print("Reshaped: (3x4)")
print(myC)
myD = myB.ravel()
print("")
print("Back to array:")
print(myD)
The array:
[0 1 2 3 4 5 6 7 8
Reshaped (2x6):
[[0 1 2 3 4 5]
[6 7 8 9 10 11]]
Reshaped: (3x4)
[[0 1 2 3]
 [4 5 6 7]
 [8 9 10 11]]
Back to array:
```

Looping through arrays

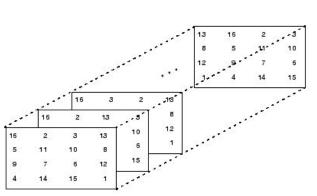
np.ndarray.flat

returns an iterator, allowing to loop through the elements as if they were 1D.

```
import numpy as np
                                  myA = np.arange(12)
                                  print(myA)
                       8 9 10 11] print("")
                                  print("Matrix:")
Matrix:
                                  myA = myA.reshape((4,3))
[[ 0 1 2]
  3 4 5]
                                  print(myA)
  6 7 81
  9 10 1111
                                  print("Looping through elements:")# equivalent to:
Looping through elements:
                                  for el in myA.flat:
                                                                         # for el in myA.ravel():
Element: 0
                                      print("Element:", el)
                                                                               print("Element:",el)
Element: 1
Element: 2
Element: 3
Element: 4
                                  print("Looping row by row:")
Element: 5
                                  for el in myA:
Element: 6
Element: 7
                                      print("Row: ", el, "is a", type(el))
Element: 8
                                      for j in el:
Element: 9
                                           print("\tel:", j)
Element: 10
Element: 11
Looping row by row:
Row: [0 1 2] is a <class 'numpy.ndarray'>
       el: 0
       el: 1
       el: 2
Row: [3 4 5] is a <class 'numpy.ndarray'>
       el: 3
       el: 4
       el: 5
Row: [6 7 8] is a <class 'numpy.ndarray'>
       el: 6
       el: 7
       el: 8
Row: [ 9 10 11] is a <class 'numpy.ndarray'>
       el: 9
       el: 10
       el: 11
```

N-Dimensions

Note that np.ndarray[0,:,:] is the whole first matrix. np.ndarray[:,0,:] is all the first rows, while
np.ndarray[:,:,0] is all the first columns. Regarding slicing and indexing, the same reasoning
applies to n-dimensional matrices. For example, myB below is a 3x3x3 matrix.



```
np.ndarray[M, R, C]

column (can be: for all)

matrix (can be: for all)
```

```
[[3 7 9 3]
 [5 2 4 7]
 [6 8 8 1]]
myA[2,2] = 8
myA[1,3] = 7
mvA[0,3] = 3
second row: [5 2 4 7]
3D matrix
 - shape: (3, 3, 3)
[[[6 7 7]
  [8 1 5]
  [9 8 9]]
 [[4 3 0]
  [3 5 0]
  [2 3 8]]
 [[1 3 3]
 [3 7 0]
  [1 9 9]]]
mvB[0,2,2] = 9
Second matrix:
 [3 5 0]
 [2 3 8]]
Third row of second matrix:
[2 3 8]
Second column of second matrix:
[3 5 3]
```

```
import numpy as np
myA = np.random.randint(0,10, size = (3,4))
print(myA)
print("")
print("myA[2,2] = ", myA[2,2])
print("myA[1,3] = ", myA[1,3])
print("myA[0,3] = ", myA[0,3])
print("second row:", myA[1,:])
print("")
print("3D matrix ",)
myB = np.random.randint(0,10, size = (3,3,3))
print(" - shape: ", myB.shape)
print(myB)
print("")
print("myB[0,2,2] = ", myB[0,2,2])
print("Second matrix:")
print(myB[1,:,:])
print("Third row of second matrix:")
print(myB[1,2,:])
print("Second column of second matrix:")
print(myB[1,:,1])
```

Operator broadcasting

```
[7 3]
                                                                     A = np.random.randint(0,10, size = (3,2))
                            [2 7]]
                                                                     B = np.random.randint(0,10, size = (3,3,3))
                           Matrix B 3x3x3
                                                                     C = np.random.randint(0,10, size = (3,1))
                           [[[2 0 0]
                                                                     print("Matrix A 3x2")
                             [4 5 5]
                                                                     print(A)
                             [6 8 4]]
                                                                     print("")
                            [[1 4 9]
                                                                     print("Matrix B 3x3x3")
                             [8 1 1]
B + C
                                                                     print(B)
                             [7 9 9]]
[[[6 4 4]
                                                                     print("")
 [10 11 11]
                             [[3 6 7]
 [10 12 8]]
                                                                     print("Matrix C 3x1")
                             [2 0 3]
                                                                     print(C)
                             [5 9 4]]]
[[ 5 8 13]
                                                                     print("")
 [14 7 7]
                           Matrix C 3x1
 [11 13 13]]
                                                                     print("A squared")
                           [[4]
                                                                     print(A**2)
                            [6]
[[ 7 10 11]
                            [4]]
                                                                     print("")
 [8 6 9]
 [ 9 13 8]]]
                                                                     print("A square-rooted")
                           A squared
                                                                     print(np.sqrt(A))
                           [[ 0 16]
                            [49 9]
[[[2 0 0]
                            [ 4 49]]
 [4 5 5]
                                                                     print("")
 [6 8 4]]
                                                                     print("B square-rooted")
                           A square-rooted
                           [ 0.
                                                                     print(np.sqrt(B))
[[1 4 9]
                              2.64575131 1.73205081]
 [8 1 1]
                             [ 1.41421356 2.64575131]]
 [7 9 9]]
                                                                     print("A + C ")
                           B square-rooted
                                                                     print(A + C)
[[3 6 7]
                           [[[ 1.41421356 0.
 [2 0 3]
                                                                     print("")
                                         2.23606798 2.236067981
 [5 9 4]]]
                             [ 2.44948974 2.82842712 2.
Sub array B - 20
                                                                     print("B + C ")
[[[-18 -20 0]
                            [[ 1.
 [-16 -15 5]
                                                                     print(B + C)
                             [ 2.82842712 1.
 [ 6 8 4]]
                             [ 2.64575131 3.
                                                            11
                                                                     print("")
[[-19 -16 9]
                            [[ 1.73205081 2.44948974 2.64575131]
                                                                     print("B")
 [-12 -19 1]
                             [ 1.41421356 0.
                                                   1.732050811
 [ 7 9 9]]
                                                                     print(B)
                             [ 2.23606798 3.
                                                            111
                           A + C
                                                                     print("Sub array B - 20")
[[-17 -14 7]
                           [[ 4 8]
 [-18 -20 3]
                                                                     B[:, 0:2, 0:2] = 20
                            [13 9]
 [ 5 9 4]]]
                                                                     print(B)
                            [ 6 11]]
```

Matrix A 3x2 [[0 4] import numpy as np

Linear algebra

```
import numpy as np
from numpy import linalg

A = np.random.randint(0,10, size = (4,4))
print("Matrix A:")
print(A)
print("")
print("inv(A)")
A_1 = linalg.inv(A)
print(A_1)
print(A_1)
print("")
print(np.dot(A,A_1))
```

```
Matrix A:
[[3 7 5 5]
 [0 1 5 9]
[3 0 5 0]
 [1 2 4 2]]
inv(A)
0.09537572 -0.10115607 -0.16763006 0.216763011
 [-0.13872832 -0.03468208 -0.02890173 0.50289017]
  0.06647399 0.1416185 0.03468208 -0.30346821]]
   1.00000000e+00
                   0.00000000e+00
                                  2.77555756e-17
                                                  0.00000000e+001
   0.00000000e+00
                  1.00000000e+00
                                  0.00000000e+00
                                                  0.00000000e+001
   0.00000000e+00
                  0.00000000e+00
                                  1.00000000e+00
                                                  0.00000000e+001
                                  6.93889390e-17
                                                  1.00000000e+00]]
  -2.77555756e-17
                   0.00000000e+00
```

```
import numpy as np

a = np.array([1, 2, 3, 1, 2, 3,1, 1,1])
A = a.reshape((3,3))
B = np.random.randint(0,10, size = (3,2))

print("A (3x3)")
print(A)
print("")
print("B (3x2)")
print(B)
print("")
print("AxB (3x2)")
print(A.dot(B))
print("")
print("A transposed:")
print(A.T)
```

```
A (3x3)
[[1 2 3]
[1 2 3]
[1 1 1]]
B (3x2)
[[4 3]
[4 4]
 [8 4]]
AxB (3x2)
[[36 23]
[36 23]
 [16 11]]
A transposed:
[[1 1 1]
[2 2 1]
 [3 3 1]]
```

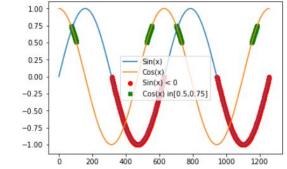
Filtering

It is possible to **filter** np.ndarrays to **retrieve the indexes** (or the values) meeting specific conditions. The method where **provides the index** of those values.

If the np.ndarray is a matrix, where returns a tuple of indexes that are respectively the i and j coordinates of the elements fulfilling the condition.

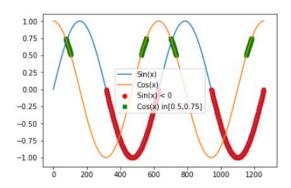
```
import numpy as np
import matplotlib.pyplot as plt
A = np.arange(-2* np.pi, 2*np.pi, 0.01)
sA = np.sin(A)
cA = np.cos(A)
plt.plot(sA)
plt.plot(cA)
s0A Y = sA[sA < 0]
s0A X = np.where(sA < 0)
c0A Y = cA[np.all( [cA > 0.5 , cA < 0.75], axis = 0)]
c0A X = np.where(np.all([cA > 0.5, cA < 0.75], axis = 0))
plt.scatter(s0A X,s0A Y, marker='o', c = 'red')
plt.scatter(c0A X,c0A Y, marker='X', c = 'green')
plt.legend(["Sin(x)", "Cos(x)", "Sin(x) < 0", "Cos(x) in[0.5, 0.75]"])
plt.show()
```

Note that in the code above, np.all tests if the two conditions are True at the same time (i.e. AND). If we want to test if at least one is True we use np.any.



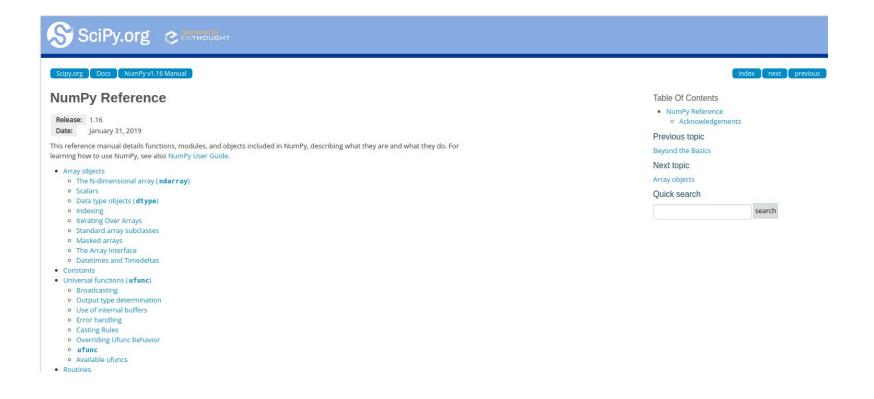
Any / All

Note that in the code above, np.all tests if the two conditions are True at the same time (i.e. AND). If we want to test if at least one is True we use np.any.



```
import numpy as np
v1 = [True, False, False, True]
v2 = [False, False, True, True]
v3 = [False, False, False, True]
print("vals:")
vals = np.array([v1, v2, v3])
print(vals)
print("\nANY(vals):")
print(np.any(vals, axis=0))
print("\nANY(vals) on rows:")
print(np.any(vals, axis=1))
print("\nALL(vals):")
print(np.all(vals, axis=0))
print("\nALL(vals) on rows:")
print(np.all(vals, axis=1))
vals:
[[ True False False True]
 [False False True True]
 [False False True]]
ANY(vals):
[ True False True True]
ANY(vals) on rows:
[ True True True]
ALL(vals):
[False False False True]
ALL(vals) on rows:
[False False False]
```

https://docs.scipy.org/doc/numpy-1.16.1/reference/



http://qcbsciprolab2019.readthedocs.io/en/latest/practical9.html

Exercises

- 1. Create the following functions:
 - a. createRadomList: with parameters, N, min, max. Creates a list of N random integers ranging from min to max;
 - b. getIdentical: with parameters two lists of integers L1 and L2 having the same size. It returns the list of indexes I where L1[I] == L2[I]
 - c. check: gets lists L1, L2, identities (as computed by getIdentical) and a number N and prints if the first N and last N values in identities correspond to indexes of identical values in L1 and L2;
 - d. implement getIdentical using numpy.ndarrays. Call it getIdenticalNpy (hint: subtract the
 two arrays and find zeros).

Test the software creating two lists of 100,000 random numbers from 0 to 10.

Show/Hide Solution

2. Write a function that converts a numpy ndarray of temperatures expressed in Degrees Celsius into Degrees Farenheit. The formula to convert a temperature C in Celsius into F in Farenheit is the following:

$$F = C * 9/5 + 32$$

Write then a function that converts a numpy ndarray of temperatures in Farenheit into Celsius.