

UECM1703 Introduction to Scientific Computing

Topic 2: Arrays Manipulation

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Programming with basic data types and imperative programming is not convenient and efficient for numeric array data. For example, to create a sine function for the range 0 to 4 .

```
# Performing calculation with basic data types and imperative programming
from math import pi, sin
xvals = [i*0.1 for i in range(int(4*pi/0.1))]
yvals = [sin(x) for x in xvals]

# Plotting
import matplotlib.pyplot as plt
plt.plot(xvals, yvals)
plt.show()
```

The Numpy module gains popularity because it makes the above calculation shorter (as well as making arithmetic, etc. with arrays much simpler).

```
# Performing calculation with Numpy
import numpy as np      # Must memorise
xvals = np.arange(0, 4*np.pi, 0.1)
yvals = np.sin(xvals)
```

CO1: perform vector and matrix operation using computer software

1. Numpy Array Data Types

Array = multi-index, homogeneous (elements are of the **same data type**) data structure.

Python's Numpy array `numpy.ndarray` is an n-dimensional (nD) array object which is also known as tensor in the tensorflow machine learning package.

1.1. Numpy Array Construction: Creating Vectors, Matrices, ...

1.1.1. Constructing arrays with no particular pattern

```
# Vector --- can be used to represent one stock price vs time
A1 = np.array([1.0, 3.5, 4.2, 2.3, 3.4, 1.5]) # All double
A2 = np.array([10,11,12,13,14,15])           # All integer
A3 = np.array([7, 19, 19, 18], dtype='double') # All double
A4 = np.array([True,False,True,False,True])   # All Boolean

# Matrix of integers --- can be used to represent gray image
B1 = np.array([ [7,19],
                 [19,18] ]) # We usually just write in one line

# Matrix of doubles
B2 = np.array([[7,19],[19,18]], dtype='double')

# 3-D arrays --- can be used to represent coloured image
C1 = np.array([[[1,2],[1,4],[5,1]], [[7,2],[9,3],[8,8]])
#
```

```

#      C1[0,:,:)      C1[1,:,:) =
#      1  2          7  2
#      1  4          9  3
#      5  1          8  8
#

```

Note that Python's ImageIO module has a class called `Image` which is a subclass of `np.array` to represent coloured images.

1.1.2. Constructing arrays with particular patterns --- identity matrices, diagonal matrices, etc.

```

# Vector --- One dimensional (1D) array
A5 = np.zeros(10)          # 10 zeros of data type double
A6 = np.ones(10)           # 10 ones of data type double
A7 = np.full(10,100)       # 10 hundreds of data type integer
A8 = np.linspace(0,np.pi,num=51,endpoint=True)
A9 = np.arange(0,10,2)     # or np.r_[0:10:2]

# Matrix --- Two dimensional (2D) array
B3 = np.zeros((2,4))
B4 = np.ones((4,2))
B5 = np.full((3,5),100)
B6 = np.eye(4)             # 4 x 4 identity matrix
B7 = np.eye(3,2)           # 3 x 2 identity matrix
B8 = np.diag([5,7,-3,4])   # Create a diagonal matrix
B9 = np.diag(np.arange(6,2,-1))
B10 = B13.diagonal()       # Get the diagonal of a matrix!
B11 = np.diag(B13)         # Same: Get the diagonal of a matrix!

# Three dimensional (3D) arrays
C3 = np.zeros((2,4,3))
C4 = np.ones((4,2,3))
C5 = np.full((3,5,3),100)

```

The command `np.linspace` is usually used in the creation of a 1-D array for the interval of a particular function f . In particular,

$$A8 = 0, \frac{2}{50}, \frac{4}{50}, \dots, \frac{49}{50}, \dots$$

Note that interval $[0, \pi]$ is cut into 50 intervals with 51 points.

1.1.3. Constructing arrays with advanced patterns

Constructing arrays with regular but complex patterns:

```
from math import tan, sin, cos, pi, log, exp
B12 = np.array([[tan(pi/3), 3/sin(pi/4)],
               [log(cos(pi/6)), 1+exp(1.5)]])
B13 = np.array([sin(x) for x in
               np.linspace(0,5*pi/14,6)]).reshape((2,3))
               # 13 12 11 10
B14 = np.vander([1,3,2,5]) # 33 32 31 30
               # 23 22 21 20
               # 53 52 51 50

#
# Grid is for vectorised evaluations of n-D scalar/vector fields
#
# Two dimensional grids:
B15a, B15b = np.meshgrid([1,2,3],[2,5,7,9]) # return two 4x3 matrices
# [1, 2, 3] [2, 2, 2]
# [1, 2, 3] [5, 5, 5]
# [1, 2, 3] [7, 7, 7]
# [1, 2, 3] [9, 9, 9]
# Note: default indexing = 'xy' for computer graphics (Topic 4)

#
# A three dimensional grid
#
# X x Y x Z = [x1,x2] x [y1,y2,y3] x [z1,z2]
#
XR, YR, ZR = [1,2], [3,5,7], [8,9] # R for range
XP, YP, ZP = np.meshgrid(XR, YR, ZR,indexing='ij') # P for grid points
C6          C7          C8
|           |           |
V           V           V
[[[1 1]      [[3 3]      [[8 9]
 [1 1]      [5 5]      [8 9]
 [1 1]]     [7 7]]     [8 9]]

[[2 2]      [[3 3]      [[8 9]
 [2 2]      [5 5]      [8 9]
 [2 2]]     [7 7]]     [8 9]]

#
# It can be used for the computation of the scalar field  $f(x,y,z)=x^2+y^2+z^2$ 
#
# def f(X, Y, Z): return X**2 + Y**2 + Z**2
# f = np.vectorize(f)
# arr = f(XP, YP, ZP)
#
# Related: np.mgrid[1:3,3:8:2,8:10] # mgrid does not accept list
# Related: np.ogrid[1:3,3:8:2,8:10] # => (2,1,1), (1,3,1), (1,1,2)
```

Constructing an array with random patterns:

```
# Random matrices
B16 = np.random.rand(3, 2) # 3x2 random matrix uniform over [0,1)
B17 = np.random.random((3,2)) # 3x2 random matrix uniform over [0,1)
B18 = np.random.randn(3, 2) # 3x2 random matrix Normal(0,1)

# Random three dimensional arrays
C13 = np.random.rand(3,2,4) # ~ Uniform[0,1)
C14 = np.random.random((3,2,4)) # ~ Uniform[0,1)
```

```
C15 = np.random.randn(3,2,4)      # ~ Normal(0,1)
```

1.2. Basic Array Attributes (Shape, Size)

Arrays are created with a particular shape and data type. The information or attributions associated with arrays can be obtained from the Numpy array.

- * Get the dimension of an array: `A.ndim`.
- * Get the shape of an array: `A.shape`.
- * Get the number of elements in an array: `A.size`.
- * Get the total number of bytes used: `A.nbytes`, it is defined as `A.size*A.itemsize`. For example, if there are n elements in `A` and all the elements are 64-bit floating numbers, then the total number of bytes used in `A` to store array data is $8n$.

There are a few operations which are related to the attributes of an array:

- * **Transpose:** It works by reversing the 'indices' but for real-world application, it is used to transpose a matrix `A` to `A.T`, for example:

```
# 1D transpose: No change
[ a b c d ] ---> [ a b c d ]

# 2D transpose: Change a matrix to its transpose
[ a b c ]
[ d e f ]      [ a d g j ]
[ g h i ] --->  [ b e h k ]
[ j k l ]      [ c f i l ]

[ a ]
[ b ]      --->  [ a b c ]
[ c ]

* Change from  $n$ -D array to 1-D array: A.ravel(), A.flatten()

# 1D ravel/flatten: No change
[ a b c d ] ---> [ a b c d ]

# 2D ravel/flatten
[ a b c ]
[ d e f ]      ---> [ a b c d e f g h i ]
[ g h i ]

* Change an array to a compatible shape: A.reshape(( $d_1, d_2, \dots, d_r$ ))

# np.array([1,3,5,7,9,5]).reshape((2,3))
[ 1 3 ]
[ 1 3 5 7 9 5 ] ---> [ 5 7 ]
[ 9 5 ]

* Change an array to any shape: np.resize(A, ( $d_1, d_2, \dots, d_r$ ))

# A = np.array([1,3,5,7,9,5])
# B = np.resize(A, (2,2))
[ 1 3 ]
[ 1 3 5 7 9 5 ] ---> [ 5 7 ]

# C = np.resize(A, (3,5))
[ 1 3 5 7 9 ]
[ 1 3 5 7 9 5 ] ---> [ 5 1 3 5 7 ]
[ 9 5 1 3 5 ]
```

1.3. Numpy Array Formatting

Get the current format: `np.get_printoptions()`
"Default values:" precision = 8, threshold = 1000, edgeitems = 3, linewidth = 75 characters per line, suppress = False, i.e. do not print small floating point values using scientific notation, nanstr = 'nan', infstr = 'inf', formatter = None (a dictionary of types to set the formatting options), sign = '-', floatmode = 'maxprec'.
Set the format: `set_printoptions(args)`
args are the keywords above. We usually need to set the linewidth for printing a nicer matrix.
Print the matrix: `print(A)`

Example. Print the matrix

```
[ 1/2  1/3  1/4  1/5  1/6  1/7  1/8  1/9 ]
[ 1/8  1/9  1/8  1/7  1/6  1/5  1/4  1/3 ]
```

using 'printoptions'.

Sample Solution 1:

```
A = np.array([[1/2, 1/3, 1/4, 1/5, 1/6, 1/7, 1/8, 1/9],
              [1/8, 1/9, 1/8, 1/7, 1/6, 1/5, 1/4, 1/3]])
print(A)
# Temporarily set the options
with np.printoptions(precision=4, linewidth=100):
    print(A)
print(A)
```

Sample Solution 2:

```
A = np.array([[1/2, 1/3, 1/4, 1/5, 1/6, 1/7, 1/8, 1/9],
              [1/8, 1/9, 1/8, 1/7, 1/6, 1/5, 1/4, 1/3]])
print(A)
default_printoptions = np.get_printoptions()
# Permanently set the options
np.set_printoptions(precision=4, linewidth=100)
print(A)
np.set_printoptions(**default_printoptions)
print(A)
```

1.4. Numpy Array Applications

- * **Array of numbers** can be used to represent
 - time series, audio / sound signals (mostly 1D)
 - black-and-white images, grayscale images (2D)
 - Colour images (3D)
 - + RGB colour = $M \times N \times 3$ with values in [0,1] or 0--255;
 - + RGBA colour = $M \times N \times 4$ with values in [0,1] or 0--255 with A=transparency

Note that out-of-range RGB(A) values are clipped.

* **Array of characters** can be used to represent

- ASCII / Unicode arts

* **Array of Booleans** can be used for selection as to be discussed later.

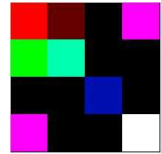
Python tools to visualise a matrix as an image:

```
matplotlib.pyplot.spy(Z) # 2D array only
matplotlib.pyplot.imshow(X, cmap=None, norm=None, *, aspect=None,
    interpolation=None, alpha=None, vmin=None, vmax=None, origin=None,
    extent=None, interpolation_stage=None, filternorm=True,
    filterrad=4.0, resample=None, url=None, data=None, **kwargs)
```

For grayscale images, use `cmap='gray'`, `vmin=0`, `vmax=255`.

Example. (Array of Numbers) A 4x4 pixel coloured image below can be represented as Numpy array:

```
P3
4 4
15
# https://paulbourke.net/dataformats/ppm/
255 0 0 100 0 0 0 0 0 255 0 255
0 255 0 0 255 175 0 0 0 0 0 0
0 0 0 0 0 0 0 15 175 0 0 0
255 0 255 0 0 0 0 0 0 255 255 255
```



The following is how we can read and display the 4x4 pixel image.

```
import numpy as np
# https://liaohaohui.github.io/UECM1703/test.ppm
fp = open("test.ppm", "r")
lines = []
while True:
    line = fp.readline()
    if not line: break # Break out of loop when no more lines
    # We skip any empty line and lines with are comment
    if len(line)>0 and line[0] != '#':
        lines.append(line.strip())
if lines[0][0]=="P" and int(lines[0][1:])==3: # P3=Coloured image
    W, H = lines[1].split()
    W = int(W)
    H = int(H)
    m = int(lines[2])
    if m == 255:
        imgarr = np.zeros((H,W,3), dtype='uint8')
    elif m == 65535:
        imgarr = np.zeros((H,W,3), dtype='uint16')
    image_contents = [int(c) for c in " ".join(lines[3:]).split()]
    for y in range(H):
        for x in range(W):
            imgarr[y,x,:] = image_contents[(y*3*W+3*x):(y*3*W+3*x+3)]
print(imgarr)

from PIL import Image
img = Image.fromarray(imgarr)
import matplotlib.pyplot as plt
plt.imshow(img)
plt.show()
```

Example. (ASCII ART) Consider a bat in ASCII art:

```

      /\          /\
    /  \\' _   (\_/)   _.' /  \
    | .'' _.'--(o.o)--' .'' |
     \_ /' ;=/' " \;=' \_ /'_
       '\___|_____|____|'\
jgs              \"-|-)/
                \" \" \"

```

It can be expressed as Numpy array of 'characters' but it is not very useful.

[illegible]

2. Array Mathematical Functions and Numpy Ufuncs

When we encounter an array below:

```
from math import sin
A = np.array([sin(1), sin(2), sin(3), sin(4), sin(5), sin(6)])
B = np.array([[sin(1), sin(2), sin(3)],
              [sin(4), sin(5), sin(6)]])
```

we would hope to **abbreviate** it as

```
fA = sin(np.array([1,2,3,4,5,6]))
fB = sin(np.array([[sin(1), sin(2), sin(3)],
                  [sin(4), sin(5), sin(6)]]))
```

However, the sine function from math module would **complain**.

Numpy provides two solutions:

- * Build the commonly use mathematical functions in. For example, use `np.sin` instead of `sin`
- * ‘Vectorise’ the function (using Numpy’s universal function framework with 1 input and 1 output):
`arsin = np.vectorize(sin)`
- * `np.frompyfunc(func, nin, nout, *[, identity])` Note that `nin` and `nout` are the number of inputs and number of outputs of the function `func` respectively. In this case, `arsin = np.frompyfunc(sin,1,1)`

Example. (Application: Plotting) By use the plotting functions `plt.plot` and `plt.show` to draw (a) Sine function; (b) Cosine function; and (c) floor function for the domain $[-2i, 2i]$.

Solution: The question does not say how small is the step size, we will just split $[-2\pi, 2\pi]$ to 100 equal intervals.

```
import numpy as np, matplotlib.pyplot as plt
xr = np.linspace(-2*np.pi, 2*np.pi, 101) # x range
y1 = np.sin(xr)
y2 = np.cos(xr)
y3 = np.floor(xr)
plt.plot(xr, y1, xr, y2, xr, y3)
plt.show() # This is not needed in Spyder/Jupyter
```

If we have a computer to plot the graph, we can see that floor looks ugly, this is because `plt.plot` just join points and we need break the domain into more intervals to make the plot of floor function nice.

Exercise. Try and see if you can define a ‘vectorise’ function for

$$\operatorname{sinhc}(x) = \begin{cases} \frac{e^x - e^{-x}}{2x}, & x \neq 0, \\ 1, & x = 0. \end{cases}$$

so that you can use it to calculate `sinhc(np.linspace(-2*np.pi, 2*np.pi, 101))`.

□

Example. (Final Exam Oct 2018, Q1(b)) The dot product of two vectors $\mathbf{x} = (x_1, x_2, \dots, x_n)$ and $\mathbf{y} = (y_1, y_2, \dots, y_n)$, $\mathbf{x} \cdot \mathbf{y}$, is defined as

$$\mathbf{x} \cdot \mathbf{y} = x_1 y_1 + x_2 y_2 + \dots + x_n y_n.$$

The angle between two arrays is defined by the following relation

$$\cos \theta = \frac{\mathbf{x} \cdot \mathbf{y}}{\|\mathbf{x}\| \|\mathbf{y}\|}.$$

Implement a **Python function** `theta` to calculate the angle (in **degree**) if you are given two arrays

$a=[a_1,a_2,a_3,a_4]$ and $b=[b_1,b_2,b_3,b_4]$. You **must** write down the proper import statements. If you use the Numpy module, you must prefix the Numpy functions with “np.” or marks will be heavily deducted. Use scientific calculator to find the return value of the Python command `theta([1,2,3,4],[2,1,3,4])` to 4 decimal places.

Sample Solution:

```
# Appropriate import when writing scripts          1    mark
import numpy as np
from math import degrees, acos, sqrt
# Able to define a function and return a value:      1.5 marks
# Correct translation of mathematical formula to Python: 2.5 marks
def theta(x, y):
    # We are using the single-line for loop from Topic 1
    # The size of x and y may be different, so we need to
    # check it in real-world programming but it is fine
    # to assume x and y the same size in exam
    num = sum(x[i]*y[i] for i in range(x.size))
    sxx = sqrt(sum(x[i]*x[i] for i in range(x.size)))
    syy = sqrt(sum(y[i]*y[i] for i in range(y.size)))
    return degrees(acos(num/sxx/syy))

print(theta(np.array([1,2,3,4]),np.array([2,1,3,4])))
```

The question also test the understanding of manual calculation and the use of calculator:

$$= \cos^{-1} \frac{2+2+9+16}{1^2+2^2+3^2+4^2} \times \frac{180^\circ}{\sqrt{2^2+1^2+3^2+4^2}} \quad [1 \text{ mark}]$$

$$= \cos^{-1} \frac{29}{30} = 0.258922 \times \frac{180^\circ}{14.8351} = 14.8351^\circ \quad [2+1=3 \text{ marks}]$$

Example. Consider the heart disease data from https://bookdown.org/brianmachut/uofm_analytics_r_hw_sol_2/logreg.html by analysing the relation between $X=\text{fast_food_spend}$ and $Y=\text{heart_disease}$.

One mathematical model for fitting the data is called logistic regression model:

$$P(Y = 1|X = x) = \frac{1}{1 + \exp(-(-10.651330614 + 0.002199567x))}$$

By using the array processing knowledge, write a Python script to read `heart_data.csv` and express the logistic regression model as Python function.

Sample Python Script Solution:

```
import numpy as np
data = np.loadtxt("heart_data.csv", delimiter=",",
                 skiprows=1, dtype=np.double)
col1 = data[:,0]
col3 = data[:,2]
from matplotlib.pyplot import plt
plt.plot(col3,col1,"*")
plt.show()

# Expressing logistic regression model as Python functions
def log_reg(x):
    return 1.0/(1.0+np.exp(-(-10.651330614 + 0.002199567*x)))
```


3. Array Indexing: Sub-arrays, ...

Indexing is an important way to assess the data in an n -D array. Indexing an array with an integer / integers will lead to the reduction of dimension by default. To keep the dimension, we either use a range $m:n:s$ or use an 'extra' index called 'None' to keep the dimension. We need to note that indexing an array A on gives us a **view** of the array A .

- * Return a "view" of A with a given shape (m_1, \dots, m_k) . Note that $m_1 \times \dots \times m_k$ must be equal to $A.size$: `A.reshape((m1, ..., mk))`.
- * Return a "view" of (m_1, m_2, \dots, m_k) -array A as a transpose with a shape (m_k, \dots, m_2, m_1) : `A.T` (alternatively, `np.transpose(A)`).

Making any changes to the **view** will be reflected on the original array. If we need a **copy** of the sub-array from A , we need to use the `.copy()` method or stacking commands:

- * Return a "copy" of A with a specific type: `A.astype(sometype)`, here `sometype` can be 'double', 'bool', 'int8', etc.
- * Return a new array by stacking existing array(s): `np.hstack` (stacking array horizontally) and `np.vstack` (stacking array vertically).

```
np.hstack((A_1,A_2,...,A_k)) : A_1 A_2 ... A_k
```

```
np.vstack((A_1,A_2,...,A_k)) : A_1
                             A_2
                             .
                             .
                             A_k
```

3.1. Usual Indexing :n, m:n, m:, m:n:k, :

- * In this section, m and n are assumed to be **non-negative**.
- * Python's index starts from 0
- * Python's ending index $m:n$ will never reach n

Example.

- * `:` is similar to 'take all' (this depends on the shape of the array)
- * `:12` is similar to `0,1,2,3,4,5,6,7,8,9,10,11` or `range(12)`
- * `5:12` is similar to `5,6,7,8,9,10,11` or `range(5,12)`
- * `2:12:3` is similar to `2,5,8,11` or `range(2,12,3)`
- * `12:2:-2` is similar to `12,10,8,6,4` (2 will not be reached) or `range(12,2,-2)`

Without loss of generality, we consider a 2-D array A .

(I) `A[m-1,n-1]` : Indexing an element of A at (m,n) (dim=0)

(II) `A[m-1,:]` : Indexing A at m -row (dim=1)

(III) `A[:,n-1]` : Indexing A at n -column (dim=1)

(IV) `A[m1-1:m2,n1-1:n2]` :

Indexing a sub-array of A bounded by $m1$ -row to $m2$ -row and $n1$ -column to $n2$ -column

(V) `A[m1-1:m2:ms,n1-1:n2:ns]` :

Indexing a sub-array of A from $m1$ -row to row- $m2$ by step ms and from $n1$ -column to $n2$ -column by step ns . When $m1-1$ is ignored, it assumes 0 and when $m2$ is ignored, it assumes the last row and when ms is ignored, it assumes 1. The situations are similar for $n1-1$, ns and $n2$.

(VI) `A[[r1-1,...,rk-1],:[c1-1,...,cl-1]]` :

Indexing a sub-array of A using rows $r1, \dots, rk$, columns $c1, \dots, cl$.

Numpy provides alternative indexing functions `take` and `put` to take and assign values to a slice of an array. They are less convenient to use, we will skip them:

- (a) `A.item(3,4)`
- (b) `A.take(indices=[3],axis=0)`
- (c) `A.take(indices=[4],axis=1)`
- (d) `A.take(range(3,7),axis=1).take(range(1,3),axis=0)`
- (d) `A.take([3,5,7],axis=1).take([1,3,5],axis=0)`

Example. (Final Exam Sept 2015, Q3(a)) The following vector is defined in Python

```
V = np.array([2,7,-3,5,0,14,-1,10,-6,8])
```

What will be displayed if the following variables B, C and D are printed.

- (i) `B = V[[1,3,4,5,6,9]]`

Solution: We first index the array V:

	0	1	2	3	4	5	6	7	8	9	<-- indices for V
V =	2	7	-3	5	0	14	-1	10	-6	8	
B =	[7	5	0	14	-1	8]					

- (ii) `C = V[[8,2,1,9]]`

Solution: `C = [-6 -3 7 8]`

- (iii) `D = np.array([V[[0,2,4]],V[[1,3,5]],V[[2,5,8]])`

Solution: `D = [[2, -3, 0], [7, 5, 14], [-3, 14, -6]]`

Example. Consider the array generated with `A = np.arange(1,55,dtype='double').reshape(6,9).`

```
A =
  1   2   3   4   5   6   7   8   9
10  11  12  13  14  15  16  17  18
19  20  21  22  23  24  25  26  27
28  29  30  31  32  33  34  35  36
37  38  39  40  41  42  43  44  45
46  47  48  49  50  51  52  53  54
```

Write down the output of the following commands:

- (a) `print(A[3,4])` Indexing (I)
- (b) `print(A[3,:])` Indexing (II)
- (c) `print(A[:,4])` Indexing (III)
- (d) `print(A[1:3,3:7])` Indexing (IV)
- (e) `print(A[1:6:2,:][:,3:8:2])` Indexing (V) & (VI)
- (f) `print(A[3,None])` (It is the same as `A[None,3]`)
- (g) `print(A[:,4,None])` or `print(A[:,4:5])`

Example. (Final Exam Sept 2015, Q1(a)) The following matrix is defined in Python:

```
M =
  6   9  12   4   3   0
  4   4  15   2   1   1
  2   1  18  -5   8   2
 -6  -4  21   1  -5   2
```

What will be displayed if the following variables A in (i) to C in (iii) are printed?

- (i) A = M[[0,2],:][:,[1,3]]
- (ii) B = M[:,[0,3,4,5]]
- (iii) C = M[1:3,:]

We have to be careful with the indexing in Numpy because it only create **views** and does not create **copies**.

Example. (View vs Copy of a sub-array) Study the following Python instructions and explain what is each output:

Assign the 'view'	Assign the 'copy'
<pre>import numpy as np A = np.array([[1,2,3],[4,5,6]]) B = A[:,0:2] B[0,0] = 8 print("A=",A) print("B=",B)</pre>	<pre>import numpy as np A = np.array([[1,2,3],[4,5,6]]) B = A[:,0:2].copy() B[0,0] = 8 print("A=",A) print("B=",B)</pre>
<pre>A = [8 2 3] [4 5 6] B = [8 2] [4 5]</pre>	<pre>A = [1 2 3] [4 5 6] B = [8 2] [4 5]</pre>

3.2. Usual Indexing vs For-Loops

Example. (Combining Programming and Array Indexing in Solving Differential Equations Numerically) In applying finite difference approximation to the type 1 ODE-BVP:

$$\ddot{y}(x) + p(x)\dot{y}(x) + q(x)y(x) = r(x), \quad a < x < b, \quad y(a) = y_a, y(b) = y_b$$

we obtain matrix

$$C = \begin{bmatrix} 1 - \frac{h}{2} p(x_1) & (h^2 q(x_1) - 2) & 1 + \frac{h}{2} p(x_1) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \vdots & 1 - \frac{h}{2} p(x_{n-1}) & (h^2 q(x_{n-1}) - 2) & 1 + \frac{h}{2} p(x_{n-1}) \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad x_i = a + i \cdot h, \quad h = \frac{b-a}{n}.$$

Write a Python script to generate the matrix C.

Sample Solution 1:

```
C1 = np.eye(n+1)
```

```

x = a
h = (b-a)/n
for i in range(1,n):
    x = x+h
    C1[i,i-1] = 1.0-p(x)*h/2.0
    C1[i,i] = h**2*q(x)-2.0
    C1[i,i+1] = 1.0+p(x)*h/2.0

```

Sample Solution 2:

```

C2 = np.eye(n+1)
idx = np.r_[1:n]
h = (b-a)/n
x = a + h*idx
C2[idx,idx-1] = 1.0-p(x)*h/2.0      # Using elementwise arithmetic: idx-1
C2[idx,idx] = h**2*q(x)-2.0
C2[idx,idx+1] = 1.0+p(x)*h/2.0

```

Example. (Combining Programming and Array Indexing in Technical Analysis of Financial Data) In the past, it is possible for us to download a lot of stock price data from Yahoo!Finance. However, Yahoo!Finance is providing less and less stock price data for data and is transforming itself to pay-per-use service. The stock price data of Telekom Malaysia (a listed company which provides the most expensive broadband service in South East Asia) below was downloaded a few years ago.

```

Date,Open,High,Low,Close,Volume,Adj Close
2016-12-30,6.06,6.09,5.81,5.95,5842300,5.95
2016-12-29,6.05,6.12,5.98,6.06,6777900,6.06
2016-12-28,5.96,6.06,5.96,6.03,2503700,6.03
2016-12-27,5.93,5.99,5.92,5.99,922400,5.99
2016-12-26,5.95,5.95,5.95,5.95,000,5.95
2016-12-23,5.91,5.97,5.91,5.95,838100,5.95
2016-12-22,5.97,5.97,5.92,5.95,1065000,5.95
2016-12-21,6.02,6.02,5.92,5.95,3405900,5.95
2016-12-20,5.95,6.07,5.94,5.98,3101400,5.98
2016-12-19,5.97,6.00,5.91,5.95,2006000,5.95
2016-12-16,5.90,5.96,5.89,5.95,3975600,5.95
2016-12-15,5.91,5.95,5.90,5.90,3987400,5.90
2016-12-14,5.96,6.00,5.93,5.95,5128000,5.95
2016-12-13,6.04,6.05,5.94,5.96,4111000,5.96
2016-12-12,6.03,6.03,6.03,6.03,000,6.03
2016-12-09,6.11,6.11,6.01,6.03,1573000,6.03
2016-12-08,6.16,6.20,6.11,6.11,3189800,6.11
2016-12-07,6.13,6.15,6.09,6.11,4564800,6.11
2016-12-06,6.12,6.15,6.09,6.12,2976600,6.12
2016-12-05,6.15,6.19,6.13,6.14,3303800,6.14
2016-12-02,6.15,6.22,6.09,6.13,2134000,6.13
2016-12-01,6.17,6.24,6.14,6.15,6188400,6.15

```

By using the closing price, write a Python program to calculate

- * the price difference between the next day and today for December 2016;
- * the three-day (moving) average for December 2016.

Sample Solution 1:

```

import numpy as np
dclose = np.array([6.15, 6.13, 6.14, 6.12, 6.11, 6.11, 6.03,
                   6.03, 5.96, 5.95, 5.9, 5.95, 5.95, 5.98,
                   5.95, 5.95, 5.95, 5.95, 5.99, 6.03, 6.06, 5.95])
price_diff = np.zeros(dclose.size-1)
moving3 = np.zeros(dclose.size-2)
for today in range(price_diff.size):
    next_day = today + 1
    price_diff[today] = dclose[next_day]-dclose[today]
for today in range(moving3.size):

```

```

next_day = today + 1
next_2day = today + 2
moving3[today] = (dclose[today]+dclose[next_day]+dclose[next_2day])/3
print("Price difference between next day and today for December 2016: ")
print(price_diff)
print("3-D moving average for December 2016:", moving3)

```

Sample Solution 2:

```

import numpy as np
dclose = np.array([6.15, 6.13, 6.14, 6.12, 6.11, 6.11, 6.03,
                  6.03, 5.96, 5.95, 5.9, 5.95, 5.95, 5.98,
                  5.95, 5.95, 5.95, 5.95, 5.99, 6.03, 6.06, 5.95])
price_diff = np.diff(dclose)
idx = np.r_[: (dclose.size-2)]
moving3 = (dclose[idx]+dclose[idx+1]+dclose[idx+2])/3.0
print("Price difference between next day and today for December 2016: ")
print(price_diff)
print("3-D moving average for December 2016:", moving3)

```

You can also use the information from https://rosettacode.org/wiki/Averages/Simple_moving_average to write a better Python script.

Example. (More Complex Array Indexing) Write a Python function `spiral(n)` to generate an $n \times n$ clockwise spiral matrix using Python. For example, `spiral(5)` gives

```

[  0  1  2  3  4 ]
[ 15 16 17 18  5 ]
[ 14 23 24 19  6 ]
[ 13 22 21 20  7 ]
[ 12 11 10  9  8 ]

```

Sample Solution: It is inspired by https://rosettacode.org/wiki/Spiral_matrix

```

def spiral(n,m=None):
    _n,_m = (n,m) if m is not None else (n,n)
    _nl,_ml=0,0
    dx,dy = 0,1          # Starting increments
    x,y = 0,0            # Starting location
    import numpy as np
    myarray = np.zeros((_n,_m),dtype='int')
    for i in range(_n*_m):
        myarray[x,y] = i
        nx,ny = x+dx, y+dy # (dx,dy) = direction to update array
        if _nl<=nx<_n and _ml<=ny<_m:
            x,y = nx,ny
        else:
            if dx==0 and dy==1:
                _nl+=1; dx,dy=1,0
            elif dx==1 and dy==0:
                _m-=1; dx,dy=0,-1
            elif dx==0 and dy==-1:
                _n-=1; dx,dy=-1,0
            elif dx==-1 and dy== 0:
                _ml+=1; dx,dy=0,1
            else:
                return None # Should not reach this state
            x,y = x+dx,y+dy
    return myarray

```

3.3. Negative Indexing: Index from End

Indexing array with the usual bounded index is often enough but Python provides “**Negative**” indexing which is used to index an array “from last element”. For example, `-1` refers to the last index, `-n` refers to the `n` last index. Note that going beyond index bound can cause error!

Example. Consider the following integer array:

```
A =
    10  11  12  13  14  15  16  17  18
    19  20  21  22  23  24  25  26  27
    28  29  30  31  32  33  34  35  36
    37  38  39  40  41  42  43  44  45
    46  47  48  49  50  51  52  53  54
```

What is the output of the following commands:

- (a) `print(A[-2,4])`
- (b) `print(A[-2,:])`
- (c) `print(A[:,-4])`
- (d) `print(A[1:-3,3:-4])`
- (e) `print(A[1:-1:2,:][: ,2:-2:2])`
- (f) `print(A[-2,None])`
- (g) `print(A[:,-4:-5:-1])`

Solution:

- (a) 41 (second last row, fifth column)
 - (b) [37, 38, 39, 40, 41, 42, 43, 44, 45] (second last row)
 - (c) [6, 15, 24, 33, 42, 51] (fourth last column = sixth column)
 - (d) [[13 14] [22 23]] (second row to the row before the last third row **and** fourth column to before the last fourth column)
 - (e) [[12 14 16] [30 32 34]] (second and fourth rows **and** third, fifth and seventh columns)
 - (f) [[37 38 39 40 41 42 43 44 45]] (different from part (b) in terms of dimension, this is a 1x9 ‘matrix’)
 - (g) [[6] [15] [24] [33] [42] [51]] (we obtain a 6x1 column ‘matrix’ rather than a 1-D array as in part (c))
-

4. Arithmetic, Logical and Relational Operations

The basic arithmetic and logical operations for “numbers” such as +, −, ×, /, power, not, and, or, equality, etc. can be generalised to operate on “arrays”. In this section, we will see how to generalise them to “element”-wise operations.

4.1. Elementwise Arithmetic Operations and Reduction Operations

The basic arithmetic +, −, ×, / and power for **two arrays of the same shape** A and B are just element-wise addition, subtraction, multiplication, division and power of numbers in the array as:

* −A: elementwise negation

1-D example	2-D example
A = [1.2 1.3 1.4]	A = [3.2 -5.3]
−A = [−1.2 −1.3 −1.4]	[−5.5 4.0]
	−A = [−3.2 5.3]
	[5.5 −4.0]

* A + B, A − B: elementwise addition and subtraction

1-D example	2-D example
A = [1.2 1.3 1.4]	A = [1 -2]
B = [2.1 2.3 3.4]	[-3 4]
A+B =	B = [8 7]
[3.3 3.6 4.8]	[-6 -5]
A−B =	A+B =
[−0.9 −1.0 −2.0]	[9 5]
	[−9 −1]
	A−B =
	[7 -9]
	[3 9]

* A * B, A / B, A ** B: elementwise multiplication, division and ‘power’

1-D example	2-D example
A = [1.3 1.2 1.4]	A = [8 -7]
B = [2 3 4]	[-6 5]
A*B =	B = [4 2]
[2.6 3.6 5.6]	[-3 -4]
A/B =	A*B =
[0.65 0.4 0.35]	[32 -14]
A**abs(B) =	[18 -20]
[1.69 1.728 3.8416]	A/B =
	[2. -3.5]
	[2. -1.25]
	A**abs(B) =
	[4096 49]
	[-216 625]

Together with the ufunc, the array arithmetic allows us to handle computations like $\sin(x^2 + x + 2)$:

```
np.sin(x**2 + x + 2)
```

Example. Write a Python script to plot the functions

$$y_1 = \frac{x^3}{2} + 3x^2 - 1, \quad y_2 = 2\sin x, \quad y_3 = \sin(2x)$$

in one diagram for the range $-\pi \leq x \leq \pi$.

Sample Solution:

```
import numpy as np, matplotlib.pyplot as plt
x = np.arange(-np.pi, np.pi, 0.0001)
y1 = x*x*x/2 + 3*x*x - 1
y2 = 2*np.sin(x)
y3 = np.sin(2*x)
plt.plot(x,np.vstack((y1,y2,y3)).T); plt.show()
```

Numpy's elementwise arithmetic can work on arrays with **compatible shapes**. For example, shape (3,4) and shape (4,) are compatible but not shape (3,4) against shape (2,) or shape (3,). Consider

```
* A = np.arange(1,13).reshape(3,4)
* B = np.array([5,4,8]) (Shape=(3,))
* C1 = np.array([9,4,8,7]) (Shape=(4,)), C2 = np.array([9,4]) (Shape=(2,))
* A + C1 is OK but A + B and A + C2 are not OK. However, reshaping B to (3,1) will make it compatible with A.
```

By expanding A, B, C1 and C2, we can see:

$$\begin{aligned}
 A + C1 &= \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \end{bmatrix} + \begin{bmatrix} 9 & 4 & 8 & 7 \end{bmatrix} \\
 &= \begin{bmatrix} 1+9 & 2+4 & 3+8 & 4+7 \\ 5+9 & 6+4 & 7+8 & 8+7 \\ 9+9 & 10+4 & 11+8 & 12+7 \end{bmatrix}
 \end{aligned}$$

$$\begin{aligned}
 A + C2 &: \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \end{bmatrix} + \begin{bmatrix} 9 & 4 \end{bmatrix} \quad ??? \\
 A + B &: \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \end{bmatrix} + \begin{bmatrix} 5 & 4 & 8 \end{bmatrix} \quad ???
 \end{aligned}$$

$$A + B.reshape((3,1)) : \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \end{bmatrix} + \begin{bmatrix} 5 \\ 4 \\ 8 \end{bmatrix}$$

Example. Write down two Python commands which allows us to transform the left matrix *A* to the right matrix *B* using index operations and array arithmetic:

$$A = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & 2 & 3 & 4 \\ 0 & -4 & -8 & -12 \\ 0 & -8 & -16 & -24 \end{bmatrix} = B$$
Sample Solution:

```
A[1,:] = A[1,:] - 5*A[0,:]
A[2,:] = A[2,:] - 9*A[0,:]
```

4.2. Logical Operations

“Boolean arrays” arise when we are “comparing” number arrays. The logical operations for Boolean arrays are similar to the arithmetic operations for numeric arrays. They are just the generalisation of logical operations from Boolean values (True, False) to Boolean arrays (arrays of True and/or False) of compatible arrays)

Let *C* and *D* be Boolean array of the same shape, the element-wise negation, conjunction and disjunction for the Boolean array are:

```
* Check and make sure that C.dtype and D.dtype are bool.
* ~C: elementwise negation
* C & D: elementwise conjunction
* C | D: elementwise disjunction
```


In Numpy, the logical operations also work on **two arrays of the compatible shape**. For example, Shape (2,3) and shape (3,) are compatible but not shape (2,)

```
* C = np.array([[True, False, True], [False, True, False]]) (Shape = 2x3)
* D1 = np.array([True, False]) (Shape = 2)
* D2 = np.array([False, False, True]) (Shape = 3)
* C & D2 is OK but C & D1 is not OK
```

Note that Python allows us to use -, * and + to denote ~, & and | respectively. However, it is not recommended to prevent confusion because Boolean will be converted to integers when other arithmetic operations are involved.

Example. (Final Exam Sept 2015, Q2(a)(iv)) What will display if the following commands are executed?

```
np.array([not False, False, not True]) & np.array([True]*3) (2 marks)
```

Solution: = [True False False] & [True True True] = [True False False]

4.3. Relational Operations

Let A and B be arrays of compatible shape. The ordering of real numbers allows us to compare numbers by the relational operations ==, ~=, <, <=, > and >=.

Example. (Final Exam Sept 2013, Q1(c)) Given that `x = np.array([1,3,4,2,5,0,-3])` and `y = np.array([6,3,2,4,1,0,6])`, list the results of the following commands (i) to (iii):

(i) `x - 2*(y>3)`

Solution: Let T denote True and F denote False. The calculation is as follows.
`= x - 2*[T F F T F F T]`
`= x - [2 0 0 2 0 0 2]`
`= [-1 3 4 0 5 0 -5]`

(ii) `(x!=0) & (y==0)`

Solution: Let T denote True and F denote False. The calculation is as follows.
`[T T T T T F T] & [F F F F F T F]`
`= [F F F F F F F]`

(iii) `(x==y) | (y<x)`

Solution:
`= [F T F F F T F] | [F F T F T F F]`
`= [F T T F T T F]`

4.4. Fancy Indexing with Boolean Array

The ‘Boolean’ array for an array A generated with the use of relational operations (or more general predicates) can be used as a kind of **fancy indexing** called **Boolean indexing** for A.

This kind of indexing is widely used in statistics, image processing, signal processing, etc. because it allows us to **select** the array data of interest.

Example. Consider the 2-D array

```
A = [ [-1  2  1 -3 ]
      [ 2 -4 -4  0 ]
      [ 0  0 -1 -2 ]
```

Write the Python commands to

- list all the values in A which are **non-negative**.
- replace the negative values in A by -10.

Sample Solution:

1. We select those array elements which are 0:

```
[-1>=0  2>=0  1>=0 -3>=0] [F T T F] [ 2  1 ]
[ 2>=0 -4>=0 -4>=0  0>=0] --> [T F F T] --> [ 2  0 ]
[ 0>=0  0>=0 -1>=0 -2>=0] [T T F F] [ 0  0 ]
--> [2  1  2  0  0  0]
```

Answer: `A[A>=0]` # or `A[~(A<0)]`

2. `A[A<0] = -10`

Here's how it works for assignment:

```
[-1,  2,  1, -3]  [T, F, F, T]      [-10,  2,  1, -10]
[ 2, -4, -4,  0]  [F, T, T, F]  --> [  2, -10, -10,  0]
[ 0,  0, -1, -2]  [F, F, T, T]      [  0,  0, -10, -10]
```

Example. (Final Exam Sept 2013, Q1(b) with modification) Write a Python script to perform the following actions:

- * Generate a 2-by-3 array of random numbers using `rand` command and,
- * Move through the array, element by element, and set any value that is less than 0.2 to 0 and any value that is greater than or equal to 0.2 to 1.

Solution: The intention of the lecturer who set the question is to ask you to express this in for loop but in reality, everyone use the array functions from Topic 2 to achieve the stated requirements.

Open up a notepad (or Spyder), type in the following text and then save it:

```
import numpy as np
A = np.random.rand(2,3) # A 2x3 array of random numbers
A[A<0.2] = 0
A[A>=0.2] = 1
```

Run the above script a few times and explain what do you observe?

Example. Extract from the array `B=np.array([3,4,6,10,24,89,45,43,46,99,100])` those numbers

- * which are not divisible by 3;
- * which are divisible by 5;
- * which are divisible by 3 and 5;
- * which are divisible by 3 and set them to 42.

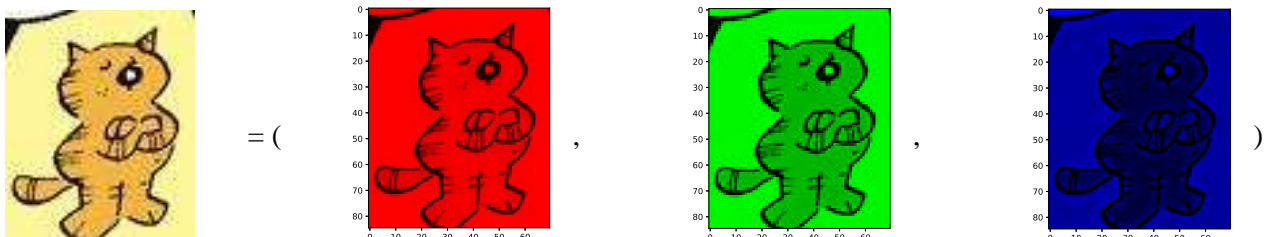
Sample Solution:

```
def is_divisible_by(n): return lambda x: x % n == 0

udiv3 = np.frompyfunc(is_divisible_by(3),1,1)
print("Not divisible by 3 =>", B[~udiv3(B).astype('bool')])
udiv5 = np.frompyfunc(is_divisible_by(5),1,1)
print("Divisible by 5 =>", B[udiv5(B).astype('bool')])
print("Divisible by 3 and 5 =>", B[udiv3(B).astype('bool') &
    udiv5(B).astype('bool')])
B[udiv3(B).astype('bool')] = 42
```

Example. (Simple Image Processing) We can regard an array of Booleans, `M`, of the same shape as a number array `A` like a new layer above the array `A`, called a **mask**.

Consider a heathcliff image `A` below:



The Boolean indexing can be used to extract the red, green and blue components of a coloured image.

```

from PIL import Image
import numpy as np
import matplotlib.pyplot as plt
# https://liaohaohui.github.io/UECM1703/heathcliff2.jpg
f = Image.open("heathcliff2.jpg")
orig = np.array(f)
fig, (ax0, ax1, ax2) = plt.subplots(nrows=1, ncols=3)
ax0.hist(orig[:, :, 0])
ax0.set_title("Red")
ax1.hist(orig[:, :, 1])
ax1.set_title("Green")
ax2.hist(orig[:, :, 2])
ax2.set_title("Blue")
fig.tight_layout()
plt.show()

fig, (ax0, ax1, ax2) = plt.subplots(nrows=1, ncols=3)
arr = orig.copy()
arr[:, :, 1:] = 0 # red
img = Image.fromarray(arr)
ax0.imshow(img)
arr = orig.copy()
arr[:, :, [0, 2]] = 0 # green
img = Image.fromarray(arr)
ax1.imshow(img)
arr = orig.copy()
arr[:, :, :2] = 0 # blue
img = Image.fromarray(arr)
ax2.imshow(img)
fig.tight_layout()
plt.show()

```

We can also use the Boolean indexing to mask part of the image. For example, we can use it to create a ‘elliptic frame’ (in black) as follows.



using Boolean indexing (and array grid boardcasting)

```

arr = orig.copy()
# Using np.ogrid allows array indexing and broadcasting for calculation
x, y = np.ogrid[:arr.shape[0], :arr.shape[1]]
centre = np.array(arr.shape)/2
mask_ellip = (x-centre[0])**2/centre[0]**2+(y-centre[1])**2/centre[1]**2>1.0
arr[mask_ellip, :] = 0
plt.imshow(arr)
plt.savefig("heathcliff2_ell.eps")
plt.show()

```

In the practical, try to convert the coloured image 3-D array to gray colour 2-D array using the formula below:

$$\text{gray} = 0.2989 \text{ red} + 0.5870 \text{ green} + 0.1140 \text{ blue}$$

The Boolean indexing can also be used in thresholding to select regions the boundaries of a character.

5. Array Reduction Operations

When we want to work on the elements of arrays along some **axis** or multiple axes, we can regard as **reducing** the array data to some values. We will explore some classes of reduction operations below.

‘Reduction’ Operations for Filtering and Construction

- * `np.choose(J, A)` picks `A[J[i]]` into `J`. It complements `np.compress()`, `np.select()`, `np.extract()`, etc.
- * `np.putmask(A, mask, values)`: works similar to Boolean masking. Closely related to `np.take()`, `np.place()`, `np.put()`, `np.copyto()`.
`np.putmask(A, A<0, 0)` # Same as `A[A<0] = 0`
- * `np.correlate(x, y)` correlates two 1-D arrays

$$z_j = \sum_{i=\max(j-M, 0)}^{\min(j, K)} x_i y_{j+i}, \quad j = 0, \dots, K+M$$

- * `np.convolve(x, y)` convolves two 1-D arrays

$$z_j = \sum_{i=\max(j-M, 0)}^{\min(j, K)} x_i y_{j-i}, \quad j = 0, \dots, \max(K, M)$$

Here x and y are two 1-D arrays with $K = x.size-1$ and $M = y.size-1$. The last two items are used in **signal processing**.

Ordering ‘Reduction’ Operations

- * `np.max`, `np.min`: returns the largest value and the smallest value
- * `ptp`: return the range of values, i.e. the difference of maximum and minimum
- * `np.argmax`, `np.argmin`: returns the index of the largest value and the smallest value
- * `sort`: return a sorted copy of an array
- * `np.argsort`: return indices of sorted array
- * `searchsorted`: find indices where elements should be inserted to maintain order

Statistical ‘Reduction’ Operations

- * `np.sum(X)`: It is used for summation. When X is the data x_1, x_2, \dots, x_n , the sum returns

$$x_1 + x_2 + \dots + x_n.$$

Together with array mathematical functions (Ufuncs), the for loop from Topic 1:

$$f(1) + f(2) + f(3) + \dots + f(n)$$

can be written as

$$f(\text{np.r_[1:(n+1)]}).\text{sum}() \quad \# \text{ or } \text{np.sum}(f(\text{np.r_[1:(n+1)]}))$$

Related: `np.cumsum`, `np.prod`, `np.cumprod`, ...

- * `np.mean(X)`: The mean is $\bar{X} = \frac{x_1 + \dots + x_n}{n}$.
- * `np.average(X, weights=W)` generalises mean and allows weighted mean.
- * `np.median(X)`: Find the median of data X .
- * `np.var(X)` (and `np.std(X) = \sqrt{\text{var}(X)}`): By default, it is the **population variance** (and standard deviation)

$$\text{Var}[X] = \frac{(x_1 - \bar{X})^2 + \dots + (x_n - \bar{X})^2}{n}.$$

Note that for **sample variance** (and sample population), the n needs to be changed to $n-1$ (set `ddof=1`).

- * `np.cov(X)`: Compute the covariance matrix of data in X based on the mathematical formulation:

$$\text{Cov}[X] = E[(X - E[X])(X - E[X])^H].$$

Example. (General and Statistical ‘Reduction’ Operations) Consider the array

```
M = [ 6  9 12  4  3  0 ]
     [ 4  4 15  2  1  1 ]
     [ 2  1 18 -5  8  2 ]
     [-6 -4 21  1 -5  2 ]
```

Let us investigate the sum, prod, cumsum, cumprod, min, max, range, mean, var (population variance), std (population standard deviation), etc. along the whole array, along the row and along the column.

Solution: Let’s investigate how the axis work with the various given reduction operations.

```
M = np.array([[ 6,  9, 12,  4,  3,  0],
              [ 4,  4, 15,  2,  1,  1],
              [ 2,  1, 18, -5,  8,  2],
              [-6, -4, 21,  1, -5,  2]])

#
# Along the whole array
#
M.sum()           # 96 (all numbers add)
M.prod()          # 0  (all numbers multiply)
M.cumsum()        # 6, 6+9, 6+9+12, ...
M.cumprod()       # 6, 6*9, 6*9*12, ...
M.min()           # -6
M.max()           # 21
M.ptp()           # 27
M.mean()          # 4.0
M.var()           # 46.25
M.std()           # 6.800735254367722
#
# NOTE: There is a 'nan' version for the above commands which
# skips nan, e.g. np.nanmean(x), np.nanvar(x), etc.
#

#
# Along the rows (axis = 1)
#
M.sum(axis=1)     # It will sum along the row return 1-D array
M.prod(axis=1, keepdims=1) # use keepdims=1 if we want 2-D array
M.cumsum(axis=1)  # [6,6+9,...], [4,4+4,...], [2,2+1,...], ...
M.cumprod(axis=1) # [6,6*9,...], [4,4*4,...], [2,2*1,...], ...
M.min(axis=1)     # [ 0,  1, -5, -6]
M.max(axis=1)     # [12, 15, 18, 21]
M.ptp(axis=1)
M.mean(axis=1)
M.var(axis=1)     # for sample variance, use ddof=1
M.std(axis=1)

#
# Along the columns (axis = 0)
#
M.sum(axis=0, keepdims=1)
M.prod(axis=0)
M.cumsum(axis=0)
M.cumprod(axis=0)
M.min(axis=0)
M.max(axis=0)
M.ptp(axis=0)
M.mean(axis=0)
M.var(axis=0)
M.std(axis=0)
```

Example. (Final Exam Sept 2015, Q1(b)(i)) Write down and explain the values of C for the following commands

```
import numpy as np
A = np.array([4,6,8],dtype='double')
B = np.array([2,0,4])
C = np.sum(A/B)
```

Solution: $C = \text{sum}([4/2 \ 6/0 \ 8/4]) = \text{sum}([2 \ \text{Inf} \ 2]) = \text{Inf}$

Lessons learned: Be careful about the division by zero. We may get into infinity.

Example. (scipy.stats.gmean) The geometric mean implementation in Scipy is listed below.

```
def gmean(a, axis=0, dtype=None, weights=None):
    r"""Compute the weighted geometric mean along the specified axis.
```

The weighted geometric mean of the array :math:`a_i` associated to weights :math:`w_i` is:

$$\exp\left(\frac{\sum_{i=1}^n w_i \ln a_i}{\sum_{i=1}^n w_i}\right)$$

and, with equal weights, it gives:

$$\sqrt[n]{\prod_{i=1}^n a_i}.$$

Parameters

```
a : array_like
    Input array or object that can be converted to an array.
axis : int or None, optional
    Axis along which the geometric mean is computed. Default is 0.
    If None, compute over the whole array 'a'.
dtype : dtype, optional
    Type to which the input arrays are cast before the calculation is
    performed.
weights : array_like, optional
    The 'weights' array must be broadcastable to the same shape as 'a'.
    Default is None, which gives each value a weight of 1.0.
```

Returns

```
gmean : ndarray
    See 'dtype' parameter above.
```

See Also

```
numpy.mean : Arithmetic average
numpy.average : Weighted average
hmean : Harmonic mean
```

References

```
.. [1] "Weighted Geometric Mean", *Wikipedia*,
    https://en.wikipedia.org/wiki/Weighted_geometric_mean.
.. [2] Grossman, J., Grossman, M., Katz, R., "Averages: A New Approach",
    Archimedes Foundation, 1983
```

Examples

```
>>> from scipy.stats import gmean
>>> gmean([1, 4])
2.0
>>> gmean([1, 2, 3, 4, 5, 6, 7])
3.3800151591412964
>>> gmean([1, 4, 7], weights=[3, 1, 3])
2.80668351922014
```

"""

```
a = np.asarray(a, dtype=dtype)
```

```
if weights is not None:
    weights = np.asarray(weights, dtype=dtype)
```

```
with np.errstate(divide='ignore'):
    log_a = np.log(a)
```

```
return np.exp(np.average(log_a, axis=axis, weights=weights))
```

Note the programming techniques used:

- * Function with default values
- * Defining 'help documentation' for a function using """ ... """.
- * If statement
- * Array mathematical functions and reduction operations.

Example. (Final Exam Oct 2018, Q1(a), CO1) The output of the Python commands below

```
>>> import numpy as np
>>> A = np.arange(1,36).astype('float').reshape(5,7)
>>> print(A)
```

is

```
[[ 1.  2.  3.  4.  5.  6.  7.]
 [ 8.  9. 10. 11. 12. 13. 14.]
 [15. 16. 17. 18. 19. 20. 21.]
 [22. 23. 24. 25. 26. 27. 28.]
 [29. 30. 31. 32. 33. 34. 35.]]
```

Use the above information to write down the output to the following Python commands for item (i) to item (iv).

(i) `print(A[2,:])`

Solution: `[15. 16. 17. 18. 19. 20. 21.]`

(ii) `print(A[1:4,3:5])`

Solution:

```
[[ 11.  12.]
 [ 18.  19.]
 [ 25.  26.]]
```

(iii) `print(A[2:4,4:6].mean())`

Solution: `A[2:4,4:6]` `[[19., 20.], [26., 27.]]`
$$\frac{19+20+26+27}{4} = 23.0$$

(iv) `print(A[:,2]>10)`

Solution: `[False False True True True]`

(v) Write down the Python command to **count** the number of elements in A who are larger than 20.

Solution: `(A>20).sum()`

Example.

- (a) Write down the Python command to subtract the each column of a matrix A by the mean of the data of each column vector.

```
A - A.mean(axis=0)
```

- (b) The 'shortest' Python command to subtract the each row of a matrix A by the mean of the data of each row vector is probably

```
(A.T - A.mean(1)).T
```

Do you know other slightly longer Python command which achieves the same outcome for A?

```
A - A.mean(axis=1, keepdims=True)
```

```
A - A.mean(1).reshape(-1,1)
```

Example. (Magic Square using Integer Array from Topic 1) Using numpy integer array, a magic square can be made simpler. The Python function to check if an object is a magic square can be simplified as follows.

```
def is_magic_square(arr):
    sums_from_every_row = arr.sum(axis=1)
    sums_from_every_col = arr.sum(axis=0)
    #Two diagonals
    diag1 = arr.diagonal().sum()    # Using reduction 'sum'
    n = arr.shape[0]
    diag2 = arr[:,n::-1].diagonal().sum()
    return diag1==diag2 and \
        (sums_from_every_row == diag1).all() and \
        (sums_from_every_col == diag1).all()

m=[[7, 12, 1, 14], [2, 13, 8, 11], [16, 3, 10, 5], [9, 6, 15, 4]]
print(is_magic_square(np.array(m)))
print(is_magic_square(np.array([[2, 7, 6], [9, 5, 1], [4, 3, 8]])))
print(is_magic_square(np.array([[2, 7, 6], [9, 5, 1], [4, 3, 7]])))
```

The generation of magic square algorithm from Topic 1 can be simplified as follows.

```
def magic_sqr_method1(n):
    if n % 2 == 0: return None    # Only works with odd n
    magic_square = np.zeros((n,n))
    cnt, i, j = 1, 0, n//2
    while cnt <= n**2:
        magic_square[i,j] = cnt
        cnt += 1
        newi, newj = (i-1)%n, (j+1)%n
        if magic_square[newi,newj]:
            i += 1
        else:
            i, j = newi, newj
    return magic_square
```

Example. (Final Exam Sept 2019, Q1)

- (a) Given
- ```
A = [[4 9 8 0 2 9]
 [3 1 9 1 2 8]
 [7 2 2 3 7 8]
 [3 5 0 7 9 7]
 [9 4 6 7 9 8]
```

Use the above information to **execute** the following Python commands for item (i) to item (iv) and write down the output of the execution.

- (i) `print(A[:,1])`

**Solution:** `[9 1 2 5 4]`

- (ii) `print(A[1:4,[1,2,3]])`

**Solution:**

```
[[1 9 1]
 [2 2 3]]
```



```
[5 0 7]]
```

(iii) `print(A[A<5].sum())`

**Solution:**  $(4+0+2) + (3+1+1+2) + (2+2+3) + (3+0) + 4 = 27$

(iv) `print(A[:4,:3].sum(axis=0))`

**Solution:**  $[4+3+7+3, 9+1+2+5, 8+9+2+0] = [17, 17, 19]$

(v) Write down the Python command which gives the mean of rows in A after execution.

**Solution:** `print(A.mean(axis=1))`

(vi) Write down the warning message that the command

`print(A[1,:]/A[0,:].astype(np.float64))` will raise when it is executed.

**Solution:** Since `A[0,3]` is zero, a division by zero error will be produced.

(b) Use Numpy array operations such as `np.arange`, etc. to write a computer program in no more than 3 lines and without using any semicolon to print the following output:

```
1 1 1 1
2 4 8 16
3 9 27 81
4 16 64 256
5 25 125 625
6 36 216 1296
7 49 343 2401
8 64 512 4096
9 81 729 6561
10 100 1000 10000
```

**Sample Solution:**

```
coll = np.arange(1,11).reshape(10,1) # [1.5 marks]
B = np.hstack((coll, coll**2, coll**3, coll**4)) # [2 marks]
print(B) # [0.5 mark]
```

**Example.** (Course Outcome 3: Write program script) The following function is used to generate a moving sequence (with a particular window size, by default 4) for a one-dimensional array `a`.

```
def rolling(a, window=4):
 n = a.size
 newarray = np.zeros((n-window+1,window))
 for i in range(n-window+1):
 newarray[i,:] = a[i:i+window]
 return newarray
```

When the one-dimensional array is  $\mathbf{x} = [x_1, x_2, x_3, x_4, \dots, x_n]$ , the return moving sequence of `rolling(x)` with a widow size 4 is

$$[[x_1, x_2, x_3, x_4], [x_2, x_3, x_4, x_5], \dots, [x_{n-3}, x_{n-2}, x_{n-1}, x_n]].$$

(i) If `a = np.array([1.1, 1.34, 1.17, 1.06, 1.06, 0.94])`, write down the output of Python command `rolling(a)`.

**Solution:**

```
array([[1.1 , 1.34, 1.17, 1.06],
 [1.34, 1.17, 1.06, 1.06],
 [1.17, 1.06, 1.06, 0.94]])
```

(ii) Define a Python function `moving_average` to calculate moving average of  $\mathbf{x}$  with a window of 4 which returns the following array:

$$\left[ \frac{x_1 + x_2 + x_3 + x_4}{4}, \frac{x_2 + x_3 + x_4 + x_5}{4}, \dots, \frac{x_{n-3} + x_{n-2} + x_{n-1} + x_n}{4} \right]$$

based on the moving sequence `rolling(x)`. Write down the output of the Python command `print(moving_average(a))` where `a` is given in part (i).

**Solution:** By using Numpy array method, we have

```
def moving_average(x,w=4): return rolling(x,w).mean(axis=1)
```

Alternatively, a less elegant method is to be used for loop:

```
def moving_average(x,w=4):
 retval = np.zeros(x.size-w+1)
 data = rolling(x,w)
 for i in range(retval.size):
 retval[i] = np.mean(data[i])
 return retval
```

The output of `moving_average(a)` is `[1.1675, 1.1575, 1.0575]`

- (iii) Explain how to calculate moving variance of `a` in part (i) with a window of 4.

**Solution:** `rolling(a).var(axis=1)`

**Example.** (Final Exam Oct 2018, Q2(b), CO3) The following function from a program script is used to generate a moving sequence for a one-dimensional array

```
def rolling(a, window=4):
 n = a.size
 newarray = np.zeros((n-window+1,window))
 for i in range(n-window+1):
 newarray[i,:] = a[i:i+window]
 return newarray
```

When the one-dimensional array is  $\mathbf{x} = [x_1, x_2, x_3, x_4, \dots, x_n]$ , the return moving sequence of `rolling(x)` is

$$[[x_1, x_2, x_3, x_4], [x_2, x_3, x_4, x_5], \dots, [x_{n-3}, x_{n-2}, x_{n-1}, x_n]].$$

- (i) If `a = np.array([0.95, 0.87, 0.87, 0.98, 1.04, 1.08])`, write down the output of `rolling(a)`.

**Solution:**

```
array([[0.95, 0.87, 0.87, 0.98],
 [0.87, 0.87, 0.98, 1.04],
 [0.87, 0.98, 1.04, 1.08]])
```

- (ii) Define a Python function `moving_average` to calculate moving average of  $\mathbf{x}$  with a window of 4 which returns the following array:

$$\left[ \frac{x_1 + x_2 + x_3 + x_4}{4}, \frac{x_2 + x_3 + x_4 + x_5}{4}, \dots, \frac{x_{n-3} + x_{n-2} + x_{n-1} + x_n}{4} \right]$$

based on the moving sequence `rolling(x)`. Write down the output of the Python command `print(moving_average(a))` where `a` is given in part (i).

**Sample Solution:** By using Numpy array method, we have

```
def moving_average(x,w=4):
 return rolling(x,w).mean(axis=1)
```

Alternatively, a less elegant method is to use the for loop:

```
def moving_average(x,w=4):
 retval = np.zeros(x.size-w+1)
 data = rolling(x,w)
 for i in range(retval.size):
 retval[i] = np.mean(data[i])
 return retval
```

The output of `moving_average(a)` is `[0.9175, 0.94, 0.9925]`.

- (iii) Explain how to calculate moving variance of `a` in part (i) with a window of 4.

**Solution:** `rolling(a).var(axis=1)`

## 6. Linear Algebra Operations

### Operations for Vectors

The **length** of a vector

$$|x| = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2}$$

can be obtained using `scipy.linalg.norm(x[, ord, axis, keepdims])`.

The **angle** between a vector  $x$  and a vector  $y$  (in radian) is given by the **dot-product** `np.vdot(x, y)`:

$$x \cdot y = x_1y_1 + x_2y_2 + \cdots + x_ny_n = |x||y|\cos \theta$$

**Example.** (Linear Algebra Operations on Vectors) Find lengths and angle the vectors  $x$  and  $y$ :

```
x = np.array([3,-1, 2,-4])
y = np.array([5, 7, 3, 1])
```

**Sample Solution:**

```
import numpy as np
from scipy import linalg
xlength = linalg.norm(x)
ylength = linalg.norm(y)
angle_x_y = np.arccos(np.vdot(x,y)/linalg.norm(x)/linalg.norm(y))
```

**Example.** (Final Exam Oct 2018, Q1(b)) The dot product of two vectors  $\mathbf{x} = (x_1, x_2, \dots, x_n)$  and  $\mathbf{y} = (y_1, y_2, \dots, y_n)$ ,  $\mathbf{x} \cdot \mathbf{y}$ , is defined as

$$\mathbf{x} \cdot \mathbf{y} = x_1y_1 + x_2y_2 + \cdots + x_ny_n$$

The angle  $\theta$  between two arrays is defined by the following relation

$$\cos \theta = \frac{\mathbf{x} \cdot \mathbf{y}}{\sqrt{\mathbf{x} \cdot \mathbf{x}} \sqrt{\mathbf{y} \cdot \mathbf{y}}}$$

Implement a **Python function** `theta` to calculate the angle  $\theta$  (in **degree**) if you are given two arrays  $a=[a_1, a_2, a_3, a_4]$  and  $b=[b_1, b_2, b_3, b_4]$ . You **must** write down the proper import statements. If you use the Numpy module, you must prefix the Numpy functions with “`np.`” or marks will be heavily deducted. Use scientific calculator to find the return value of the Python command `theta([1, 2, 3, 4], [2, 1, 3, 4])` to 4 decimal places.

Try to work out the answer using dot product and vector norms.

**Sample Solution:**

```
import numpy as np
from scipy import linalg
from math import degrees, acos
def theta(a, b):
 num = np.array(a).dot(b)
 den = linalg.norm(a)*linalg.norm(b)
 return degrees(acos(num/den))
```

# [0.5 mark]  
# [0.5 mark]  
# [1 mark]  
# [1 mark]  
# [1 mark]  
# [1 mark]

### Operations for Matrices

Apart from the elementwise arithmetic mentioned earlier, the following are some operations specific to matrices:

- \* `A@B` or `np.matmul(A, B)`: Matrix product of two arrays.
- \* `np.dot(A, B)`: Dot product  $z[I, J, j] = \sum_k A[I, k]B[J, k, j]$  of  $A$  and  $B$ . It is equivalent to matrix multiplication.
- \* `np.linalg.matrix_power(A, n)`: Raise a square matrix to the (integer) power  $n$ .

\* `np.kron(A,B)` : Kronecker product of two arrays, giving  $[a_{ij...k}B]$ .

**Example.** (Linear Algebra Operations on 2-D arrays) Consider the matrices

$$A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix} \quad B = \begin{bmatrix} 7 & 8 \\ & \\ 8 & 7 \end{bmatrix} \quad C = \begin{bmatrix} 3 & -2 \end{bmatrix}$$

Find the matrix product  $AB$ , the 'matrix product'  $BC$ , the matrix power  $B^4$  and the Kronecker product  $A \otimes B$  using Python.

**Sample Solution:**

```
A = np.array([[1, 2],[3, 4],[5, 6]])
B = np.array([[7, 8],[8, 7]])
C = np.array([3,-2])

A @ B # Other: np.matmul(A, B), np.dot(A, B)
[23, 22]
A x B = [53, 52]
[83, 82]

Note: Python will cleverly regard C as column matrix
when B (2x2 matrix) is multiplied to C
B @ C # [5, 10]

B @ B @ B @ B # Other: np.linalg.matrix_power(B, 4)
[25313 25312]
B^4 = B x B x B x B = []
[25312 25313]

np.kron(A, B)
#
[7, 8, 14, 16]
[8, 7, 16, 14]
Kronecker product A (x) B = [1B, 2B] = [21, 24, 28, 32]
[3B, 4B] = [24, 21, 32, 28]
[5B, 6B] = [35, 40, 42, 48]
[40, 35, 48, 42]
```

**Example.** Explain which of the Python/NumPy instruction is most appropriate achieved the following results.

- (a) Generate the multiplication tables for 1 to 9 using Python's linear algebra operations.

**Sample Solution:** We can use the elementwise arithmetic to achieve this:

```
np.r_[1:10].reshape((9,-1)) * np.r_[1:10] # or
np.kron(np.r_[1:10].reshape((9,-1)), np.r_[1:10])
```

- (b) Let  $A = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$ . Use  $A$  to generate a matrix like this

$$\begin{bmatrix} 6 & 8 & 10 & 3 & 4 & 5 \\ 10 & 8 & 6 & 5 & 4 & 3 \\ 3 & 4 & 5 & 6 & 8 & 10 \\ 5 & 4 & 3 & 10 & 8 & 6 \end{bmatrix}$$

**Sample Solution:** There are many answers to this but requires us to observe that

$$\begin{bmatrix} 2 \begin{bmatrix} 3 & 4 & 5 \\ 5 & 4 & 3 \end{bmatrix} \\ \begin{bmatrix} 3 & 4 & 5 \\ 5 & 4 & 3 \end{bmatrix} \end{bmatrix} = 2 \begin{bmatrix} 3 & 4 & 5 \\ 5 & 4 & 3 \end{bmatrix}$$

```
A = np.array([[2,1],[1,2]])
B = np.array([[3,4,5],[5,4,3]])
np.kron(A,B)
```

**Example.** (Final Exam Sept 2019, Q2) Given the matrix

$$M = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix}$$

(a) **Execute** the following Python commands for item (i) to item (v) and write down the output of the execution.

(i) `print(M * M)`

**Solution:**

$$\begin{bmatrix} 1 & 4 \\ 9 & 16 \\ 25 & 36 \end{bmatrix}$$

(ii) `print(M @ M.T)`

**Solution:**

$$\begin{bmatrix} 5 & 11 & 17 \\ 11 & 25 & 39 \\ 17 & 39 & 61 \end{bmatrix}$$

(iii) `print(M[[2,1,0,1,2],:][:,[1,0,0,1]])`

**Solution:**

|                                                                           |        |                                                                                                                   |
|---------------------------------------------------------------------------|--------|-------------------------------------------------------------------------------------------------------------------|
| M[[2,1,0,1,2],:]                                                          |        | M[[2,1,0,1,2],:][:,[1,0,0,1]]                                                                                     |
| $\begin{bmatrix} 5 & 6 \\ 3 & 4 \\ 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix}$ | -----> | $\begin{bmatrix} 6 & 5 & 5 & 6 \\ 4 & 3 & 3 & 4 \\ 2 & 1 & 1 & 2 \\ 4 & 3 & 3 & 4 \\ 6 & 5 & 5 & 6 \end{bmatrix}$ |

(iv) `print(M[:2,:]==M[[2,1],:])`

**Solution:**

|                                                |                 |                                                |                    |                                                                                          |
|------------------------------------------------|-----------------|------------------------------------------------|--------------------|------------------------------------------------------------------------------------------|
| $\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$ | <code>==</code> | $\begin{bmatrix} 5 & 6 \\ 3 & 4 \end{bmatrix}$ | <code>-&gt;</code> | $\begin{bmatrix} \text{False} & \text{False} \\ \text{True} & \text{True} \end{bmatrix}$ |
|------------------------------------------------|-----------------|------------------------------------------------|--------------------|------------------------------------------------------------------------------------------|

(v) `print((M<3)|(M>4))`

**Solution:**

|                                                                     |                 |                                                                     |                |                                                                                                                       |
|---------------------------------------------------------------------|-----------------|---------------------------------------------------------------------|----------------|-----------------------------------------------------------------------------------------------------------------------|
| $\begin{bmatrix} 1<3 & 2<3 \\ 3<3 & 4<3 \\ 5<3 & 6<3 \end{bmatrix}$ | <code>or</code> | $\begin{bmatrix} 1>4 & 2>4 \\ 3>4 & 4>4 \\ 5>4 & 6>4 \end{bmatrix}$ | <code>=</code> | $\begin{bmatrix} \text{True} & \text{True} \\ \text{False} & \text{False} \\ \text{True} & \text{True} \end{bmatrix}$ |
|---------------------------------------------------------------------|-----------------|---------------------------------------------------------------------|----------------|-----------------------------------------------------------------------------------------------------------------------|

(b) Write a Python program with no more than 3 lines to produce the following matrices from M:

$$\begin{array}{lll} M\_1 = \begin{bmatrix} -2.5 & -1.5 \\ -0.5 & 0.5 \\ 1.5 & 2.5 \end{bmatrix} & M\_2 = \begin{bmatrix} -2 & -2 \\ 0 & 0 \\ 2 & 2 \end{bmatrix} & M\_3 = \begin{bmatrix} -0.5 & 0.5 \\ -0.5 & 0.5 \\ -0.5 & 0.5 \end{bmatrix} \end{array}$$

by using the Numpy vector operation in the Python computer software. Note that M\_1 is M subtracted by the mean of all values in M, M\_2 is a matrix such that each column in M being subtracted by the mean of corresponding column, M\_3 is a matrix such that each row in M being subtracted by the mean of corresponding row. Note that your program must work when M is changed to an arbitrary  $m \times n$  matrix.

**Sample Solution:**

```
M1 = M - M.mean() # [1 mark]
M2 = M - M.mean(axis=0)) # [2 marks]
M3 = M - M.mean(axis=1,keepdims=True) # [2 marks]
```

---

## 7. Linear Algebra Solvers

In science and engineering, we often encounter the equations involving matrices called the **linear system** or the **linear algebra problem**:

$$AX = B \quad (\text{LS})$$

where  $A$  is an  $m \times n$  matrix,  $X$  is an  $n \times k$  matrix and  $B$  is an  $m \times k$  matrix.  $X$  is unknown whereas  $A$  and  $B$  need to be given.

### 7.1. When $m = n$ and $A$ is invertible

(LS) can be solved using

```
from scipy import linalg
X = linalg.solve(A, B) # linalg.inv(A) @ B is not recommended
```

The `linalg.solve` should be able to solve (LS) with  $m = n \ll 10^4$  using the Gaussian elimination method (and Cholesky method when the matrix  $A$  is positive definite). For any larger matrix, we may need the sparse matrix solvers.

**Example.** Write down the Python script to solve the following problem:

$$\begin{bmatrix} -2 & 11 \\ 17 & -19 \end{bmatrix} \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{bmatrix} = \begin{bmatrix} 19 & 1 \\ 3 & 2 \end{bmatrix}$$

**Sample Solution:**

```
from scipy import linalg # Mentioned earlier
A = np.array([[-2, 11], [17, -19]])
B = np.array([[19, 1], [3, 2]])
X = linalg.solve(A, B)
print("X=", X)
```

The solution is

$$X = \begin{bmatrix} 2.64429530 & 0.27516779 \\ 2.20805369 & 0.14093960 \end{bmatrix}$$

---

**Example.** (Final Exam Sept 2014, Q4(a)) Given the linear system

$$\begin{aligned} 3x_1 + 7x_2 - 2x_3 + 3x_4 - x_5 &= 37 \\ 4x_1 + 3x_5 &= 40 \\ 5x_3 - 4x_4 + x_5 &= 12 \\ 2x_1 + 9x_3 + 4x_4 + 3x_5 &= 14 \\ 5x_4 + 8x_5 &= 20 \end{aligned}$$

Write a Python script to solve the linear system.

**Sample Solution:**

```
import numpy as np
from scipy import linalg
A = np.array([[3, 7, -2, 3, -1],
 [4, 0, 0, 0, 3],
 [0, 0, 5, -4, 1],
 [2, 0, 9, 4, 3],
 [0, 0, 0, 5, 8]])
x = linalg.solve(A, [37, 40, 12, 14, 20])
```

---

**Example.** (Final Exam Sept 2020 during MCO, Q1)

(a) Given that A stores the following matrix

```
[4 0 0 0 0 15 8 1 0 0]
[0 6 0 0 0 6 24 6 1 0]
[0 0 6 0 0 1 8 15 4 4]
[1 0 0 3 0 0 8 4 18 5]
[2 3 0 0 5 0 0 8 6 24]
[29 3 1 0 0 5 0 0 3 7]
[3 17 5 6 0 0 7 0 0 2]
[4 4 17 3 4 0 0 6 0 0]
[0 8 2 25 4 0 0 0 8 0]
[0 0 7 1 16 0 0 0 0 7]
```

- (i) Write down the output of the Python command `A[:, [3, 5, 2, 4]]`. Determine if it is the same as `A[[3, 5, 2, 4]]` and explain the difference.

**Solution:**

```
[[0 15 0 0]
 [0 6 0 0]
 [0 1 6 0]
 [3 0 0 0]
 [0 0 0 5]
 [0 5 1 0]
 [6 0 5 0]
 [3 0 17 4]
 [25 0 2 4]
 [1 0 7 16]]
```

`A[:, [3, 5, 2, 4]]` and `A[[3, 5, 2, 4]]` are different because the former picks the columns while the later pick the rows.

- (ii) Write the Python command to pick all the odd rows and even columns from A and write down the output of your command.

**Solution:** `A[::2, 1::2]` -> 

```
[[0 0 0 24 1]
 [1 0 0 8 18]
 [29 1 0 0 3]
 [4 17 4 0 0]
 [0 7 16 0 0]]
```

- (iii) Write the Python command to pick the intersection of the second, fifth, third columns and of the eighth, fifth and seventh rows in the given order and write down the output of your command.

**Solution:** `A[:, [1, 4, 2]][[7, 4, 6], :]` -> 

```
[[4 4 17]
 [3 5 0]
 [17 0 5]]
```

- (iv) Write the Python command to arrange the given matrix A into the following diagonally dominant form:

```
[15 8 1 0 0 4 0 0 0 0]
[6 24 6 1 0 0 6 0 0 0]
[1 8 15 4 4 0 0 6 0 0]
[0 8 4 18 5 1 0 0 3 0]
[0 0 8 6 24 2 3 0 0 5]
[5 0 0 3 7 29 3 1 0 0]
[0 7 0 0 2 3 17 5 6 0]
[0 0 6 0 0 4 4 17 3 4]
[0 0 0 8 0 0 8 2 25 4]
[0 0 0 0 7 0 0 7 1 16]
```

**Solution:** `A[:, [5, 6, 7, 8, 9, 0, 1, 2, 3, 4]]`

- (v) For an  $n \times n$  matrix A, it is said to be *diagonally dominant* if for each row the absolute value of the diagonal element is larger than the sum of the absolute value of the rest of the elements in the row:

$$|a_{ii}| > \sum_{j=1, j \neq i}^n |a_{ij}|, \quad i = 1, 2, \dots, n.$$

Write a Python function `is_diag_domin(A)` which determines whether the matrix  $A$  is diagonally dominant. The function will return True if the matrix  $A$  is diagonally dominant, False if the matrix  $A$  is not diagonally dominant, and None if the matrix is not square.

**Sample Solution:**

```
def is_diag_domin(A):
 N = A.shape[0]
 for i in range(N):
 S = sum(abs(A[i,j]) for j in range(N) if j != i)
 if abs(A[i,i]) <= S:
 print("i=", i)
 return False
 return True

#import q1
#print(is_diag_domin(q1.AA))
```

(b) Given that three  $3 \times 3$  matrices

$$P = \begin{bmatrix} 5 & 8 & 8 \\ 6 & -9 & -8 \\ 6 & -5 & 1 \end{bmatrix} \quad Q = \begin{bmatrix} 2 & 2 & -2 \\ 7 & 8 & -2 \\ 0 & 2 & 2 \end{bmatrix} \quad R = \begin{bmatrix} -2 & -8 & 8 \\ -8 & -5 & 8 \\ 6 & -9 & 4 \end{bmatrix}$$

(i) Write down the Python command to find the inverse matrix of  $Q$ ,  $Q^{-1}$ .

**Solution:** The Python command to find  $Q^{-1}$  is

```
np.linalg.inv(Q)
```

or

```
np.linalg.solve(Q, np.eye(Q.shape[0]))
```

The output is

$$\begin{bmatrix} -1.25 & 0.5 & -0.75 \\ 0.875 & -0.25 & 0.625 \\ -0.875 & 0.25 & -0.125 \end{bmatrix}$$

(ii) Write down the Python command to find matrix  $L$  if  $P^3 L Q = R$ . Write down the **matrix**  $L$ .

**Solution:**  $L = (P^3)^{-1} R Q^{-1}$

```
L = linalg.inv(P@P@P) @ R @ linalg.inv(Q)
```

```
L = linalg.solve(np.linalg.matrix_power(P,3), R)@linalg.inv(Q)
```

The matrix  $L$  is

$$\begin{bmatrix} 0.08603119 & -0.04214438 & 0.07957573 \\ 0.21360577 & -0.09753974 & 0.18129806 \\ -0.24895274 & 0.11235113 & -0.20818642 \end{bmatrix}$$

(iii) Suppose the  $3 \times 3$  matrices  $E, F, G, H$  satisfies

$$\begin{bmatrix} P & Q \\ Q & R \end{bmatrix}^{-1} = \begin{bmatrix} E & F \\ G & H \end{bmatrix}$$

First, find the matrix  $H$  by writing down the appropriate Python commands. Then, write down the appropriate Python command(s) to show that

$$(R - QP^{-1}Q)^{-1} = H.$$

**Solution:** After from `scipy import linalg`, the command

```
H = linalg.inv(R - Q@linalg.inv(P)@Q)
```

allows us to obtain

$$H = \begin{bmatrix} 0.26819736 & -0.15480007 & -0.07891041 \\ 0.69421553 & -0.3532685 & -0.42828374 \\ 1.00692917 & -0.48176952 & -0.51330189 \end{bmatrix}$$


---



## 7.2. When $m \neq n$ or $A$ is not invertible

Mathematicians have solved the general linear system (LS) with no restrictions (except that that they cannot be too large because computer memory is limited) on  $m$  and  $n$  (the price to pay is a longer computation time) using the SVD method or QR method leading to the following functions in Python:

```
from scipy import linalg
X = linalg.lstsq(A, B) # linalg.pinv(A) @ B is not recommended
```

Note that  $X$  may not be a solution but a ‘least square solution’ of the linear system (LS).

**Example.** Write down the Python script to solve the following problem:

$$\begin{bmatrix} -2 & 11 \end{bmatrix} \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{bmatrix} = \begin{bmatrix} 19 & 1 \end{bmatrix}$$

**Sample Solution:**

```
A = np.array([[-2, 11]])
B = np.array([[19, 1]])
X, _, Rank, Sing = linalg.lstsq(A, B)
print("X=", X) # Many solutions but only one return
```

---

**Example.** Solve the Least Square Problem:

$$\begin{bmatrix} -2 & 11 \\ 17 & -19 \\ 6 & 6 \end{bmatrix} \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{bmatrix} = \begin{bmatrix} 19 & 1 \\ 3 & 2 \\ 6 & 7 \end{bmatrix}$$

Note: Be careful, `linalg.solve` will not work.

**Sample Solution:**

```
A = np.array([[-2, 11], [17, -19], [6, 6]])
B = np.array([[19, 1], [3, 2], [6, 7]])
X, Err, Rank, Sing = linalg.lstsq(A, B)
print("X=", X)
print("Residue=", Err)
```

---

### 7.3. Special (Dense) Matrices and Sparse Matrices

For some linear system with special square matrices such as the **Toeplitz matrix**:

$$\begin{bmatrix} a_1 & b_1 & b_2 & \cdots & b_{n-1} & b_n \\ a_2 & a_1 & b_1 & \cdots & b_{n-2} & b_{n-1} \\ a_3 & a_2 & a_0 & \cdots & . & . \\ . & . & . & . & . & . \\ . & . & . & . & a_0 & b_1 \\ a_n & a_{n-1} & a_{n-2} & \cdots & a_1 & a_0 \end{bmatrix}$$

It can be generated using

```
linalg.toeplitz([a1, a2, a3, ..., an], [b0, b1, b2, ..., bm])
```

Mathematicians have developed special algorithms to speed up the solution of linear system with special matrices.

```
* linalg.solve_toeplitz(c_or_cr, b, check_finite=True)
```

```
* Other special cases are ignored.
```

**Example.** Construct a Toeplitz matrix from the 1-D arrays  $a=[2,3,4,5]$  and  $b=[500,6,7,8,9,10]$ .

**Sample Solution:**

```
>>> print(linalg.toeplitz([2,3,4,5],[500,6,7,8,9,10]))

[2, 6, 7, 8, 9, 10]
[3, 2, 6, 7, 8, 9]
[4, 3, 2, 6, 7, 8]
[5, 4, 3, 2, 6, 7]
```

---

**Example.** (Toeplitz System) Write a script using `linalg.toeplitz` to solve the linear system:

$$\begin{bmatrix} 1 & -1 & -2 & -3 \\ 3 & 1 & -1 & -2 \\ 6 & 3 & 1 & -1 \\ 10 & 6 & 3 & 1 \end{bmatrix} y = \begin{bmatrix} 1 \\ 2 \\ 2 \\ 5 \end{bmatrix}$$

**Sample Solution:**

```
MUST MAKE SURE linalg.toeplitz(c, r) is the same as
left matrix in order to use this.
c = np.array([1,3,6,10]) # first column of left matrix
r = np.array([1,-1,-2,-3]) # first row of left matrix
b = np.array([1,2,2,5]) # right column matrix
x = linalg.solve_toeplitz((c, r), b)
```

---

Some square matrices like the tridiagonal matrices have a lot zeros and sparse matrix is a good representation and special solvers can be applied.

**Example.** (Sparse Matrix Solver (Not working with Old Scipy))

```
import numpy as np
from scipy import sparse
N = 10
idx = np.r_[0:N]
v1 = 3*idx**2 +(idx/2)
v2 = -(6*idx**2 - 1)
v3 = 3*idx**2 -(idx/2)
A = sparse.spdiags(np.vstack((v1,v2,v3)),(-1,0,1),N,N).tocsc()
B = np.r_[N:0:-1]
X = sparse.linalg.spsolve(A, B)
```

---

## 8. Eigenvalue Problems and Matrix Functions

**Eigenvalues** are important in science and engineering because they are linked with **resonance frequencies, characteristic functions, etc.** The eigenvalue problem  $Ax = \lambda x$  has the following matrix form:

$$AX = \lambda X \quad (\text{EP})$$

Here  $A$  is an  $n \times n$  matrix. (EP) can be solved using:

```
from scipy import linalg
eigenvalues, eigenvectors = linalg.eig(A)
```

returning the eigenvalues and the normalised right eigenvectors of the square array  $A$ . For a special case where  $A$  is a Hermitian or symmetric, `linalg.eigh(A)` has a faster algorithm.

$A$  (right) **generalised matrix eigenvalue problem** has the form:

$$AX = \lambda BX \quad (\text{GEP})$$

It can be solved using

```
eigenvalues, eigenvectors = linalg.eig(A,B).
```

**Example.** Write down the Python script to solve the following eigenvalue problem:

```
[-2 11]
[] v = lambda v
[17 -19]
```

**Sample Solution:**

```
from scipy import linalg
A = np.array([-2,11],[17,-19])
lambdas, eigenvectors = linalg.eig(A)
print("/\=", lambdas)
print("X=", eigenvectors)
```

---

### 8.1. Linear Matrix Equations

There are a few matrix equations from linear control theory, signal processing, filtering, model reduction, image restoration, decoupling techniques for ordinary and partial differential equations below and the respective solvers in Python are listed.

Sylvester equations:

$$AX + BX = C$$

are solved with `linalg.solve_sylvester(A, B, C)` using the Bartels-Stewart algorithm.

A continuous-time algebraic Riccati equation (CARE):

$$XA + A^H X - XBR^{-1}B^H X + Q = 0$$

is `linalg.solve_continuous_are(A, B, Q, R[, E, S, ...])` in Python.

A discrete-time algebraic Riccati equation (DARE):

$$A^H X A - X - (A^H X B)(R + B^H X B)^{-1}(B^H X A) + Q = 0$$

is `linalg.solve_discrete_are(A, B, Q, R[, E, S, balanced])` in Python.

A continuous-time Lyapunov equation:

$$AX + XA^H = -Q$$

is `linalg.solve_continuous_lyapunov(A, -Q)` in Python.

A discrete-time Lyapunov equation:

$$AXA^H - X + Q = 0$$

is `linalg.solve_discrete_lyapunov(A, -Q[, method])` in Python.

## 8.2. Matrix Functions and Matrix Equations

A more general **nonlinear matrix problem** has the form:

$$f(X) = 0 \quad (\text{ME})$$

where  $X$  and  $0$  are  $n \times n$  square matrices. There is no simple / unified solution technique to this problem. A special case of (ME) has a quadratic left hand side leading to a 'quadratic matrix equation':

$$AX^2 + BX + C = 0$$

where  $X, A, B, C, 0$  are all  $n \times n$  matrices. For example,

$$\begin{bmatrix} -2 & 11 \\ & \end{bmatrix} X^2 + \begin{bmatrix} 19 & 1 \\ & \end{bmatrix} X + \begin{bmatrix} 0 & 13 \\ -13 & 13 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

where  $X$  is a  $2 \times 2$  matrix.

The  $f(X)$  in (ME) can be a **matrix function** defined by the Taylor series for matrix of the form

$$f(X) = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{k!} X^k.$$

Python has the exponential, logarithm, trigonometric and hyperbolic matrix functions such as `linalg.expm`, `linalg.logm`, `linalg.sinm`, `linalg.cosm`, `linalg.tanm`, `linalg.sinhm`, `linalg.coshm` and `linalg.tanhm`.

**Example.** (Final Exam Sept 2021 during MCO, Q1(d)) Given a  $2 \times 2$  matrix

$$A = \begin{bmatrix} 1 & -0.1 \\ 0.1 & 1 \end{bmatrix}.$$

Let  $X$  be a  $2 \times 2$  matrix with entries  $x_{ij}$ ,  $i, j = 1, 2$ . You are investigating the difference between the matrix exponential function

$$\exp^{[m]}(X) = I_2 + X + \frac{1}{2!} X^2 + \frac{1}{3!} X^3 + \frac{1}{4!} X^4 + \cdots + \frac{1}{k!} X^k + \cdots$$

and the elementwise exponential function

$$\exp(X) = \begin{bmatrix} e^{x_{11}} & e^{x_{12}} \\ e^{x_{21}} & e^{x_{22}} \end{bmatrix}$$

- (i) Write down the Python commands for calculating  $\exp^{[m]}(A)$  and  $\exp$ . Run the Python commands and write down the output of the commands. Then, write down the difference  $\exp^{[m]}(A) - \exp(A)$ .

**Solution:** The Python commands are respectively

```
* exp[m](A): linalg.expm(A)
* exp(A): np.exp(A)
```

The outputs are respectively

$$\begin{bmatrix} 2.70470174 & -0.27137536 \\ 0.27137536 & 2.70470174 \end{bmatrix} \quad \begin{bmatrix} 2.71828183 & 0.90483742 \\ 1.10517092 & 2.71828183 \end{bmatrix}$$

and the difference is

$$\begin{bmatrix} -0.01358009 & -1.17621278 \\ -0.83379556 & -0.01358009 \end{bmatrix}$$

- (ii) Write down the Python command to find the difference

$$\exp^{[m]}(A) - I_2 - A - \frac{1}{2!} A^2 - \frac{1}{3!} A^3$$

and write down the difference.

**Solution:** The Python command to find the difference is

$$\text{linalg.expm}(A) - \text{np.eye}(2) - A - 0.5*A*A - 1/6*A*A*A$$

and the output is

$$\begin{bmatrix} 0.04803508 & -0.02154203 \\ 0.02154203 & 0.04803508 \end{bmatrix}$$

## 9. Inline Functions, Anonymous Functions

Python does not have inline functions. Another implementation of Python called PyPy will inline functions automatically.

The lambda notion for function in Topic is the **anonymous function** in Python:

```
lambda x: an_expression_of x ...
```

It is usually used when we don't need to give an operation a function name.

**Example.** Sorting list strings reversely based on the characters and the number.

```
import re
table_data = ["vlan1", "usb0", "eth1", "vlan4", "vlan20"]
sorted(table_data, key=lambda v:
 [re.findall(r'([a-z]+)', v), -int(re.findall(r'(\d+)', v)[0])],
 reverse=True)
```

---