



# CEng 240 – Spring 2021 Week 13

Scientific and Engineering Libraries
Part 1: NumPy and SciPy

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# Error Types

- Syntax errors
- METH Computer Engreering

  Language

  Language Type errors
  - Run-time errors
  - Logical errors

```
>>> for i in range(10)
       print(i)
File "<ipython-input-1-12d72cac235a>", line 1
    for i in range(10)
SyntaxError: invalid syntax
>>> x = float(input())
>>> a = ((x+5)*12+4
File "<ipython-input-2-dead5b360d91>", line 2
  a = ((x+5)*12+4)
SyntaxError: invalid syntax
>>> S = 0
>>> for i in range(10):
     s += i
       print(i)
File "<ipython-input-3-c3ef5d622e47>", line 4
  print(i)
IndentationError: unexpected indent
>>> while x = 4:
       s += x
File "<ipython-input-4-befcf7769cec>", line 1
  while x = 4:
```

SyntaxError: invalid syntax



# Error Types

- Syntax errors
- Type errors
- Run-time errors
- METU Computer Engraeering

  Language

  Language Logical errors

```
>>> print(astr ** 3)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: unsupported operand type(s) for ** or pow(): 'str' and 'int'
>>> print(bflt[1])
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: 'float' object is not subscriptable
>>> print(cdict * 2)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: unsupported operand type(s) for *: 'dict' and 'int'
>>> cdict < astr
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: '<' not supported between instances of 'dict' and 'str'
```



# Error Types

- Syntax errors
- Type errors
- Run-time errors
- METU Computer Engracering Logical errors

```
def divisible(m, n):
  return m % n == 0
def count(m):
  sum = 0
 for i in range(1,1000):
   if divisible(i, m):
      sum += 1
  return sum
value = int(input())
print('input value is:', value)
print(value, 'divides', count(value), 'many integers in range [1, 1000]')
```

```
input value is: 0
ZeroDivisionError
                                           Traceback (most recent call last)
in ()
    12 value = int(input())
     13 print('input value is:', value)
---> 14 print(value, 'divides ', count(value), 'many integers in range [1, 1000]')
 in count(m)
      5 \quad \text{sum} = 0
      6 for i in range(1,1000):
            if divisible(i,m):
      8
              sum += 1
 in divisible(m, n)
      1 def divisible(m, n):
 ---> 2 return m % n == 0
      4 def count(m):
          sum = 0
ZeroDivisionError: integer division or modulo by zero
```

# **Exceptions**

METU Computer Engineering	Won CENG 240!	Exceptions
	Exception	Reason
	KeyboardInterrupt	User presses Ctrl-C; not an error but user intervention
	ZeroDivisionError	Right-hand side of / or % is 0
	AttributeError	Object/class does not have a member
	EOFError	input() function gets End-of-Input by user
	IndexError	Container index is not valid (negative or larger than length)
	KeyError	dict has no such key
	FileNotFoundError	The target file of open ( ) does not exist
	TypeError	Wrong operand or parameter types, or wrong number of parameters for functions
	ValueError	The given value has correct type but the operation is not supported for the given value



# **Exception Examples**

```
The company of the co
                                                                                                                               # ZeroDivisionError
                                                                                                                               # AttributeError: lists does not have a length attribute (use len(x))
                                                                                                                               # IndexError: last valid index of list x is 2
                           person = { 'name' : 'Han', 'surname': 'Solo'}
                                                                                                                    # KeyError: person does not have 'Name' key but 'name'
                           print(person['Name'])
                            fp = open("example.txt") # FileNotFoundError: file "example.txt" does not exist
                           print([1,2,3] / 12)
                                                                                                                              # TypeError: Division is not defined for lists
                           def f(x, y):
                                   return x*x+y
                           print(f(5))
                                                                                                                               # TypeError: Only one element is supplied instead of 2.
                           print(int('thirtytwo'))
                                                                                                                            # ValueError: string value does not represent an integer
                           a,b,c = [1,2,3,4]
                                                                                                                              # ValueError: too many values on the right hand side
```



# METU Computer Engreering L S L S L

# Error Types

- Syntax errors
- Type errors
- Run-time errors
- Logical errors

```
y = x / x+1
                        # you meant y = x / (x+1), forgetting about precedence
lastresult = 0
def missglobal(x):
                                  # you intend to update the global variable
  result = x*x+1
  if lastresult != result:
                                  # but you assign a local variable instead
    lastresult = result
                                  # you should have used "global lastresult"
def returnsnothing(x, y):
  y = x*x+y*y
 if x <= y:
                                   \# if x > y, the function returns nothing
    return x
                                  # does not have any value. prints "None"
print(returnsnothing(0.1, 0.1))
s = 1
while i < n:
                                   # you forgot incrementing i as i+=1
                                  # loop will run forever. "infinite loop"
   s += s*x/i
```



# How to work with errors

- Program with care
- Place controls in your code
- Handle exceptions
- METU Computer Engreering 1: 7: 4: 4: Write verification code & raise exceptions
  - Debug your code
  - Write test cases

```
work with errors.

(2) Place controls in your code

# CASE 1 with sanitization
n = int(input())
if 0 <= n < len(a):
    print(a[n])
else:
    print("n is not valid."

# CASE 2 with
name = input
if name
</pre>
                             # CASE 3 with sanitization
                             x = float(input())
                             if x >= 0:
                                y = math.sqrt(x)
                             else:
                                print("invalid for sqrt operation: ", x)
                             if x != 0:
                                y = 1 / x
                             else:
                                print("divisor cannot be 0")
```



```
work with errors.
(3) Handle Exceptions
                  # and error occurs in the function, we can handle error here
                  # when there is an error, execution jumps here
```

```
covork with errors.
(3) Handle Exceptions

import math

a = [1,2,3]
age = {'Han': 30, 'Leia': 20, 'Luke': 20}

try:
    n = int(input())
    print(a[n])

name = input()
print(age*
               y = math.sqrt(x) # will fail for x < 0
               y = 1 / x
                                        # will fail for x == 0
             except IndexError:
               print('List index is not valid')
             except KeyError:
               print('Dictionary does not have such key')
             except ValueError:
               print('Invalid value for square root operation')
             except ZeroDivisionError:
               print('Division by zero does not have value')
             except:
               print('None of the known errors. Something happened even if nothing happened')
```



# How to work with errors:

Write verification code and raise exception

- You can raise exceptions
- "raise Exception" => raise a generic exception

```
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        try:
          if !cond1:
            raise Error
          . . 1 . .
          if !cond2:
             raise Error
          ..2..
          if !cond3:
             raise Error
          . . 3 . .
          ..4.. # success
        except:
          ... Error handling
```

```
def solvesecond(a,b,c):
  det = b*b - 4*a*c
  # the following is the verification code
  if det < 0:
    print("Equation has no real roots for", a, b, c)
    raise ValueError
  . . .
```



```
work with errors.

(6) Write test cases

(x1, x2) = findre

if a*x1*
```



# Debugging

- Using debugging outputs
- Handling exception and getting more info
- Using debugger



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# CMC5401

# Debugging:

# Using debugging outputs

The following code has a bug, how can we find it?



```
def sum_and_delete(L):
    sum = 0
    try:
                                   del L[i]
                   except:
                           print(f"i: {i} len(L): {len(L)}")
                   return sum
            sum and delete([1, 2, 3, 4, 5])
```



# Debugging:

# Using debugger

```
pdb.
      pdb.set trace()
     > <ipython-input-14-110393975fb5>(7)startswith()
      -> for i in range(len(srcstr)): # check all characters of srcstr
     Documented commands (type help <topic>):
     E0F
                                         list
                                                                     undisplay
            C
                                h
                                                            rv
           cl
                       debug
                                help
                                         11
                                                   quit
                                                                     unt
      alias clear
                       disable
                               ignore
                                         longlist
                                                                     until
                                                           source
                                                   restart step
     args commands
                       display interact n
                                                                     up
           condition
                                                            tbreak
                       down
                                         next
                                                   return
                                                                     W
                       enable
     break cont
                                                   retval
                                                                     whatis
                                jump
                                         p
                                                            u
            continue
                                                            unalias
     bt
                       exit
                                                                     where
                                                   run
                                         pp
     Miscellaneous help topics:
     exec pdb
```



# Debugging: Using debugger

```
pdb.
      pdb.set_trace()
                  import pdb
                  def sum_and_delete(L):
                           sum = 0
                           pdb.set_trace()
                           for i in range(len(L)):
                                    sum += L[i]
                                    del L[i]
                           return sum
                  sum_and_delete([1, 2, 3, 4, 5])
```



## This Week

- Scientific and Engineering Libraries
  - NumPy for numerical computing
  - SciPy for scientific computing

- Next week:
  - Pandas for data handling and analysis
  - Matplotlib for plotting



## **Administrative Notes**

Lab 8

■ Midterm: 1 June, Tuesday, 17:40

Final: 8 July, 9:30







## Outline



- Overview
  Installation
  Arrays and their properties
  Working with arrays

  - Linear algebra
  - Why use NumPy?

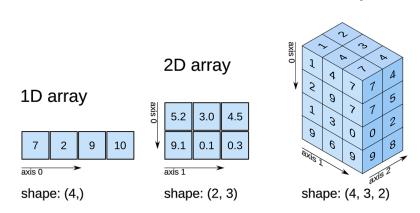


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## Overview



- A Python library for arrays & matrices and mathematical functions that work on them.
- Combination of two ancestor libraries in 2005:
   Numeric and Numarray.



3D array

Figure: https://www.oreilly.com/library/view/elegant-scipy/9781491922927/ch01.html



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## Installation



- On your Linux environment:
  - \$ pip install numpy

or

- \$ conda install numpy
- On Windows/Mac: install anaconda first
- On Colab, it is already installed



# Data types in NumPy



- Integers:
  - np.int8, np.int16, np.int32, np.int64, np.uint8, ...
- Float:
  - np.float16, np.float32, np.float64, ...
- Complex:
  - np.complex64, np.complex128, ...
- **Boolean:** 
  - np.bool8
- **Default:**

np.float64

For a full list, see:

https://numpy.org/devdocs/user/basics.types.html

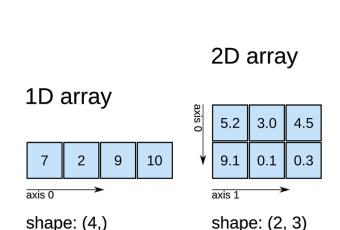
# Arrays and their properties



In essence, NumPy is a library for ndimensional arrays:

$$array1 = \begin{pmatrix} 1 & 2 & 3 \end{pmatrix}$$

$$array2 = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix}$$



3D array

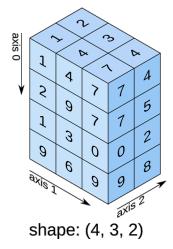


Figure: https://www.oreilly.com/library/view/elegant-scipy/9781491922927/ch01.html



# Arrays and their properties NumPy



$$array1 = \begin{pmatrix} 1 & 2 & 3 \end{pmatrix}$$

Basic array creation
$$array1 = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix}$$

$$array2 = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix}$$

```
>>> import numpy as np
                                 # Import the NumPy library
>>> array1 = np.array([1, 2, 3])
>>> array2 = np.array([[1, 2, 3], [4, 5, 6]])
>>> type(array1)
<class 'numpy.ndarray'>
>>> type(array2)
<class 'numpy.ndarray'>
>>> arrayl
array([1, 2, 3])
>>> array2
array([[1, 2, 3],
       [4, 5, 6]])
>>> print(array2)
[[1 2 3]
 [4 5 6]]
```

# Arrays and their properties NumPy



## Array Shapes, Dimensions, and Elements

$$array1 = \begin{pmatrix} 1 & 2 & 3 \end{pmatrix}$$

$$array2 = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix}$$

```
>>> arrayl.reshape((3,1))
array([[1],
       [2],
       [3]])
>>> array2.reshape((1,6))
array([[1, 2, 3, 4, 5, 6]])
```

```
>>> array1.size
3
>>> array2.size
6
```

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## Arrays and their properties



## Array Shapes, Dimensions, and Elements

## Same indexing mechanisms of Python:

```
>>> array1[-1]
>>> array2[1][2]
>>> array2[-1]
array([4, 5, 6])
```

$$array1 = \begin{pmatrix} 1 & 2 & 3 \end{pmatrix}$$

$$array2 = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix}$$

array2[1, 2] is also possible.



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## Arrays and their properties



## **Creating arrays**

- With the constructor:
  - np.array(<List>)

```
>>> array1 = np.array([1, 2, 3])
>>> array2 = np.array([[1, 2, 3], [4, 5, 6]])
```

- Arrays with constant values:
  - np.zeros(<shape>)
  - np.ones(<shape>)

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## **Creating arrays**

- Array with a range of values:
  - np.arange(start, stop, step)

- Random array:
  - np.random.randn(<shape>)



# **METH Computer Engineering**

# Working with arrays



- Arithmetic, relational and membership operations
- Mathematical functions
- Splitting and combining arrays
- Iterations with arrays



# Working with arrays



Arithmetic, relational and membership operations

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## Arithmetic operations:

Be careful about the shapes of the arrays

```
>>> A = np.arange(4).reshape((2,2))
>>> A
array([[0, 1],
       [2, 3]])
>>> B = np.arange(4, 8).reshape((2,2))
>>> B
array([[4, 5],
       [6, 7]])
>>> print(B-A)
[[4 4]
 [4 4]]
>>> print(B+A)
[[4 6]
 [ 8 10]]
>>> A
array([[0, 1],
       [2, 3]])
>>> B
array([[4, 5],
```

[6, 7]])

2020



# Working with arrays



Arithmetic, relational and membership operations

Relational operations:

Membership operations:

■ in, not in

Be careful about the shapes of the arrays

False



# Working with arrays



**Useful Functions** 

- np.sqrt(<array>)
- np.exp(<array>)
- np.sin(<array>)
- np.cos(<array>)
- <array>.min()
- <array>.max()
- <array>.sum()
- <array>.mean()
- <array>.std()



# Working with arrays



**Useful Functions** 

You may apply some of these operations on the whole array or along an axis

```
>>> A
array([[0, 1],
       [2, 3]])
>>> A.sum()
>>> A.sum(axis=0)
array([2, 4])
>>> A.sum(axis=1)
array([1, 5])
>>> A.sum(axis=2)
Traceback (most recent call last):
 File "<stdin>", line 1, in <module>
 File "/usr/local/lib/python3.7/site-packages/numpy/core/ methods.py", line 47, in sum
    return umr sum(a, axis, dtype, out, keepdims, initial, where)
numpy.AxisError: axis 2 is out of bounds for array of dimension 2
```





**Splitting and Combining Arrays** 

#### Splitting:

- horizontal split (np.hsplit)
- vertical split
  (np.vsplit)
- general splitting
  (np.array\_split)

```
>>> L = np.arange(16).reshape(4,4)
>>> L
array([[ 0, 1, 2, 3],
      [4, 5, 6, 7],
      [8, 9, 10, 11],
      [12, 13, 14, 15]])
>>> np.hsplit(L,2) # Divide L into 2 arrays along the horizontal axis
[array([[ 0, 1],
      [4, 5],
      [8, 9],
      [12, 13]]), array([[ 2, 3],
      [6, 7],
      [10, 11],
      [14, 15]])]
>>> np.vsplit(L,2)
[array([[0, 1, 2, 3],
      [4, 5, 6, 7]]), array([[ 8, 9, 10, 11],
      [12, 13, 14, 15]])]
```



**Splitting and Combining Arrays** 

#### Combining:

- horizontal stack (np.hstack)
- vertical stack (np.vstack)
- general stack (np.stack)

```
>>> A
array([[0, 1],
       [2, 3]])
>>> B
array([[4, 5],
       [6, 7]])
>>> np.hstack((A, B))
array([[0, 1, 4, 5],
       [2, 3, 6, 7]])
>>> np.vstack((A, B))
array([[0, 1],
       [2, 3],
       [4, 5],
       [6, 7]])
```





**Iterations with Arrays** 

 You can use NumPy arrays in iterations as we would be using other container data types

```
>>> L
array([[ 0, 1, 2, 3],
       [4, 5, 6, 7],
       [ 8, 9, 10, 11],
       [12, 13, 14, 15]])
>>> for r in L:
        print("row: ", r)
. . .
      [0 1 2 3]
row:
      [4 5 6 7]
row:
      [ 8 9 10 11]
row:
      [12 13 14 15]
row:
```





#### **Iterations with Arrays**

```
>>> for element in L.flat:
        print(element)
0
10
11
12
13
14
15
```

```
>>> for r in L:
        for element in r:
                 print(element)
10
11
12
13
14
15
```



#### Linear algebra with NumPy



Transpose

<array>.T or <array>.transpose()

$$A = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}$$

$$A^T = \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix}$$

```
>>> A
array([[1, 2],
       [3, 4]])
>>> A.T
array([[1, 3],
       [2, 4]])
>>> A
array([[1, 2],
       [3, 4]])
```

Original array does not change!



#### Linear algebra with NumPy



**Inverse** 

np.linalg.inv(<array>)

```
A \times A^{-1} = I.
```

```
>>> A
array([[1, 2],
       [3, 4]])
>>> A inv = np.linalg.inv(A)
>>> A inv
array([[-2., 1.],
      [1.5, -0.5]
```

#### Let's check correctness:

```
>>> np.matmul(A, A inv)
array([[1.0000000e+00, 0.0000000e+00],
       [8.8817842e-16, 1.0000000e+00]])
```





Determinant, norm, rank, condition number, trace

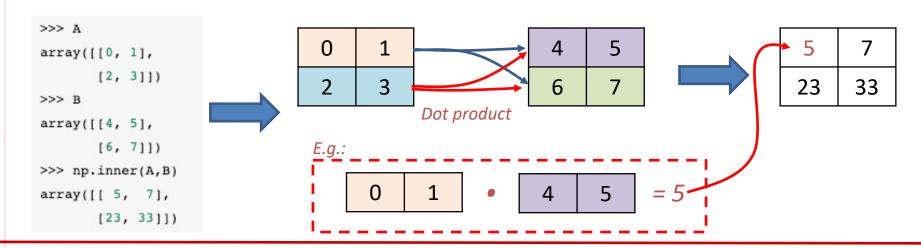
How to Calculate with NumPy
np.linalg.det(A)
np.linalg.norm(A)
np.linalg.matrix_rank(A)
np.linalg.cond(A)
np.linalg.trace(A)

#### Linear algebra with NumPy



Dot product, inner product, outer product, matrix multiplication

- np.dot(a, b)
  - For 1D arrays, this is dot product:  $\sum_{i} \mathbf{a}_{i} \mathbf{b}_{i}$
  - For nD arrays, this is matrix multiplication (see below).
- np.inner(a,b)
  - For 1D arrays, this is dot product:  $\sum_i \mathbf{a}_i \mathbf{b}_i$
  - For nD arrays, dot-product over the last axes:





Dot product, inner product, outer product, matrix multiplication

- np.matmul(a,b)
  - $result_{ij} = \sum_{k} \mathbf{a}_{ik} \mathbf{b}_{kj}$

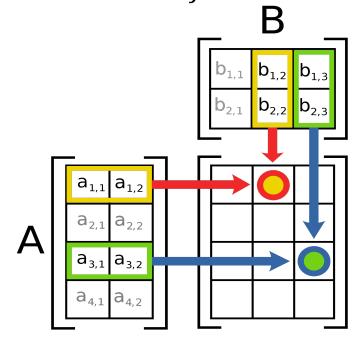


Figure source: Wikipedia



Dot product, inner product, outer product, matrix multiplication

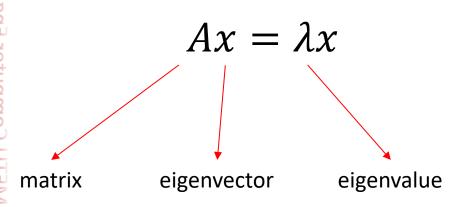
- np.outer(a,b):
  - Defined over vectors (1D arrays)
  - equivalent to matrix multiplication with ab<sup>T</sup>
  - $result_{ij} = a_i b_i$

$$\begin{bmatrix} a_1 \\ a_2 \\ \dots \\ a_n \end{bmatrix} [b_1 \ b_2 \ \dots b_m] = \begin{bmatrix} a_1b_1 & a_1b_2 & \dots & a_1b_m \\ a_2b_1 & a_2b_2 & \dots & a_2b_m \\ \dots & \dots & \dots & \dots \\ a_nb_1 & a_nb_2 & \dots & a_nb_m \end{bmatrix}$$





**Eigenvectors and Eigenvalues** 



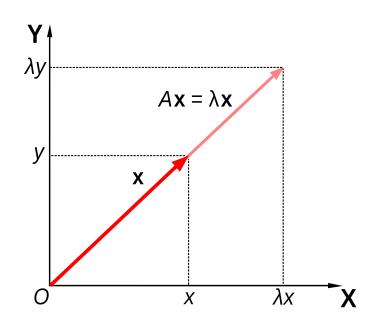


Figure source: https://en.wikipedia.org/wiki/Eigenvalues\_and\_eigenvectors



**Matrix Decomposition** 

 Matrix decomposition is highly used in solving problems in linear algebra

<b>Matrix Decomposition</b>	How to Calculate with NumPy
Cholesky decomposition	linalg.cholesky(A)
QR factorization	np.linalg.qr(A)
Singular Value Decomposition	linalg.svd(a)





Solving a linear system of equations

$$a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = b_1,$$
  
 $a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n = b_2,$   
 $\dots$   
 $a_{n1}x_1 + a_{22}x_2 + \dots + a_{nn}x_n = b_n,$ 

which can be rewritten in matrix form as:

$$ax = b$$
,

We can use np.linalg.solve(a,b), e.g.:

We can verify the solution by checking whether AX=B:

```
>>> np.inner(A, X)
array([3., 4.])
```



# Why Use NumPy?

- We can implement all functionalities of NumPy using Python datatypes and functions.
- E.g. matrix multiplication is just an iteration over the elements of two arrays.
- However, all such NumPy operations are implemented in C. Therefore, they are faster.

~1000 times difference in speed!

```
import numpy as np
from time import time
def matmul 2D(M, N):
  """Custom defined matrix multiplication for two 2D matrices M and N"""
  (H M, W M) = M.shape
  (H_N, W_N) = N.shape
  if W M != H N:
    print("Dimensions of M and N mismatch!")
    return None
  result = np.zeros((H M, W N))
  for i in range(H M):
    for j in range(W N):
     for k in range(W M):
       result[i][j] += M[i][k] * N[k][j]
  return result
27 # Now let us measure the running-time performances
28 # Create two 2D large matrices
29 M = np.random.randn(100, 100)
30 N = np.random.randn(100, 100)
31
32 # Option 1: Use NumPy's matrix multiplication
33 t1 = time()
34 result = np.matmul(M, N)
35 t2 = time()
36 print("NumPy's matmul took ", t2-t1, "ms.")
38 # Option 2: Use our matmul 2D function
39 t1 = time()
40 result = matmul 2D(M, N)
41 t2 = time()
42 print("Our matmul 2D function took ", t2-t1, "ms.")
Our matmul 2D result:
 [[1.44819064 2.44425364 3.19640633 0.98131108]
 [1.91135161 2.66745824 4.09341735 1.37928184]]
Correct result:
 [[1.44819064 2.44425364 3.19640633 0.98131108]
 [1.91135161 2.66745824 4.09341735 1.37928184]]
NumPy's matmul took 0.008047342300415039 ms.
Our matmul 2D function took 1.2613885402679443 ms.
```









#### Outline



- Overview
- Installation
- Modules



#### Overview



- A library for Scientific Computing.
  - Clustering, Fourier Transforms, Integration & differential equation solving, Linear Algebra, Optimization, Image processing ...

It is closely linked with NumPy so much that NumPy needs to be imported first to be able to use SciPy.



#### Installation



On your Linux environment:

\$ pip install scipy

or

\$ conda install scipy

- On Windows/Mac: install anaconda first
- On Colab, it is already installed



#### Modules



Module	Description
cluster	Clustering algorithms
constants	Physical and mathematical constants
fftpack	Fast Fourier Transform routines
integrate	Integration and ordinary differential equation solvers
interpolate	Interpolation and smoothing splines
io	Input and Output
linalg	Linear algebra
ndimage	N-dimensional image processing
odr	Orthogonal distance regression
optimize	Optimization and root-finding routines
signal	Signal processing
sparse	Sparse matrices and associated routines
spatial	Spatial data structures and algorithms
special	Special functions
stats	Statistical distributions and functions

#### Examples

#### From the book:

"Define functions that work like the sum, mean, min and max operations provided by NumPy. These functions should take a single 2D array and return the result as a number. You can assume that the operation applies to the whole array and not to a single axis."



### Final Words: Important Concepts

- NumPy arrays and their properties: array shape, dimensions, sizes, elements.
- Accessing and modifying elements of a NumPy array.
- Simple algebraic functions on NumPy arrays.
- SciPy and its basic capabilities.



## THAT'S ALL FOLKS! STAY HEALTHY