09 – Arrays

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Scientific Programming in Python (2026)

https://atticlectures.net/scipro/python-2026/

Modules

- Declarations (e.g functions) in a separate file
- Better **code structuring**
- Accessible in many scripts/notebooks (reusability)
- Module must be imported before first use

```
import numpy
```

- Content is accessed by prefix notation

```
module.content
```

```
grid = numpy.linspace(-1, 1, 3)
grid
array([-1.,  0.,  1.])
```

- Module name prefix can be changed at import

```
import numpy as np
grid = np.linspace(-1, 1, 3)
```

- If only a few entities are needed, they can be **imported directly** and used without prefix

```
from numpy import linspace
linspace(-1, 1, 3)
```

- Importing all entities from a module directly is possible, but discouraged

```
from numpy import *
```

Python modules, SciPy stack

Python Standard Library

- Bundled with the Python interpreter
- **Python Standard Library documentation**

Third party modules

- Not part of the official Standard Library
- Must be installed additionally to the Python interpreter (Conda, PyPI, packages)

SciPy stack

- *De facto* standard mathematical / statistical / scientific (third party) modules

Numpy: arrays & basic numerical routines
https://docs.scipy.org/doc/numpy/

Scipy: additional mathematical routines https://docs.scipy.org/doc/scipy/

Matplotlib: powerful graphical plotting routines
https://matplotlib.org/stable/users/index.html

Pandas: data analysis toolkit
http://pandas.pydata.org/pandas-docs/stable/

SymPy: symbolic mathematics
http://docs.sympy.org/latest/index.html

```
conda install numpy scipy matplotlib pandas sympy
```

Arrays

Array = Multi-dimensional storage of elements with the same type (matrix)

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

```
[1 2 3]
```

```
bb = np.array([[1, 2, 3], [4, 5, 6]])
print(bb)
```

```
[[1 2 3]
 [4 5 6]]
```

Advantages (compared to lists)

- Elements are stored sequentially in memory
  → Fast access
  (assuming the right access pattern)
- Optimized functions for array manipulation can speed up algorithm by orders of magnitude

Disadvantages (compared to lists)

- All elements must have the same type
- All strides in a multi-dimensional array must have the same length

Creating arrays

numpy.array(*expression*, dtype=*type*)

Creates an array of given type and storage order from an expression

```
np.array([1.0, 2.0], dtype=float)
```

→

```
[ 1.  2.]
```

numpy.empty(*shape*, dtype=*type*)

numpy.zeros(*shape*, dtype=*type*)

numpy.ones(*shape*, dtype=*type*)

Array with uninitialized elements / zeros / ones of given shape, type (and storage order)

```
np.ones((2, 3), dtype=float)
```

```
[[ 1.  1.  1.]
 [ 1.  1.  1.]]
```

- Data type: either intrinsic type (int, float, etc.) or numpy provided one (np.float32, np.float64, etc.)
- Storage order: C or Fortran (row-major / column-major)

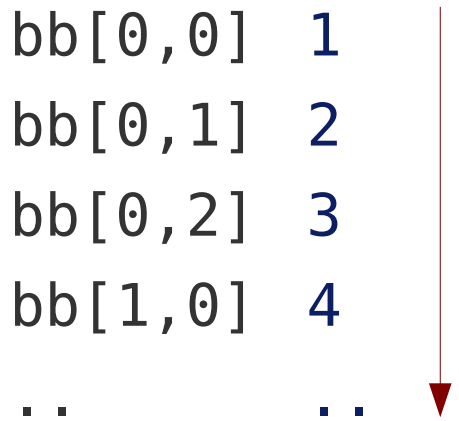
Element storage ordering

- Default is **row-major** storage(like in C):
  first index grows slowest, last index grows fastest:

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

C-storage

Memory



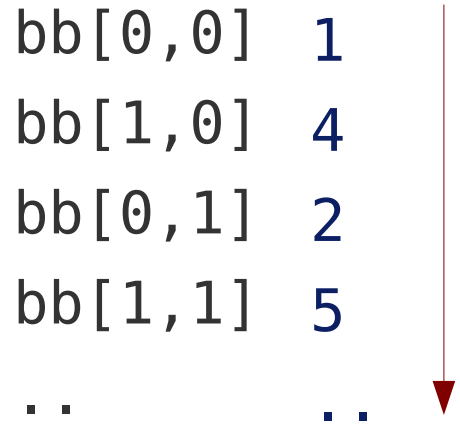
- Array manipulation is fastest, if elements are accessed in the same sequence as stored in memory (**cache coherence**)

- Optionally, **column-major** storage format (like in Fortran)
  first index grows fastest, last index grows slowest:

```
bb = np.array([[1, 2, 3], [4, 5, 6]], order='F')
```

F-storage

Memory



Querying size and shape

- Object variable **size** contains the total **number of elements in the array**

```
bb = np.array([[1, 2, 3], [4, 5, 6]])
bb.size
```

```
6
```

- Object variable **shape** contains a tuple with **number of elements along each axis**

```
bb.shape
```

```
(2, 3)
```

- Array **shape can be changed**, provided size remains constant
- Order of elements in the memory remains unchanged

```
bb.shape = (3, 2)
bb
```

```
[[1 2]
 [3 4]
 [5 6]]
```

Array element access

- Elements accessed as with nested lists
- First element indexed by 0
- Indices for multidimensional arrays collected to **index tuple**

```
bb = np.array([[1, 2, 3],
               [4, 5, 6],
               [7, 8, 9])
```

`bb[1]`

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

`bb[1, 1]`

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

~~`bb[1][1]`~~

- **Slices** analogously to lists as **[from:to:step]**
- Along arbitrary dimensions / axis

`bb[0,:]`

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

`bb[:,0]`

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

`bb[0:3:2, 0:2]`

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

Modifying arrays

- Arrays are **mutable**, be aware of side effects

```
aa = np.array([1, 2, 3])
bb = aa
```

```
bb is aa
```
→ True

```
bb[0] = -1
```

```
aa
```
→ [-1 2 3]

- Arrays slices are pointers/views, no true copies

```
aa = np.array([1, 2, 3])
bb = aa[0:2]
```

```
bb
```
→ [1 2]

```
bb[0] = -1
```

```
aa
```
→ [-1 2 3]

- True **copy** can be enforced via **array()**

```
aa = np.array([1, 2, 3])
bb = np.array(aa)
```

```
bb is aa
```
→ False

```
bb[0] = -1
```

```
aa
```
→ [1 2 3]

- True **copy** can be enforced via **array()**

```
aa = np.array([1, 2, 3])
bb = np.array(aa[0:2])
```

```
bb
```
→ [1 2]

```
bb[0] = -1
```

```
aa
```
→ [1 2 3]

Scalar operations with arrays

Arithmetic / logical operators

- Operations applied elementwise
- One of the operands must be either a scalar or operands must have identical shapes*
- Result has same shape as operand(s)

```
aa = np.array([1, 2, 3])
bb = np.array([5, 4, 3])
```

```
aa * bb
```
```
[5 8 9]
```

```
2.0 * aa
```
```
[2. 4. 6.]
```

```
aa**2
```
```
[1 4 9]
```

```
aa == bb
```
```
[False False True]
```

```
aa < bb
```
```
[True True False]
```

* or shapes which can be made identical via **broadcasting**

Universal functions (ufuncs)

- Scalar functions applicable on arrays
- Ufuncs are applied elementwise
- Result has same shape as argument

```
aa = np.array([0.0, np.pi / 2,
               -np.pi / 2])
np.sin(aa)
```

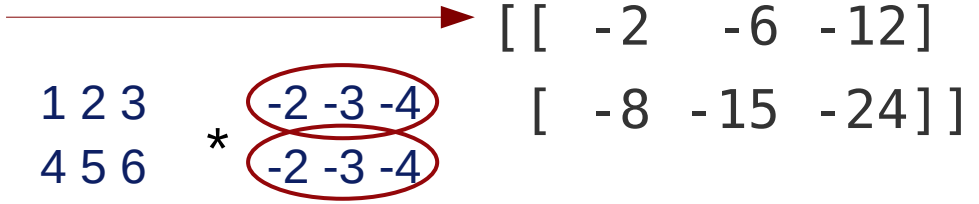
```
[0.0000e+00 1.0000e+00-1.0000e+00]
```

- Numpy module contains many useful ufuncs
  - Square root function (**sqrt**)
  - Trigonometric functions (**sin**, **cos**, …)
  - Rounding functions (**floor**, **ceil**, …)
  - etc.

Broadcasting

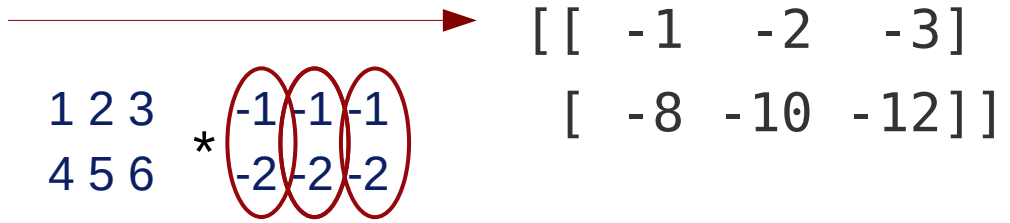
- If arrays in binary operators have different number of dimensions, numpy tries to **extend the one with less dimensions** by broadcasting:
  - **Extra dimensions inserted** before existing one(s), to equal number of dimensions
  - Array **repeated** along new dimensions to match correct shape
  - Shapes must be compatible!

```
aa = np.array([[1, 2, 3], [4, 5, 6]])
bb = np.array([-2, -3, -4])
aa * bb
```



- With **numpy.newaxis** **extra dimension(s)** can be **inserted at arbitrary position**

```
cc = np.array([-1, -2])
aa * cc[:,np.newaxis]
```



Matrix multiplication, array reduction

Matrix multiplication

- Arrays can be matrix-multiplied with the @ **operator** (eqivalent with **numpy.matmul()**)

```
aa = np.array([[1, 2], [3, 4]])
bb = np.array([5, 6])
```

```
aa @ bb
```
```
[17 39]
```

```
bb @ aa
```
```
[23 34]
```

```
bb @ bb
```
```
61
```

- **numpy.dot()** does also matrix multiplication
- For arrays with more than 2 dimensions, **numpy.dot()** and **numpy.matmul()** / @ behave differently

Array reduction

- Reduces array to scalar via given operation
- **numpy.sum(), numpy.product(), etc.**

```
vec = np.array([1.0, 2.0, 3.0])
np.sqrt(np.sum(vec**2))
```
→ `3.7416...`

- Reduction can be restricted to selected axis
- Resulting shape as before but without selected/reduced axis

```
aa = np.array([[1, 2], [3, 4]])
np.sum(aa, axis=0)
```

```
[[1, 3],
 [3, 4]]
```
→ `[4 6]`

Iterating over arrays

Arrays behave in iterations **as (nested) lists**:

- Iteration over 1D-array delivers each element
- Iteration over 2D-array delivers the rows of the 2D-array as 1D-arrays
- :

```
vec = np.array([1, 2, 3])
for ind, elem in enumerate(vec):
    print(f"{ind}: {elem}")
```

→

```
0: 1
1: 2
2: 3
```

```
aa = np.array([[1, 2, 3], [4, 5, 6]])
for ind, row in enumerate(aa):
    print(f"{ind}: {row}")
```

→

```
0: [1 2 3]
1: [4 5 6]
```