

Numpy及其应用

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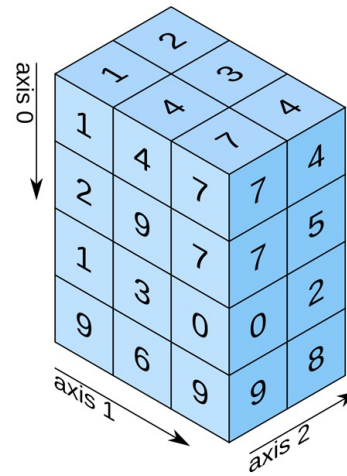


- **NumPy is the fundamental package for scientific computing in Python.**
 - **a multidimensional array object**
 - various derived objects (such as masked arrays and matrices)
 - an assortment of routines for fast operations on arrays, including mathematical, logical, shape manipulation, sorting, selecting, I/O, discrete Fourier transforms, basic linear algebra, basic statistical operations, random simulation and much more.



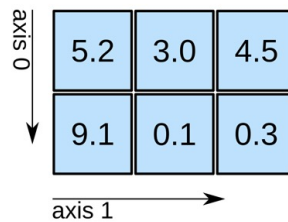
multi-dimensional array

3D array



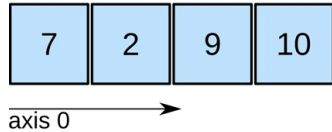
shape: (4, 3, 2)

2D array



shape: (2, 3)

1D array



shape: (4,)

$$\begin{array}{|c|} \hline \text{data} \\ \hline 1 \\ 2 \\ \hline \end{array} - \begin{array}{|c|} \hline \text{ones} \\ \hline 1 \\ 1 \\ \hline \end{array} = \begin{array}{|c|} \hline 0 \\ 1 \\ \hline \end{array}$$

$$\begin{array}{|c|} \hline \text{data} \\ \hline 1 \\ 2 \\ \hline \end{array} * \begin{array}{|c|} \hline \text{data} \\ \hline 1 \\ 2 \\ \hline \end{array} = \begin{array}{|c|} \hline 1 \\ 4 \\ \hline \end{array}$$

$$\begin{array}{|c|} \hline \text{data} \\ \hline 1 \\ 2 \\ \hline \end{array} / \begin{array}{|c|} \hline \text{data} \\ \hline 1 \\ 2 \\ \hline \end{array} = \begin{array}{|c|} \hline 1 \\ 1 \\ \hline \end{array}$$

$$\begin{array}{|c|c|} \hline \text{data} \\ \hline 1 & 2 \\ 3 & 4 \\ 5 & 6 \\ \hline \end{array} .\text{max}() = 6$$

$$\begin{array}{|c|c|} \hline \text{data} \\ \hline 1 & 2 \\ 3 & 4 \\ 5 & 6 \\ \hline \end{array} .\text{min}() = 1$$

$$\begin{array}{|c|c|} \hline \text{data} \\ \hline 1 & 2 \\ 3 & 4 \\ 5 & 6 \\ \hline \end{array} .\text{sum}() = 21$$

https://numpy.org/doc/stable/user/absolute_beginners.html

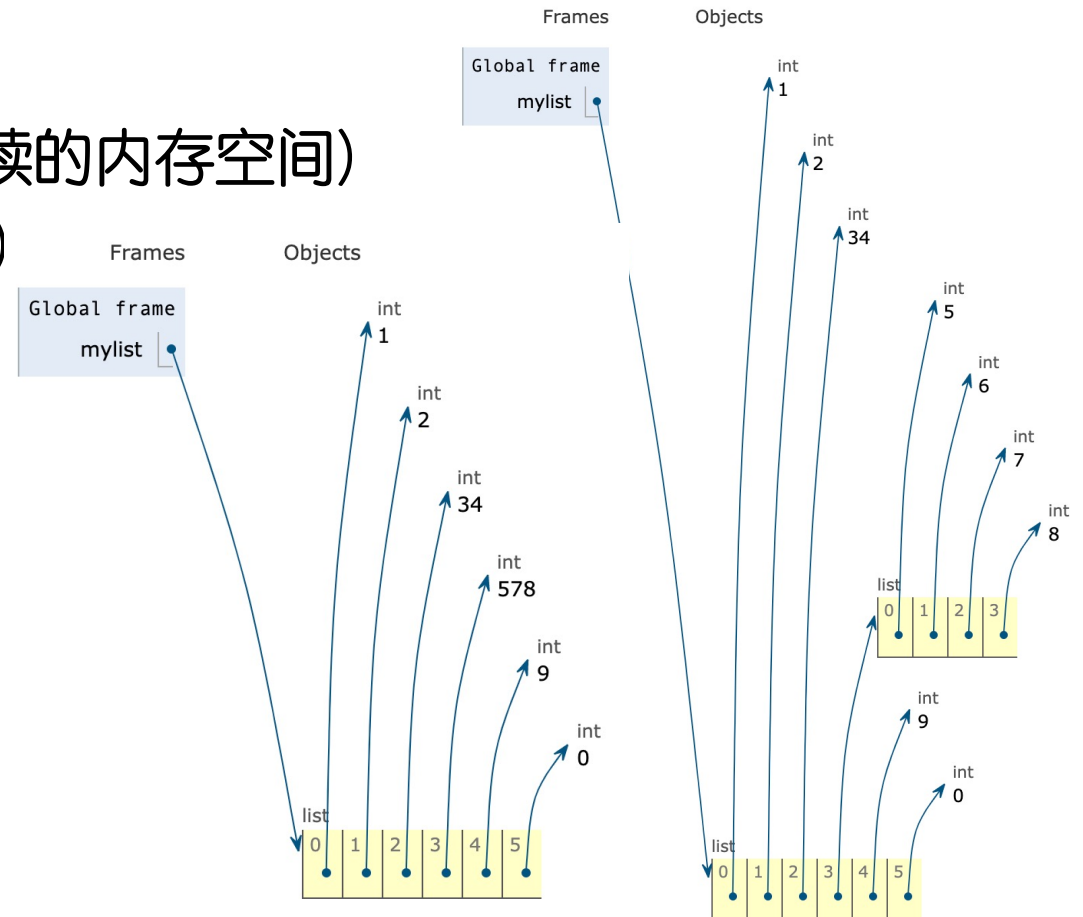
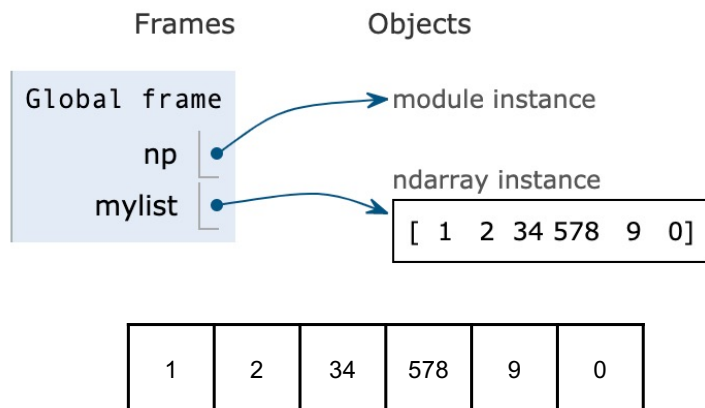


NumPy ndarray v.s. Python List

- 目标：更高的计算效率
- 更高效的数据组织
 - 同类型元素 + 固定长度
- 更高效的计算方式
 - 向量化编程 v.s. 循环
- 实现和底层支持
 - 基于C的实现
 - 利用Basic Linear Algebra Subprograms, BLAS
 - Intel MTK、Open BLAS、CUDA等

NumPy Array v.s. Python List

- 数据组织上的差异
 - 更贴近C的数组实现（连续的内存空间）
 - 同质结构（元素类型相同）



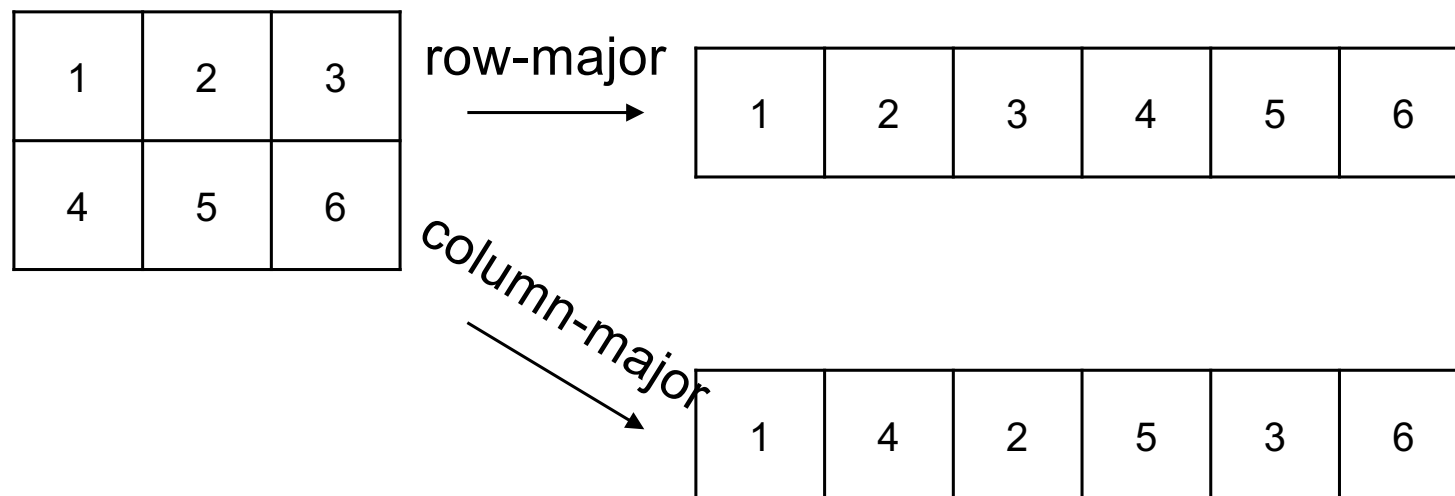
```
mylist = np.array([1, 2, 34, 578, 9 ,0])
```



数组的存储表示

- 行主序 v.s. 列主序

C++:
`int matrix[2][3]`

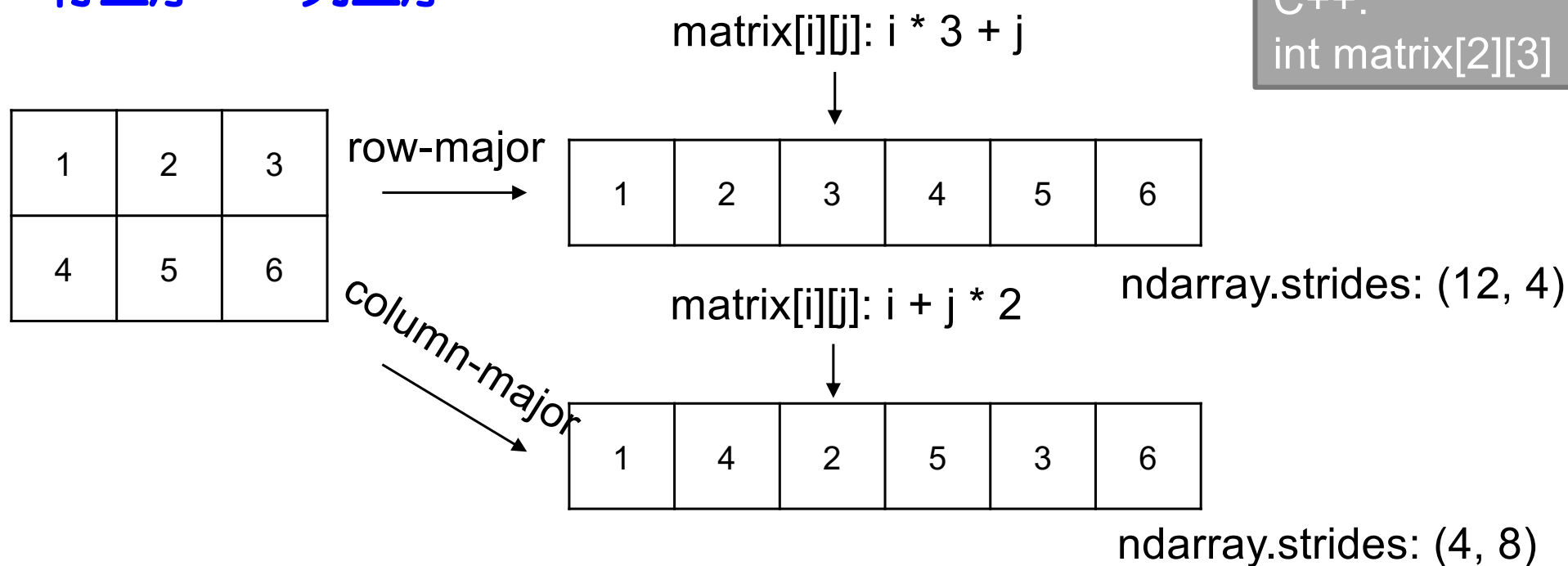


行主序是C等语言的格式，列主序是Fortran等语言的格式 6



数组的存储表示

- 行主序 v.s. 列主序



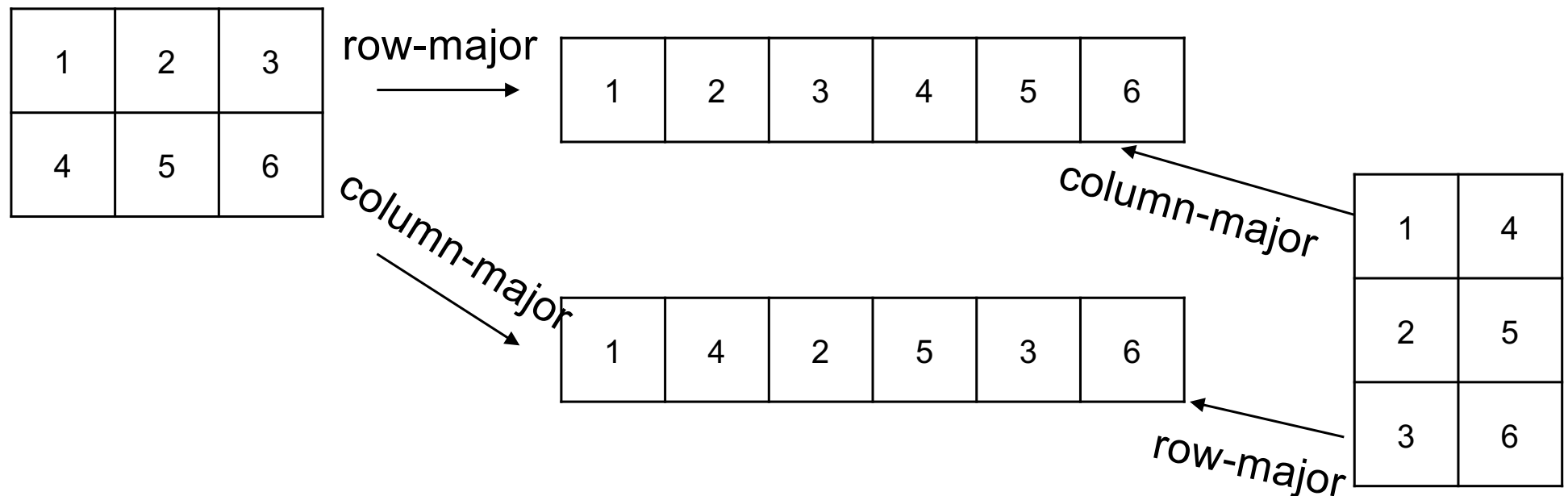
strides: 表示高维数组每一维对应的下标每次偏移时，在一维数组的存储中发生的偏移量(此处假设元素为int32，4个字节)。



数组的存储表示

- 行主序 v.s. 列主序

```
C++:  
int matrix[2][3]
```



不用改变数据表示，仅需要改变访问方式，即可完成转置！



numpy中的转置

`import numpy as np` #默认引用和别名，后续大多省略

```
def print_array(arr):  
    print(arr.dtype)  
    print(arr)  
    print(arr.strides)  
    print()  
myarray = np.array([[1,2,3],[4,5,6]])  
print_array(myarray)
```

```
myarrayT = myarray.T  
print_array(myarrayT)
```

```
myarray2 = np.array([[1,4],[2,5],[3,6]])  
print_array(myarray2)
```

同样的数组，不一样的内部表示！

数组的存储表示



```
C++:  
int matrix[2][3]
```

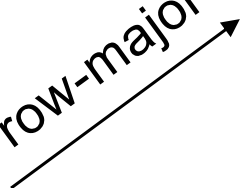
1	2	3
4	5	6

row-major



1	2	3	4	5	6
---	---	---	---	---	---

row-major



1	2
3	4
5	6

同样的内部表示，不一样的外部形式！



numpy中改变数组的形状

```
data = np.arange(1, 7)
print_array(data)

data1 = np.arange(1, 7).reshape((3,2))
print_array(data1)

data2 = np.arange(1, 7).reshape((2,3))
print_array(data2)
```

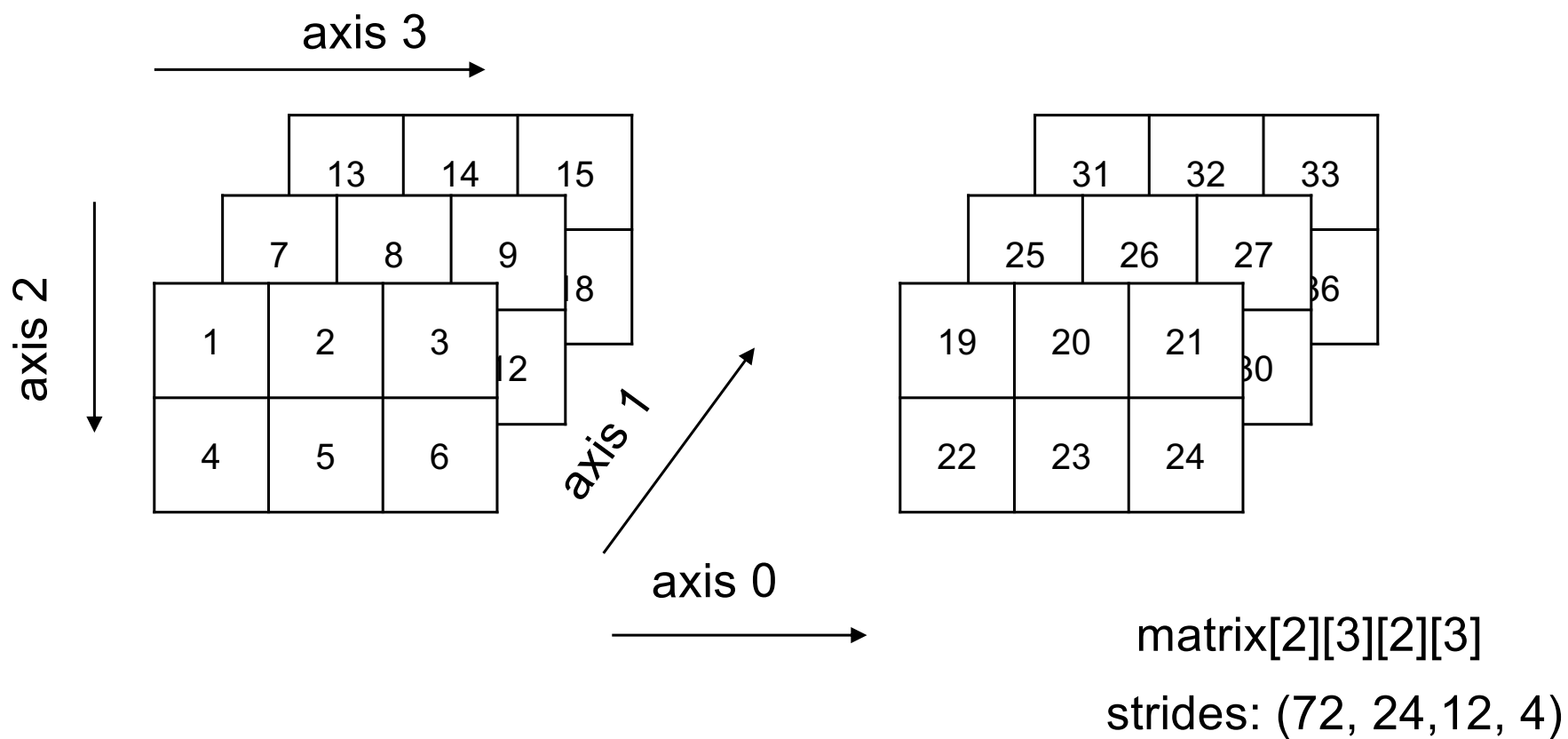
同样的数组，不一样的内部表示！
同样的内部表示，不一样的外部形式！

抽象和封装：数据内部表示 v.s. 数据的外部使用

高维数组



Tensor



```
data = np.arange(1, 19)
print_array(data)

data1 = np.arange(1, 19).reshape((3,2,3))
print_array(data1)

data2 = np.arange(1, 19).reshape((2,3,3))
print_array(data2)
```

试着自己实现一个n维矩阵类，创建任意维度的矩阵，提供元素访问操作、转置操作、reshape操作等功能。



ndarray的基本属性

- **dtype: 元素类型**
- **ndim: 维数**
- **shape: 数组形状**
 - 整数构成的元组, 如: (2, 3), (1, 4)等
 - 向量的形状是元素仅有1个的元组, 须加逗号区分, 如: (3,)
- **size: 所有元素个数**
- **itemsize: 单个元素大小 (bytes)**
- **strides: 访问规则**
- **.....**

Attributes

T : ndarray

Transpose of the array.

data : buffer

The array's elements, in memory.

dtype : dtype object

Describes the format of the elements in the array.

size : int

Number of elements in the array.

itemsize : int

The memory use of each array element in bytes.

ndim : int

The array's number of dimensions.

shape : tuple of ints

Shape of the array.

strides : tuple of ints

The step-size required to move from one element to the next in memory. For example, a contiguous ``(3, 4)`` array of type ``int16`` in C-order has strides ``(8, 2)``. This implies that to move from element to element in memory requires jumps of 2 bytes. To move from row-to-row, one needs to jump 8 bytes at a time ($2 * 4$).

`help(np.ndarray)`
`np.ndarray?`

NDARRAY的创建



ndarray的创建

- 从已有列表创建
 - 使用np.array函数

查阅 `np.array?`

```
array(object, dtype=None, copy=True, order='K', subok=False, ndmin=0)
```

```
In [62]: np.array([1, 2, 3, 4])
```

```
Out[62]: array([1, 2, 3, 4])
```

```
In [63]: a1 = np.array([1, 2, 3, 4])
```

```
Out[63]: a2 = np.array(a1, order = 'F', ndmin = 2)
```



ndarray的创建

- 从已有列表创建
- 数值自动填充
 - zeros, ones, empty, full ...
 - zeros_like, ones_like, empty_like, full_like ...
 - identity, eye
 - diag, arrange
 - linspace, logspace, meshgrid
 - fromfunction, fromfile
 - np.random.rand



```
In [58]: np.zeros(2)
Out[58]: array([0., 0.])
```

```
In [59]: np.ones(3)
Out[59]: array([1., 1., 1.])
```

```
In [60]: np.diag(range(1,5))
Out[60]:
array([[1, 0, 0, 0],
       [0, 2, 0, 0],
       [0, 0, 3, 0],
       [0, 0, 0, 4]])
```

```
In [69]: np.arange(1,6,2)
Out[69]: array([1, 3, 5])
```

more examples on [test_numpy.ipynb](#)

```
In [71]: np.linspace(0, 10, num=5)
Out[71]: array([ 0. ,  2.5,  5. ,  7.5, 10. ])
```



NumPy支持的数据类型

- 各种字长的5种基础数据类型
 - booleans, integers, unsigned integers, floating point, complex
 - 例如: bool_ , int8, int16, int32, float32, uint64, complex64 等
- 更精确指定数据类型，以获取存储和计算上的性能提升
- NumPy也可以用于支持自定义类型 (Structured arrays)
 - <https://numpy.org/doc/stable/user/basics.rec.html#structured-arrays>

索引、切片、视图

NDARRAY的访问



索引和切片

- 定位单个元素
 - 下标 (正值、负值)
- 选择多个元素
 - 切片 ((start, end, step) 序列开始、序列结尾)
- 对于高维数组, 须从0-ndim指明每个需要切片的维度
- 每个维度的索引和切片操作相互独立
 - `myarray[-3:, -3:]`

• 语法说明

```
newlist = listA[start : end : step]
```



- 结束位置元素不在结果列表中
- 步长用于跳过部分元素
- start、end 可以省略, 分别表示从列表开始、直到列表结束
- step可以省略, 表示默认步长为1



```
In [7]: myarray = np.arange(100).reshape(10, 10)
```

```
In [8]: myarray
```

```
Out[8]:
```

```
array([[ 0,  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],
       ...
```

```
In [9]: myarray[:,1]
```

```
In [10]: myarray[-3:,-3:]
```

```
In [11]: myarray[:,-3:]
```

```
In [12]: myarray[-3:]
```




切片和视图

- 切片操作得到的数据子集是原数组的一种展示方式（称为视图）
 - 视图仍然具有正常数组的行为、效率得到提升
 - 视图中的改动将影响原数组数据

```
In [19]: newarray =  
myarray[:,5,-3:]  
...: print_array(newarray)
```

```
Element Type:  int64  
Shape:      (2, 3)  
Strides:    (400, 8)  
[[ 7  8  9]  
 [57 58 59]]
```

```
In [20]: newarray2 =  
np.array([[ 7, 8, 9], [57, 58,  
59]], dtype="int32")  
...:
```

```
print_array(newarray2)
```

```
Element Type:  int32  
Shape:      (2, 3)  
Strides:    (12, 4)  
[[ 7  8  9]  
 [57 58 59]]
```

抽象和封装：数据内部表示 v.s. 数据的外部使用



```
In [21]: newarray3 = newarray[:, -2:]
```

创建切片的切片

```
In [22]: newarray3.fill(0)
```

将切片数组置零

```
In [23]: print(newarray3)
...: print(newarray)
...: print(myarray)
```

原数组也被置零，除非显式指明copy：
`newarray3 = newarray[:, -2:].copy()`

试着自己实现一个三维矩阵类，让它能进行多次slicing操作，操作结果是原矩阵的一个视图。

```
[[0 0]
 [0 0]]
[[ 7  0  0]
 [57  0  0]]
[[ 0  1  2  3  4  5  6  7  0  0]
 [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 55 56 57  0  0]
 [60 61 62 63 64 65 66 67 68 69]
 [70 71 72 73 74 75 76 77 78 79]
 [80 81 82 83 84 85 86 87 88 89]
 [90 91 92 93 94 95 96 97 98 99]]
```



fancy indexing & boolean indexing

- 花式索引

- 使用一个索引序列从ndarray中选择元素，并创建新数组

```
In [24]: myarray = np.arange(0, 100, 10)
...: indices = [1, 5, -1]
...: newarray = myarray[indices]
```

- 布尔索引

- 使用一个bool序列进行元素选择，并创建新数组

```
In [25]: myarray = np.arange(8)
...: b = [False, True, False, False, False, False, True, False]
...: myarray[b]
Out[25]: array([1, 6])
```

调整数组形状和值



改变数组维度

- 基于底层表示支持上层的高效实现（一般返回视图）
 - `np.reshape/np.ndarray.reshape`
 - `np.ravel/np.ndarry.ravel`（折叠为一维数组）
 - `np.squeeze`（删除长度为1的维度）
 - `np.expand_dims`和`np.newaxis`（增加新的维度）
 - `np.transpose/np.ndarray.transpose/np.ndarray.T`



改变数组大小、形状、内容

- 一般将会按照要求创建新的数组
 - `np.resize`
 - `np.ndarray.flatten`
 - `np.hstack`, `np.vstack`, `np.dstack`, `np.concatenate`
 - `np.append`, `np.insert`, `np.delete`

矩阵的运算

基本算术运算

- 算术运算定义为对应元素进行运算
 - 对于大小相同的矩阵，运算结果与原矩阵形状相同

$$\begin{array}{|c|} \hline \text{data} \\ \hline \begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline \end{array} + \begin{array}{|c|} \hline \text{ones} \\ \hline \begin{array}{|c|} \hline 1 \\ \hline 1 \\ \hline \end{array} = \begin{array}{|c|} \hline 2 \\ \hline 3 \\ \hline \end{array} \end{array}$$

$$\begin{array}{|c|} \hline \text{data} \\ \hline \begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline \end{array} - \begin{array}{|c|} \hline \text{ones} \\ \hline \begin{array}{|c|} \hline 1 \\ \hline 1 \\ \hline \end{array} = \begin{array}{|c|} \hline 0 \\ \hline 1 \\ \hline \end{array} \end{array}$$

$$\begin{array}{|c|} \hline \text{data} \\ \hline \begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline \end{array} * \begin{array}{|c|} \hline \text{data} \\ \hline \begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline \end{array} = \begin{array}{|c|} \hline 1 \\ \hline 4 \\ \hline \end{array} \end{array}$$

$$\begin{array}{|c|} \hline \text{data} \\ \hline \begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline \end{array} / \begin{array}{|c|} \hline \text{data} \\ \hline \begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline \end{array} = \begin{array}{|c|} \hline 1 \\ \hline 1 \\ \hline \end{array} \end{array}$$



循环 v.s. 向量化运算(vectorized operation)

- 通过python的循环依次访问每个元素并运算效率较低

- 创建访问迭代器
- 类型匹配和操作符运算函数调用

```
c = np.empty(a.size)
for i in range(a.size):
    c[i] += a[i] + b[i]
```

- 将对矩阵中每个元素的运算 封装为 对矩阵整体的运算
 - 通过基于c的实现和底层优化提升计算效率
- 提供一系列封装好的计算函数 (Universal functions, **ufunc**) ,
避免显式使用元素遍历循环



```
In [27]: size = 10000
...: a = np.random.rand(size)
...: b = np.random.rand(size)
...:
...: %timeit c = np.add(a, b)
...:
...: def myadd(a , b):
...:     c = np.empty(a.size)
...:     for i in range(a.size):
...:         c[i] += a[i] + b[i]
...:     return c
...:
...: %timeit myadd(a, b)
```

5.39 $\mu\text{s} \pm 39.7 \text{ ns}$ per loop (mean \pm std. dev. of 7 runs, 100000 loops each)
5.43 ms $\pm 22.5 \mu\text{s}$ per loop (mean \pm std. dev. of 7 runs, 100 loops each)

```
In [28]: size = 10000
...: a = np.random.rand(size)
...: b = np.random.rand(size)
...:
...: %timeit c = np.dot(a, b)
...:
...: def mydot(a , b):
...:     c = 0
...:     for i in
range(a.size):
...:         c += a[i] * b[i]
...:     return c
...:
...: %timeit mydot(a, b)
```

2.41 $\mu\text{s} \pm 140 \text{ ns}$ per loop (mean \pm std. dev. of 7 runs, 100000 loops each)
4.13 ms $\pm 23.7 \mu\text{s}$ per loop (mean \pm std. dev. of 7 runs, 100 loops each)



Universal functions (ufuncs)

- **Math operations 数学运算**
 - add, subtract, multiply, matmul, divide, power, remainder, ...
- **Trigonometric functions 三角函数**
 - sin, cos, tan, sinh, cosh, tanh, arcsin, arccos, ...
- **Bit-twiddling functions 位运算**
 - bitwise_add, bitwise_or, bitwise_xor, invert, left_shift, ...
- **Comparison functions 比较运算**
 - greater, greater_equal, less, equal, logical_and, logical_or, ...
- **Floating functions**
 - isfinite, isinf, isnan, fabs, fmod, floor, ceil, ...

<https://numpy.org/doc/stable/reference/ufuncs.html>



Calling ufuncs:

from np.ufunc?

=====

`op(*x[, out], where=True, **kwargs)`

Apply ``op`` to the arguments ``*x`` elementwise, broadcasting the arguments.

Parameters

`*x` : array_like

Input arrays.

`out` : ndarray, None, or tuple of ndarray and None, optional

指定输出位置

Alternate array object(s) in which to put the result; if provided, it must have a shape that the inputs broadcast to. A tuple of arrays (possible only as a keyword argument) must have length equal to the number of outputs; use ``None`` for uninitialized outputs to be allocated by the ufunc.

指定作用元素

`where` : array_like, optional

This condition is broadcast over the input. At locations where the condition is True, the ``out`` array will be set to the ufunc result. Elsewhere, the ``out`` array will retain its original value. Note that if an uninitialized ``out`` array is created via the default ``out=None``, locations within it where the condition is False will remain uninitialized.

`**kwargs`

For other keyword-only arguments, see the :ref:`ufunc docs <ufuncs.kwargs>`. 36



操作数匹配和广播 (Broadcasting)

- 当运算的两个操作数矩阵形状不同时，运算需要重新定义
 - NumPy通过广播机制自动扩展小矩阵，以匹配大矩阵
 - 将不同大小的矩阵转换为同样大小，便于进行统一运算

$$\begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline \end{array} * 1.6 = \begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline \end{array} * \begin{array}{|c|} \hline 1.6 \\ \hline 1.6 \\ \hline \end{array} = \begin{array}{|c|} \hline 1.6 \\ \hline 3.2 \\ \hline \end{array}$$

$$\text{data} + \text{ones_row} = \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & 4 \\ \hline 5 & 6 \\ \hline \end{array} + \begin{array}{|c|c|} \hline 1 & 1 \\ \hline \hline \hline \end{array} = \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & 4 \\ \hline 5 & 6 \\ \hline \end{array} + \begin{array}{|c|c|} \hline 1 & 1 \\ \hline 1 & 1 \\ \hline 1 & 1 \\ \hline \end{array} = \begin{array}{|c|c|} \hline 2 & 3 \\ \hline 4 & 5 \\ \hline 6 & 7 \\ \hline \end{array}$$

<https://numpy.org/doc/stable/user/basics.broadcasting.html>



广播和向量化运算

- 广播后的计算可以采用通用的ufunc进行，以保证运算效率



```
In [26]: x = np.arange(10000)
....: %timeit x * 1.6
....: %timeit [i * 1.6 for i in x]
```

9.38 μs \pm 68 ns per loop (mean \pm std. dev. of 7 runs, 100000 loops each)

19.8 ms \pm 109 μs per loop (mean \pm std. dev. of 7 runs, 100 loops each)



Broadcasting广播

- 从右到左依次匹配两个矩阵各维度的长度：
 - 当 两个维度长度相等 或者 其中一个为1 时，两者compatible
 - 当 其中一个矩阵维度不足 时，用长度为1的新维度进行补充
- 广播：
 - 将长度为1的维度内容复制匹配另一矩阵对应长度
 - strides = 0

$$\begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline \end{array} * 1.6 = \begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline \end{array} * \begin{array}{|c|} \hline 1.6 \\ \hline 1.6 \\ \hline \end{array} = \begin{array}{|c|} \hline 1.6 \\ \hline 3.2 \\ \hline \end{array} \quad \begin{array}{l} (1,) \rightarrow (2, 1) \\ (2, 1) \end{array}$$

$$\begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & 4 \\ \hline 5 & 6 \\ \hline \end{array} + \begin{array}{|c|c|} \hline 1 & 1 \\ \hline 1 & 1 \\ \hline 1 & 1 \\ \hline \end{array} = \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & 4 \\ \hline 5 & 6 \\ \hline \end{array} + \begin{array}{|c|c|} \hline 1 & 1 \\ \hline 1 & 1 \\ \hline 1 & 1 \\ \hline \end{array} = \begin{array}{|c|c|} \hline 2 & 3 \\ \hline 4 & 5 \\ \hline 6 & 7 \\ \hline \end{array} \quad \begin{array}{l} (1, 2) \rightarrow (3, 2) \\ (3, 2) \end{array}$$

Broadcasting广播



- 常见的广播是用于扩展标量、向量和低维矩阵

A	(2d array):	5 x 4
B	(1d array):	1
Result	(2d array):	5 x 4

A	(2d array):	5 x 4
B	(1d array):	4
Result	(2d array):	5 x 4

A	(3d array):	15 x 3 x 5
B	(2d array):	3 x 5
Result	(3d array):	15 x 3 x 5



Broadcasting广播

- 常见的广播是用于扩展标量、向量和低维矩阵
 - 可能扩展的是中间的维度
 - 或扩展多个不连续维度

A	(3d array):	15 x 3 x 5
B	(2d array):	15 x 1 x 5
Result	(3d array):	15 x 3 x 5

A	(3d array):	15 x 3 x 5
B	(2d array):	3 x 1
Result	(3d array):	15 x 3 x 5



Broadcasting广播

- 常见的广播是用于扩展标量、向量和低维矩阵
 - 可能扩展的是中间的维度
 - 或扩展多个不连续维度
 - 广播也可能同时扩展两个矩阵

A	(4d array):	8 x 1 x 6 x 1
B	(3d array):	7 x 1 x 5
Result	(4d array):	8 x 7 x 6 x 5



Broadcasting广播

- 一些广播失败的例子

- ValueError: operands could not be broadcast together

A (1d array): 3

B (1d array): 4 # *trailing dimensions do not match*

A (2d array): 2 x 1

B (3d array): 8 x 4 x 3 # *second from last dimensions mismatched*



```
In [3]: x = np.arange(4)
....: xx = x.reshape(4,1)
....: y = np.ones(5)
....: z =
np.ones((3,4))
```

```
In [4]: x + y
ValueError: operands could not be
broadcast together with shapes (4,)
(5,)
```

```
In [5]: xx + y
Out[5]:
array([[1., 1., 1., 1., 1.],
       [2., 2., 2., 2., 2.],
       [3., 3., 3., 3., 3.],
       [4., 4., 4., 4., 4.]])
```

```
In [6]: x + z
Out[6]:
array([[1., 2., 3., 4.],
       [1., 2., 3., 4.],
       [1., 2., 3., 4.]])
```



ufuncs

- ufunc中的out参数用于指定结果存储位置

```
In [32]: x = np.arange(1000000)
....: %time y = x * 2
....: %time x = x * 2
....: %time x *= 2
CPU times: user 2.33 ms, sys:
3.06 ms, total: 5.39 ms
Wall time: 4.74 ms
CPU times: user 2.17 ms, sys:
3.43 ms, total: 5.6 ms
Wall time: 5.64 ms
CPU times: user 858 µs, sys: 0
ns, total: 858 µs
Wall time: 862 µs
```

```
In [33]: y = np.random.rand(100,100)
....:
....: %time np.round(y, decimals = 4)
....: %time np.round(y, decimals = 4,
out = y)
CPU times: user 775 µs, sys: 970 µs, total:
1.74 ms
Wall time: 3.73 ms
CPU times: user 58 µs, sys: 6 µs, total:
64 µs
Wall time: 60.1 µs
```

- ufunc中的where参数用于指定参与运算的元素

```
In [1]: x = np.arange(5)
...: y = [True, True, False, True, False]
...:
...: #z = np.add(x, 5, where = y)
...: z = np.add(x, 5, where = (x%3==0))
...: print(x)
...: print(z)
```



其他ufunc的相关功能

- **aggregates**

- np.add.reduce(x)
- np.add.accumulate(x)
- reduceat等

- **outer products**

- np.multiply.outer(x, x)

```
In [41]: x = np.arange(1, 5)
...: xacc = np.multiply.accumulate(x)
...: xred = np.multiply.reduce(x)
...:
...: print(xacc, xred)
[ 1  2  6 24] 24
```

```
In [40]: x = np.arange(1,10)
...: print(np.multiply.outer(x, x))
[[ 1  2  3  4  5  6  7  8  9]
 [ 2  4  6  8 10 12 14 16 18]
 [ 3  6  9 12 15 18 21 24 27]
 [ 4  8 12 16 20 24 28 32 36]
 [ 5 10 15 20 25 30 35 40 45]
 [ 6 12 18 24 30 36 42 48 54]
 [ 7 14 21 28 35 42 49 56 63]
 [ 8 16 24 32 40 48 56 64 72]
 [ 9 18 27 36 45 54 63 72 81]]
```



其他ufunc的相关功能

- 创建一个ufunc
 - `np.vectorize(myfunc)`

```
In [42]: def myfunc(x, y):
...:     return x**2 + y**2
...:
...: myfunc_vectorized = np.vectorize(myfunc)
...:
...: x = np.random.rand(5, 5)
...: y = np.random.rand(5, 5)
...:
...: %timeit myfunc_vectorized(x, y)
...: %timeit x**2 + y**2
```

21.6 μ s \pm 199 ns per loop (mean \pm std. dev. of 7 runs, 10000 loops each)

2.05 μ s \pm 7.78 ns per loop (mean \pm std. dev. of 7 runs, 100000 loops each)



聚合函数

- 用于对数组进行聚合计算
 - np.mean, std, var, sum, prod, cumsum, cumprod,
 - min, max, argmin, argmax
 - all (所有元素不为零, 返回True)
 - any (任一元素不为零, 返回True)
- 默认对整个输入数组进行聚合, 也可以用axis关键字参数指定聚合的轴
 - data.max(axis=0)
 - data.max(axis=(0, 2))



data

1	2
3	4
5	6

`.max()` = 6

data

1	2
3	4
5	6

`.min()` = 1

data

1	2
3	4
5	6

`.sum()` = 21

data

1	2
5	3
4	6

`.max(axis=0)` =

1	2
5	3
4	6

=

5	6
---	---

data

1	2
5	3
4	6

`.max(axis=1)` =

1	2
5	3
4	6

=

2
5
6



```
In [89]: data = np.random.normal(size=(15,15))
...: np.mean(data) # data.mean()
Out[89]: 0.07822575388685046
```

```
In [90]: data = np.random.normal(size=(5, 10, 15))
...:
...: print(data.sum(axis=0).shape)
...: print(data.sum(axis=(0, 2)).shape)
```

```
(10, 15)
(10,)
```



条件计算函数

- **np.where**
 - 从两个数组中选取值
- **np.choose**
 - 根据给定的索引数组从数组列表中选取值
- **np.select**
 - 根据条件列表从数组列表中选取值
- **np.nonzero**
 - 返回非零元素的索引



```
x = np.linspace(-4, 4, 9)
...:
...: np.where(x < 0, x**2, x**3)
...:
...: np.select([x < -1, x < 2, x >= 2],
...:           [x**2, x**3, x**4])
...:
...: np.choose([0, 0, 0, 1, 1, 1, 2, 2, 2],
...:           [x**2, x**3, x**4])
```



其他效率相关问题

```
In [30]: a = np.random.rand(5000,
5000)
...: %timeit a[0, :].sum()
...: %timeit a[:, 0].sum()
...: b = a.T
...: %timeit b[0, :].sum()
...: %timeit b[:, 0].sum()
...: c = np.array(a, copy = True,
order = 'F')
...: %timeit c[0, :].sum()
...: %timeit c[:, 0].sum()
...: d = np.array(a, copy = True,
order = 'C')
...: %timeit d[0, :].sum()
...: %timeit d[:, 0].sum()
```

对行与列求和的差别:

3.77 $\mu\text{s} \pm 42.3 \text{ ns}$ per loop (mean \pm std. dev. of 7 runs, 100000 loops each)
35.7 $\mu\text{s} \pm 149 \text{ ns}$ per loop (mean \pm std. dev. of 7 runs, 10000 loops each)
35.4 $\mu\text{s} \pm 180 \text{ ns}$ per loop (mean \pm std. dev. of 7 runs, 10000 loops each)
3.76 $\mu\text{s} \pm 24.8 \text{ ns}$ per loop (mean \pm std. dev. of 7 runs, 100000 loops each)
35.3 $\mu\text{s} \pm 162 \text{ ns}$ per loop (mean \pm std. dev. of 7 runs, 10000 loops each)
3.75 $\mu\text{s} \pm 15.2 \text{ ns}$ per loop (mean \pm std. dev. of 7 runs, 100000 loops each)
3.76 $\mu\text{s} \pm 20.3 \text{ ns}$ per loop (mean \pm std. dev. of 7 runs, 100000 loops each)
35.3 $\mu\text{s} \pm 177 \text{ ns}$ per loop (mean \pm std. dev. of 7 runs, 10000 loops each)



```
In [31]: a = np.arange(6).reshape(2,3)
....:
....: def print_nditer(b):
....:     #print_array(b)
....:     #print(b.ravel())
....:     print("Iter: ")
....:     for x in np.nditer(b):
....:         print(x, end = ' ')
....:     print("\n")
....:
....: print_nditer(a)
....: print_nditer(a.T)
....: print_nditer(a.T.copy(order = 'C'))
```

np.nditer是numpy中用于高效遍历矩阵元素的对象，遍历顺序可以由数据存储方式决定。

Iter:

0 1 2 3 4 5

Iter:

0 1 2 3 4 5

Iter:

0 3 1 4 2 5



numpy应用示例（一）

- 计算两个给定序列的均方误差。

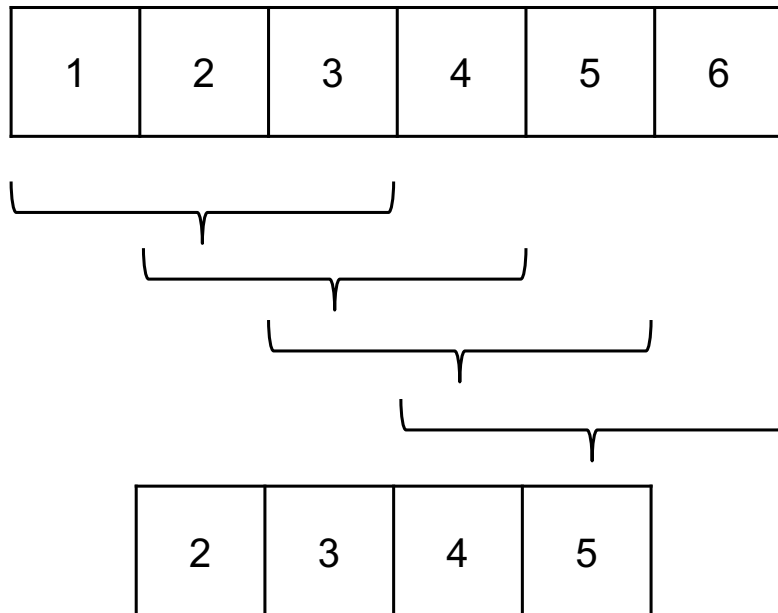
$$MeanSquareError = \frac{1}{n} \sum_{i=1}^n (Y_prediction_i - Y_i)^2$$

```
In [48]: def mean_square_error(y_hat, y):  
        ...:     return np.average(np.square(y_hat - y), axis = 0)
```




numpy应用示例（二）

- 计算数组中连续三个值的平均值



```
x = np.arange(6)
ave = (x[:-2] + x[1:-1] + x[2:]) / 3
```

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

如何计算给定窗口大小w中的元素的平均值？



numpy应用示例（三）

- 计算给定矩阵的平方根矩阵。其中，负数的平方根为其绝对值的平方根的相反数。

```
x = np.random.randint(-100, 101, (5,5))
```

```
np.sqrt(x)
```

- 组合现有ufunc，自定义ufunc?



```
In [46]: def method1(x):
...:     x = np.array(x, dtype = "float32")
...:     np.sqrt(x, where = x > 0, out = x)
...:     np.sqrt(-x, where = x < 0, out = x)
...:     return x
...:
...: def method2(x):
...:     mysqrt = np.vectorize(lambda x: np.sqrt(x) if x > 0 else np.sqrt(-x))
...:     return mysqrt(x)
```

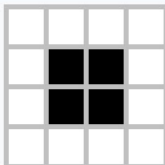
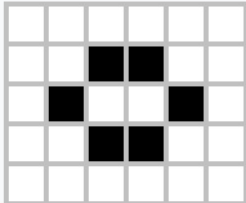
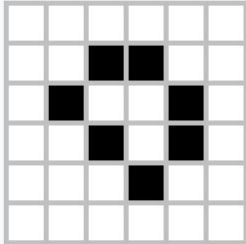
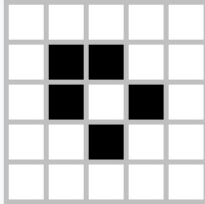
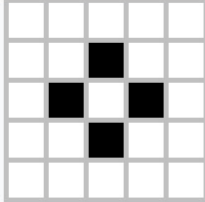
```
In [47]: %timeit method1(x)
...: %timeit method2(x)
7.88  $\mu$ s  $\pm$  120 ns per loop (mean  $\pm$  std. dev. of 7 runs, 100000 loops each)
44.6  $\mu$ s  $\pm$  174 ns per loop (mean  $\pm$  std. dev. of 7 runs, 10000 loops each)
```



numpy应用示例（四）

- **The Game of Life**
- **These rules, which compare the behavior of the automaton to real life, can be condensed into the following:**
 - Any live cell with two or three live neighbours survives.
 - Any dead cell with three live neighbours becomes a live cell.
 - All other live cells die in the next generation. Similarly, all other dead cells stay dead.
- **由随机初始的矩阵开始，输出每一代的生物存活情况**

https://en.wikipedia.org/wiki/Conway%27s_Game_of_Life

Still lifes	
Block	
Bee-hive	
Loaf	
Boat	
Tub	

- **NumPy**
 - 对高维数组的一种抽象：高效存储和计算
 - 数据创建，索引、切片和视图
 - 向量化运算、广播、聚合函数



- **其他教程阅读**

- https://numpy.org/doc/stable/user/absolute_beginners.html
- https://www.numpy.org.cn/article/basics/understanding_numpy.html

- **100 numpy exercises**

- <https://github.com/rougier/numpy-100>