



Data Science Lab

Numpy: Numerical Python

Andrea Pasini Flavio Giobergia Elena Baralis

DataBase and Data Mining Group







- Numpy (Numerical Python)
 - Store and operate on dense data buffers
 - Efficient storage and operations
- Features
 - Multidimensional arrays
 - Slicing/indexing
 - Math and logic operations
- Applications
 - Computation with vectors and matrices
 - Provides fundamental Python objects for data science algorithms
 - Internally used by scikit-learn and SciPy







Summary

- Numpy and computation efficiency
- Numpy arrays
- Computation with Numpy arrays
 - Broadcasting
- Accessing Numpy arrays
- Working with arrays, other functionalities







- array is the main object provided by Numpy
- Characteristics
 - Fixed Type
 - All its elements have the same type
 - Multidimensional
 - Allows representing vectors, matrices and n-dimensional arrays







- Numpy arrays vs Python lists:
 - Also Python lists allow defining multidimensional arrays
 - E.g. my_2d_list = [[3.2, 4.0], [2.4, 6.2]]
- Numpy advantages:
 - Higher flexibility of indexing methods and operations
 - Higher efficiency of operations



Python lists vs NumPy



 "Build two randomly initialized NxN matrices A and B, then add them element-wise and place the output in C"

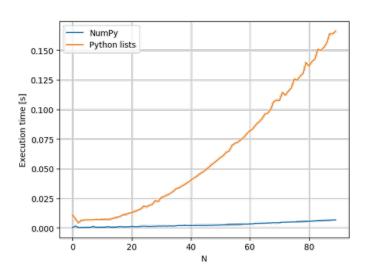
Python lists

```
from random import random
def build_random_matrix(n):
    mat = []
    for i in range(n):
        row = []
        for j in range(n):
            row.append(random())
        mat.append(row)
    return mat
n = 100
A = build random matrix(n)
B = build random matrix(n)
C = [1]
for i in range(n):
    row = []
    for j in range(n):
        row.append(A[i][j] + B[i][j])
    C.append(row)
```

NumPy

```
import numpy as np

n = 100
A = np.random.random((n, n))
B = np.random.random((n, n))
C = A + B
```

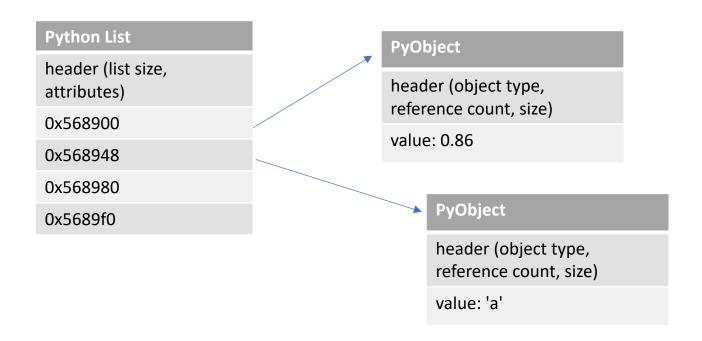








- Since lists can contain heterogeneous data types,
 they keep overhead information
 - E.g. my_heterog_list = [0.86, 'a', 'b', 4]

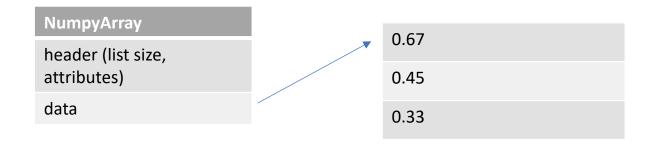








- Characteristics of numpy arrays
 - Fixed-type (no overhead)
 - Contiguous memory addresses (faster indexing)
 - E.g. $my_numpy_array = np.array([0.67, 0.45, 0.33])$









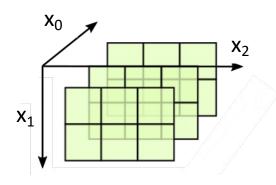
- Numpy data types
 - Numpy defines its own data types
 - Numerical types
 - int8, int16, int32, int64
 - uint8, ..., uint64
 - float16, float32, float64
 - Boolean values
 - bool







- Collections of elements organized along an arbitrary number of dimensions
- Multidimensional arrays can be represented with
 - Python lists
 - Numpy arrays









Multidimensional arrays with Python lists

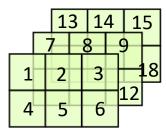
Examples:

vector

2D matrix

1	2	3
4	5	6

3D array

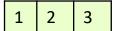


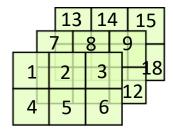






- Multidimensional arrays with Numpy
 - Can be directly created from Python lists
 - Examples:





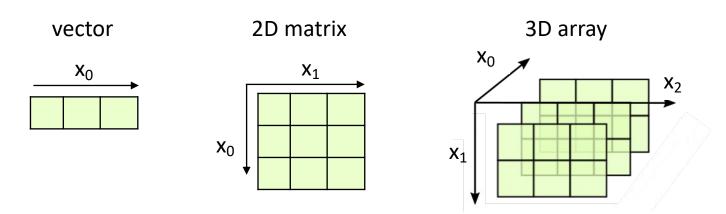
```
import numpy as np
arr1 = np.array([1, 2, 3])
```







- Multidimensional arrays with Numpy
 - Characterized by a set of axes and a shape
 - The axes of an array define its dimensions
 - a (row) vector has 1 axis (1 dimension)
 - a 2D matrix has 2 axes (2 dimensions)
 - a ND array has N axes

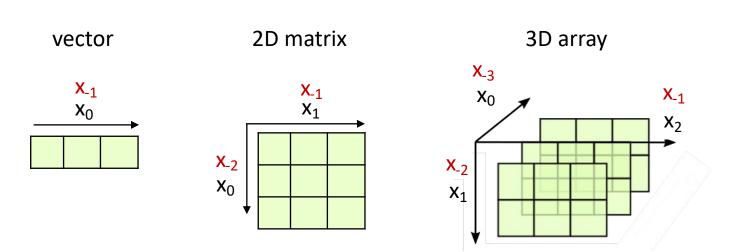








- Multidimensional arrays with Numpy
 - Axes can be numbered with negative values
 - Axis -1 is always along the row

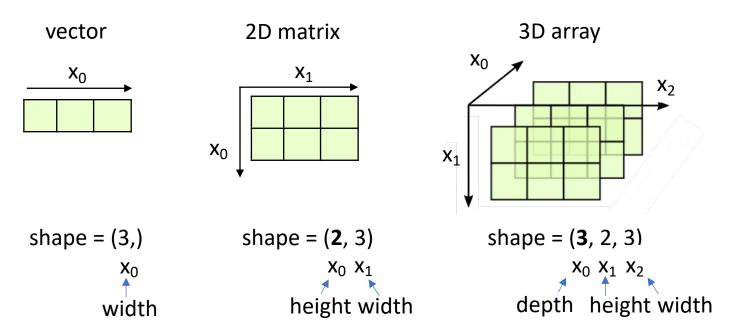








- Multidimensional arrays with Numpy
 - The shape of a Numpy array is a tuple that specifies the number of elements along each axis
 - Examples:









Column vector vs row vector

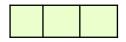
e.g. np.array([[0.1], [0.2], [0.3]])

[0.1] [0.2] [0.3]

shape = (3, 1)

Column vector is a 2D matrix!

e.g. np.array([0.1, 0.2, 0.3])



shape = (3,)







- Creation from list:
 - np.array(my_list, dtype=np.float16)
 - Data type inferred if not specified
- Creation from scratch:
 - np.zeros(shape)
 - Array with all O of the given shape
 - np.ones(shape)
 - Array with all 1 of the given shape
 - np.full(shape, value)
 - Array with all elements to the specified value, with the specified shape







Creation from scratch: examples









Creation from scratch:



- np.linspace(start, stop, num)
 - Generates num samples from start to stop (included)
 - np.linspace(0,1,11) \rightarrow [0.0, 0.1, ..., 1.0]
- np.arange(start, stop, step)
 - Generates numbers from start to stop (excluded), with step step
 - np.arange(1, 7, 2) \rightarrow [1, 3, 5]
- np.random.normal(mean, std, shape)
 - Generates random data with normal distribution
- np.random.random(shape)
 - Random data uniformly distributed in [0, 1]











- Consider the array
 - x = np.array([[2, 3, 4], [5, 6, 7]])
- x.ndim: number of dimensions of the array
 - Out: 2
- x.shape: tuple with the array shape
 - Out: (2,3)
- x.size: array size (product of the shape values)
 - Out: 2*3=6







Summary:

- Universal functions (Ufuncs):
 - Binary operations (+,-,*,...)
 - Unary operations (exp(),abs(),...)
- Aggregate functions
- Sorting
- Algebraic operations (dot product, inner product)







- Universal functions (Ufuncs): element-wise operations
 - Binary operations with arrays of the same shape
 - +, -, *, /, % (modulus), // (floor division), **
 (exponentiation)







Example:

```
In [1]: x=np.array([[1,1],[2,2]])
    y=np.array([[3, 4],[6, 5]])
    x*y
```







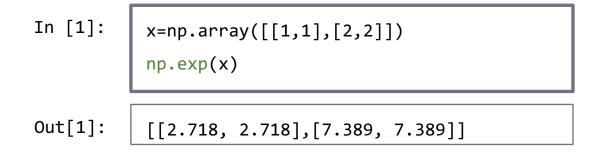
- Universal functions (Ufuncs):
 - Unary operations
 - np.abs(x)
 - np.exp(x), np.log(x), np.log2(x), np.log10(x)
 - np.sin(x), cos(x), tan(x), arctan(x), ...
 - They apply the operation separately to each element of the array

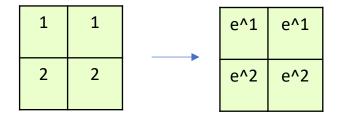






Example:





Note: original array (x) is not modified







Aggregate functions

- Return a single value from an array
 - np.min(x), np.max(x), np.mean(x), np.std(x), np.sum(x)
 - \blacksquare np.argmin(x), np.argmax(x)
- Or equivalently:
 - x.min(), x.max() x.mean(), x.std(), x.sum()
 - x.argmin(), x.argmax()
- Example

```
In [1]: x=np.array([[1,1],[2,2]])
    x.sum()
```

Out[1]: 6



np.argmin(), np.argmax()





For 1-dimensional array x → position of the smallest/largest element of x

```
x = np.array([5, 3, 9, 0, 7])
x.argmin()
```

- For N-dimensional array x → position of the smallest/largest element of the *flattened* version of x
 - Flattened = collapsed into one dimension, x.flatten()

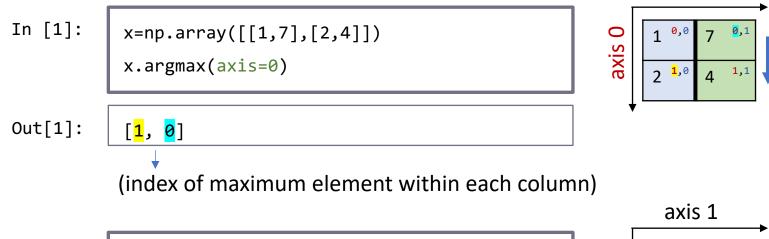


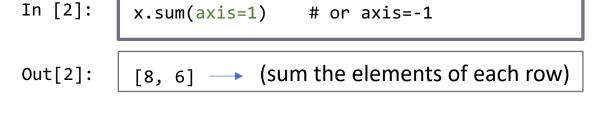


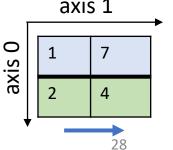


Aggregate functions along axis

- Allow specifying the axis along with performing the operation
- Examples







axis 1

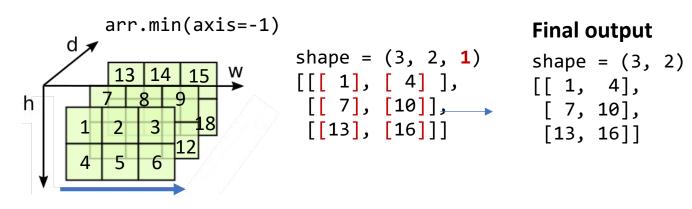


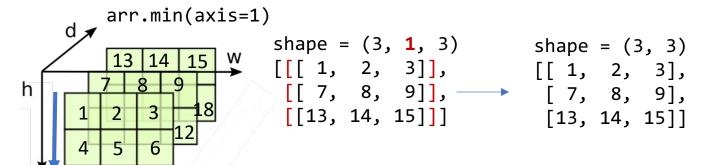




Aggregate functions along axis

The aggregation dimension is removed from the output











Sorting

- np.sort(x): creates a sorted copy of x
 - x is not modified
- x.sort(): sorts x inplace (x is modified)

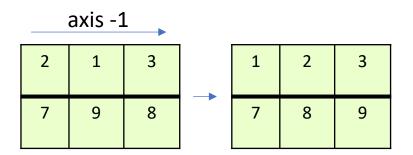






Sorting

Array is sorted along the last axis (-1) by default









Sorting

Allows specifying the axis being sorted

Out[1]: [[2,2,1], [7,7,3]]

axis 0		2	7	3	→	2	2	1
	,	7	2	1		7	7	3

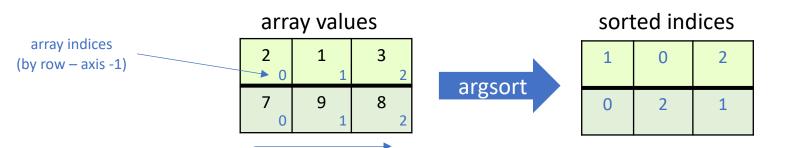






Sorting

np.argsort(x): return the position of the indices of the sorted array (sorts by default on axis -1)









Algebraic operations

- np.dot(x, y)
 - inner product if x and y are two 1-D arrays

Out[1]: 7







Algebraic operations

- np.dot(x, y)
 - matrix multiplied by vector

```
In [1]: x=np.array([[1,1],[2,2]])
    y=np.array([2, 3]) # works even if y is a row vector
    np.dot(x, y)
```

Out[1]: [5, 10] # result is a **row** vector







Algebraic operations

- np.dot(x, y)
 - matrix multiplied by matrix

```
In [1]: x=np.array([[1,1],[2,2]])
    y=np.array([[2,2],[1,1]])
    np.dot(x, y)
```

Out[1]: [[3,3],[6,6]]



Notebook Examples

- 2-Numpy Examples.ipynb
 - 1) Computation with arrays









Pattern designed to perform operations between arrays with different shape

c)
$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$$
 + $\begin{bmatrix} [1] \\ [2] \end{bmatrix}$ $\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$ + $\begin{bmatrix} 1 & 1 \\ 2 & 2 \end{bmatrix}$







- Rules of broadcasting
 - 1. The shape of the array with **fewer dimensions** is **padded** with <u>leading</u> ones

x.shape =
$$(2, 3)$$
, y.shape = (3) y.shape = $(1, 3)$

If the shape along a dimension is 1 for one of the arrays and >1 for the other, the array with shape = 1 in that dimension is stretched to match the other array



x.shape =
$$(2, 3)$$
, y.shape = $(1, 3) \rightarrow \text{stretch}$: y.shape = $(2, 3)$

 If there is a dimension where both arrays have shape >1 and those shapes differ, then broadcasting cannot be performed







Example: compute x + y

$$x = np.array([1, 2, 3])$$

$$z = x + y$$

y.shape =
$$(3,1)$$

[13]

x.shape =
$$(1,3)$$

y.shape =
$$(3,1)$$

- Apply Rule 1
 - x.shape becomes (1, 3): x=[[1,2,3]]
- Apply Rule 2:
 - extend x on the vertical axis, y on the horizontal one

1	2	3		11	11	11		12	13	14
1	2	3	+	12	12	12	=	13	14	15
1	2	3		13	13	13		14	15	16







Example: compute x + y

-
$$x = np.array([[1, 2],[3,4],[5,6]])$$

$$y = np.array([11, 12, 13])$$

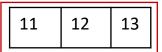
$$z = x + y$$

- Apply Rule 1
 - y.shape becomes (1, 3): y=[[11,12,13]]
- Apply Rule 3
 - shapes (3, 2) and (1, 3) are incompatibles
 - Numpy will raise an exception

	•	•		•
v cha	no -	12	١	

x.shape = (3, 2)

y.shape =
$$(3,)$$



1	2
3	4
5	6



Notebook Examples

- 2-Numpy Examples.ipynb
 - 2) Broadcasting: dataset normalization









- Numpy arrays can be accessed in many ways
 - Simple indexing
 - Slicing
 - Masking
 - Fancy indexing
 - Combined indexing
- Slicing provides views on the considered array
 - Views allow reading and writing data on the original array
- Masking and fancy indexing provide copies of the array







Simple indexing: read/write access to element



```
x[i, j, k, ... ]
```



```
Out[1]: el = 7
```







- Simple indexing: returning elements from the end
- Consider the array
 - x = np.array([[2, 3, 4], [5,6,7]])
- x[0, -1]
 - Get last element of the first row: 4
- x[0, -2]
 - Get second element from the end of the first row: 3







- Slicing: access contiguous elements
 - x[start:stop:step, ...]
 - Creates a view of the elements from start (included) to stop (excluded), taken with fixed step
 - Updates on the view yield updates on the original array
 - Useful shortcuts:
 - omit start if you want to start from the beginning of the array
 - omit stop if you want to slice until the end
 - omit step if you don't want to skip elements







Slicing: access contiguous elements

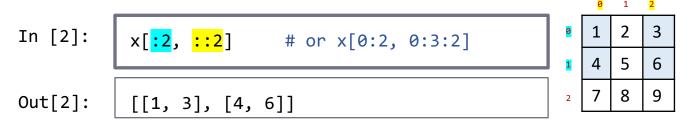


Select all rows and the last 2 columns:

In [1]:
$$x = \text{np.array}([[1,2,3],[4,5,6],[7,8,9]])$$
 $x[:, 1:]$ # or $x[0:3, 1:3]$ 4 5 6 7 8 9

Out[1]: $[[2,3],[5,6],[8,9]]$

Select the first two rows and the first and third columns









Update a sliced array



```
In [1]: x = np.array([[1,2,3],[4,5,6],[7,8,9]])
x[:, 1:] = 0
print(x)
```

Out[1]: [[1,0,0], [4,0,0], [7,0,0]]







Update a view



- To avoid updating the original array use .copy()
 - x1=x[:,1:].copy()







- Masking: use boolean masks to select elements
 - x[mask]
 - mask
 - boolean numpy array that specifies which elements should be selected (select if True)
 - same shape as the original array
 - The result is a one-dimensional vector that is a copy of the original array elements selected by the mask







Mask creation

- x op value (e.g x==4)
- where op can be >, >=, <, <=, ==, !=</p>

Examples

```
In [1]: x = np.array([1.2, 4.1, 1.5, 4.5])
x > 4
```

Out[1]: [False, True, False, True]

In [2]: x2 = np.array([[1.2, 4.1], [1.5, 4.5]])
x2 >= 4

Out[2]: [[False, True], [False, True]]









Operations with masks (boolean arrays)

- Numpy allows boolean operations between masks with the same shape (bitwise operators)
 - & (and), | (or), ^ (xor), ~ (negation)
- Example
 - mask = \sim ((x < 1) | (x > 5)) \Leftrightarrow ((x >= 1) & (x <= 5))
 - elements that are between 1 and 5 (included)







Masking examples



Even if the shape of x2 is (2, 2), the result is **a one-dimensional** array containing the elements that satisfy the condition







Update a masked array



Out[1]: [1.2, 0, 1.5, 0]







Masking does not create views, but copies



```
Out[2]: [1.2, 4.1, 1.5, 4.5]
```







- Fancy indexing: specify the index of elements to be selected
 - Example: select elements from 1-dimensional array

```
x[1] x[3]

In [1]: x = np.array([7.0, 9.0, 6.0, 5.0])
x[[1, 3]]

Out[1]: [9.0, 5.0]
```







Fancy indexing: selection of rows from a 2dimensional array







- Fancy indexing: selection of elements with coordinates
 - Result contains a 1-dimensional array with selected elements

```
In [1]: x = np.array([[0.0, 1.0, 2.0], [3.0, 4.0, 5.0], [6.0, 7.0, 8.0]])

x[[1, 2], [0, 2]] \longrightarrow [1, 0] (indices being selected)
```

Out[1]: [3.0, 8.0]







Similarly to masking, fancy indexing provides
 copies (not views) of the original array

```
In [1]:
         x = np.array([1.2, 4.1, 1.5, 4.5])
          x[[1, 3]] = 0 # Assignment is allowed
          Χ
Out[1]:
         [1.2, 0, 1.5, 0]
In [2]:
         x = np.array([1.2, 4.1, 1.5, 4.5])
          sel = x[[1, 3]] # sel is a copy of x
          sel[:] = 0  # Assignment does not affect x
          Χ
Out[2]:
          [1.2, 4.1, 1.5, 4.5]
```







Combined indexing:

- Allows mixing the indexing types described so far
- Important rule:
 - The number of dimensions of selected data is:
 - The same as the input if you mix:
 - masking+slicing, fancy+slicing
 - Reduced by one for each axis where simple indexing is used
 - Because simple indexing takes only 1 single element from an axis







- Combined indexing: masking+slicing, fancy+slicing
 - Output has the same numer of dimensions as input

```
x = np.array([[0.0, 1.0, 2.0], [3.0, 4.0, 5.0], [6.0, 7.0, 8.0]])
```

```
x[[True,False,True], 1:]
# Masking + Slicing: [[1.0,2.0],[7.0,8.0]]
```

0.0	1.0	2.0
3.0	4.0	5.0
6.0	7.0	8.0

```
x[[0,2], :2]
# Fancy + Slicing: [[0.0,1.0],[6.0,7.0]]
```

0.0	1.0	2.0
3.0	4.0	5.0
6.0	7.0	8.0







- Combined indexing: simple+slicing, simple+masking
 - Simple indexing reduces the number of dimensions

```
x = np.array([[0.0, 1.0, 2.0], [3.0, 4.0, 5.0], [6.0, 7.0, 8.0]])
```

```
x[0, 1:]
# Simple + Slicing: [1.0, 2.0]
```

0.0	1.0	2.0
3.0	4.0	5.0
6.0	7.0	8.0

```
x[[True, False, True], 0]
# Simple + Masking: [0.0, 6.0]
```

0.0	1.0	2.0
3.0	4.0	5.0
6.0	7.0	8.0

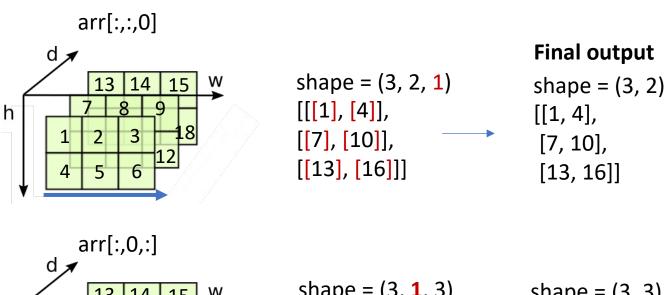


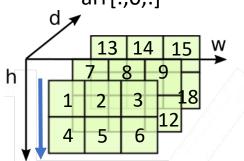




Simple indexing + slicing

 The dimension selected with simple indexing is removed from the output





```
shape = (3, 1, 3) shape = (3, 3) 
[[[1,2,3]], [[1, 2, 3], [7, 8, 9], [7, 8, 9], [13, 14, 15]]
```



Notebook Examples

- 2-Numpy Examples.ipynb
 - 3) Accessing Numpy Arrays









Summary:

- Array concatenation
- Array splitting
- Array reshaping
- Adding new dimensions







- Array concatenation along existing axis
 - The result has the same number of dimensions of the input arrays

```
In [1]:     x = np.array([[1,2,3],[4,5,6]])
     y = np.array([[11,12,13],[14,15,16]])
     np.concatenate((x, y))  # Default axis: 0
```

```
Out[1]: [[1,2,3],[4,5,6],[11,12,13],[14,15,16]]
```

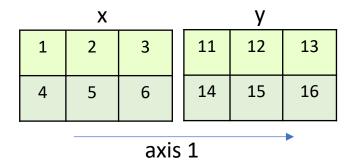






Array concatenation along existing axis

Concatenation along rows (axis=1)



```
In [1]: x = np.array([[1,2,3],[4,5,6]])
y = np.array([[11,12,13],[14,15,16]])
np.concatenate((x, y), axis=1)
```

Out[1]: [[1,2,3,11,12,13],[4,5,6,14,15,16]]

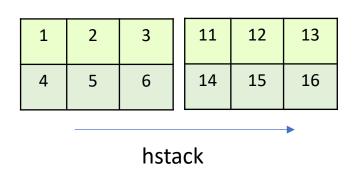


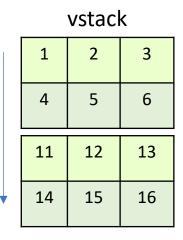




Array concatenation: hstack, vstack

Similar to np.concatenate()





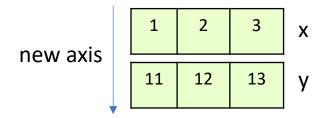






Array concatenation: hstack, vstack

vstack allows concatenating 1-D vectors along new axis (not possible with np.concatenate)









Splitting arrays (split, hsplit, vsplit)

- np.split(arr, N, axis=0)
 - outputs a list of Numpy arrays
 - If N is integer: divide arr into N equal arrays (along axis), if possible!
 - if N is a 1d array: specify the entries where the array is split (along axis)

```
x index 0 1 2 3 4 5 values 7 7 9 9 8 8
```

Out[1]: [array([7, 7]), array([9, 9]), array([8, 8])]

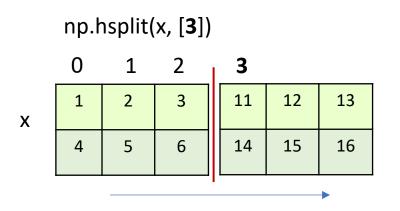


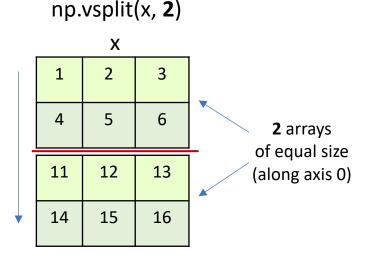




Splitting arrays (split, hsplit, vsplit)

- hsplit, vsplit with 2D arrays
 - return a list with the arrays after the split





In both examples output is:

Out: [array([[1,2,3],[4,5,6]]), array([[11,12,13],[14,15,16]])]







Reshaping arrays

0	1	2
3	4	5

y is filled following the index order:

$$y[0,0] = x[0], y[0,1] = x[1], y[0,2] = x[2]$$

$$y[1,0] = x[3], y[1,1] = x[4], y[1,2] = x[5]$$

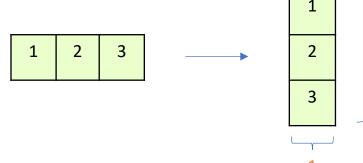






Reshaping arrays

- At most one dimension can be -1 ("unknown")
- If present, the size is inferred from
 - The source array
 - The other dimensions



The first dimension (rows) is inferred to be 3, considering that the second dimension (columns) is 1 and x.size = 3

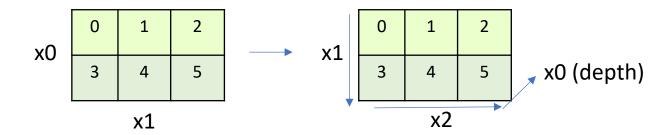






Adding new dimensions

np.newaxis adds a new dimension with shape=1 at the specified position









Adding new dimensions

- Application: row vector to column vector
 - Alternative approach to .reshape(-1,1)