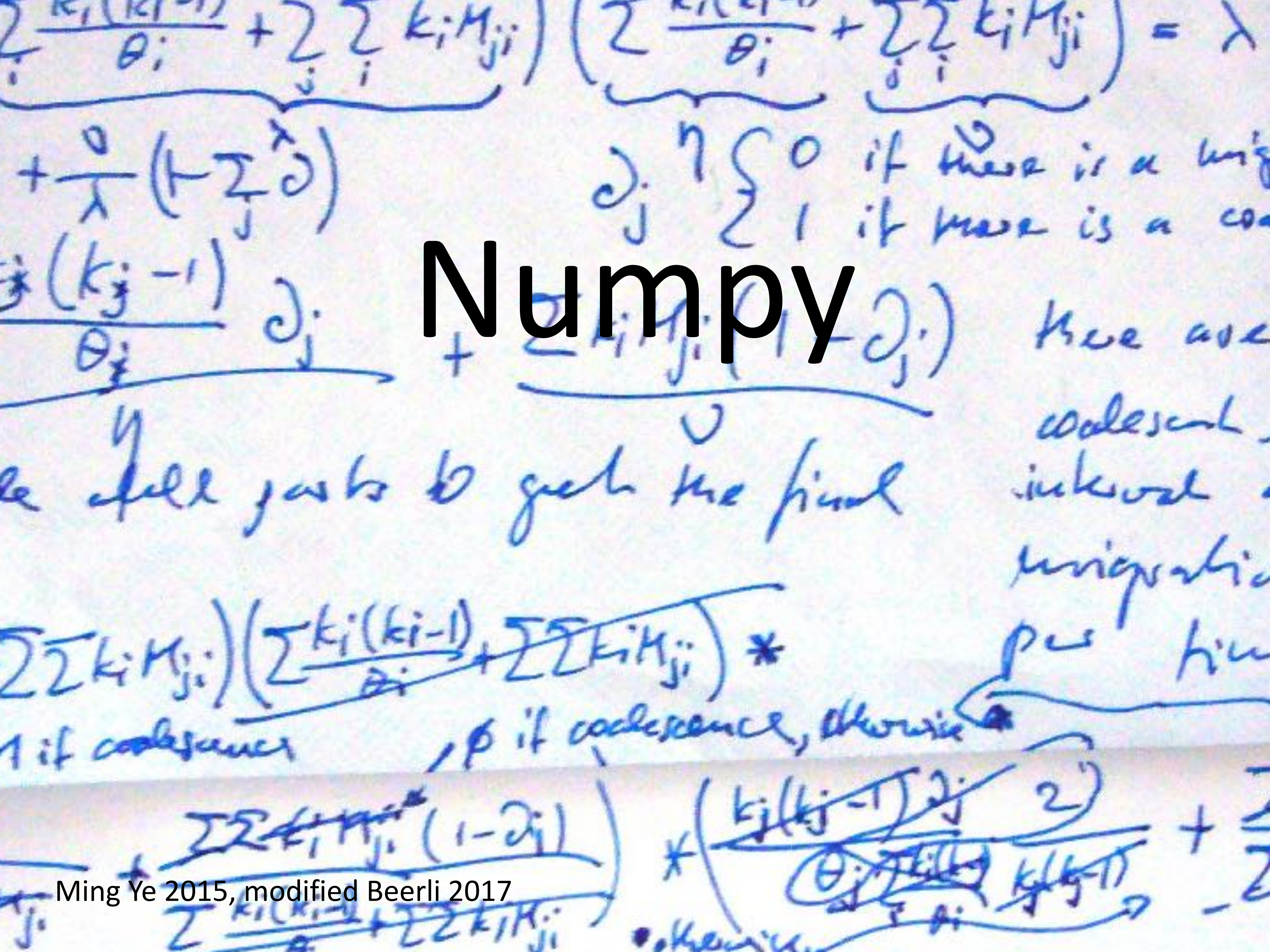


Numpy

Ming Ye 2015, modified Beerli 2017

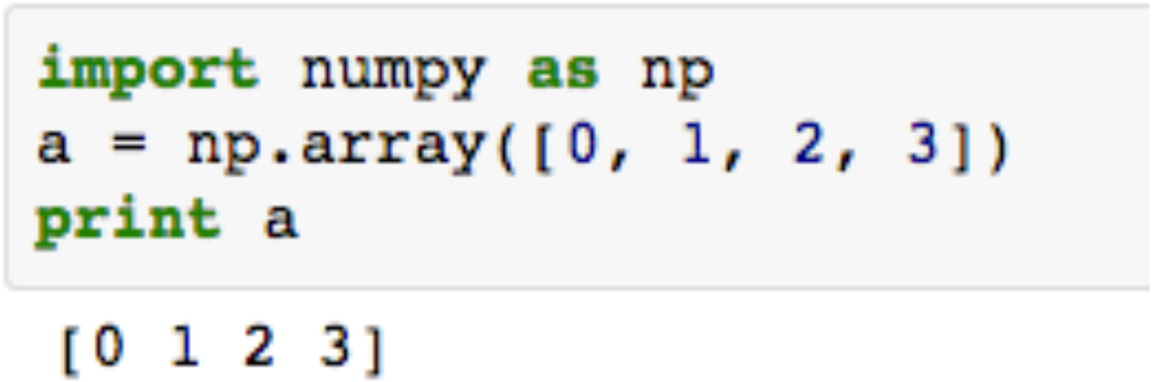
NumPy is fundamental package for scientific computing with Python

- powerful N-dimensional array object
- sophisticated functions
- basic linear algebra functions
- basic Fourier transforms
- sophisticated random number capabilities
- tools for integrating Fortran code.
- tools for integrating C/C++ code.

Numpy provides

- extension package to Python for multi-dimensional arrays
- closer to hardware (efficiency)
- designed for scientific computation (convenience)
- Also known as array oriented computing

Numpy Array



```
import numpy as np
a = np.array([0, 1, 2, 3])
print a
```

```
[0 1 2 3]
```

```python
a = np.arange(10)  # 0 .. n-1
print a
```

```
[0 1 2 3 4 5 6 7 8 9]
```

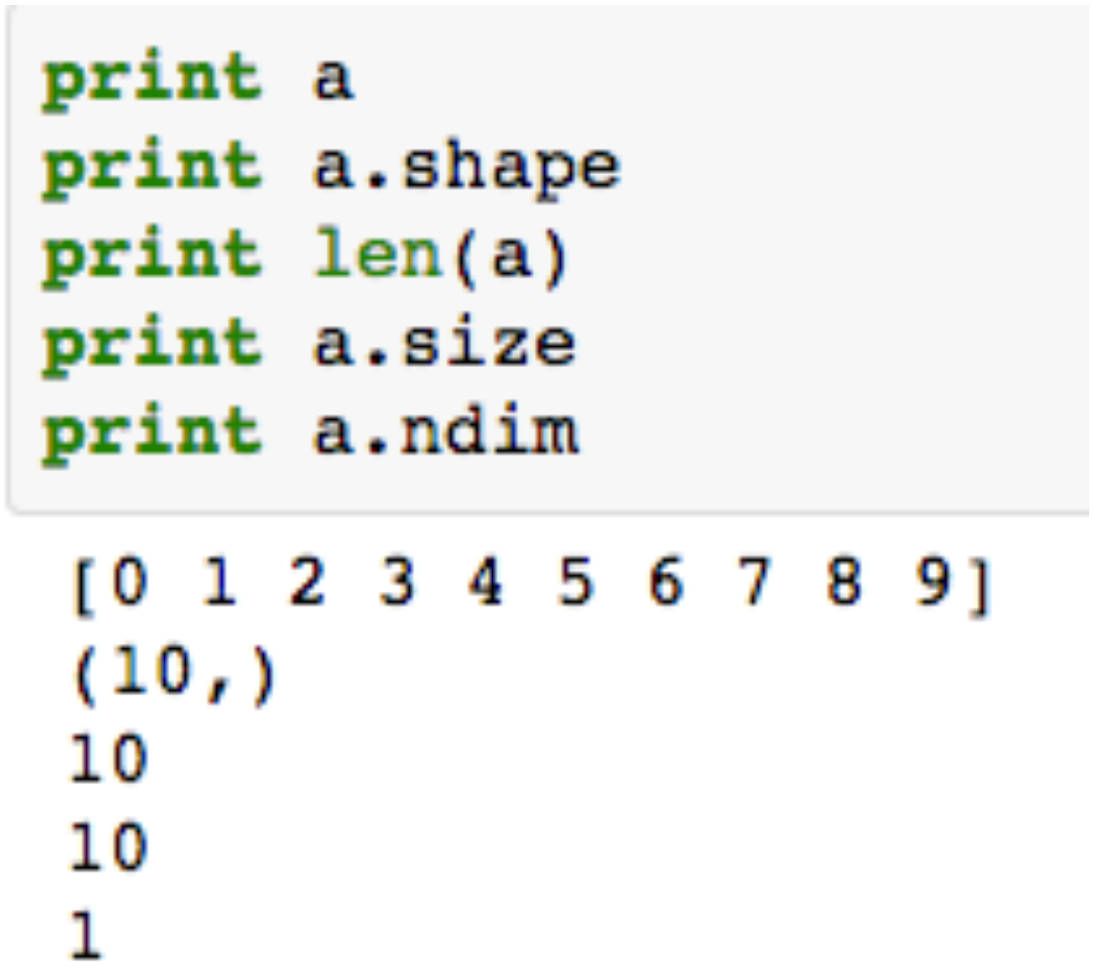
```python
b = np.arange(1, 9, 2) # start, end (exclusive), step
print b
```

```
[1 3 5 7]
```

```python
c = np.linspace(0, 1, 6) # start, end, num-points
print c
```

```
[ 0.   0.2  0.4  0.6  0.8  1. ]
```

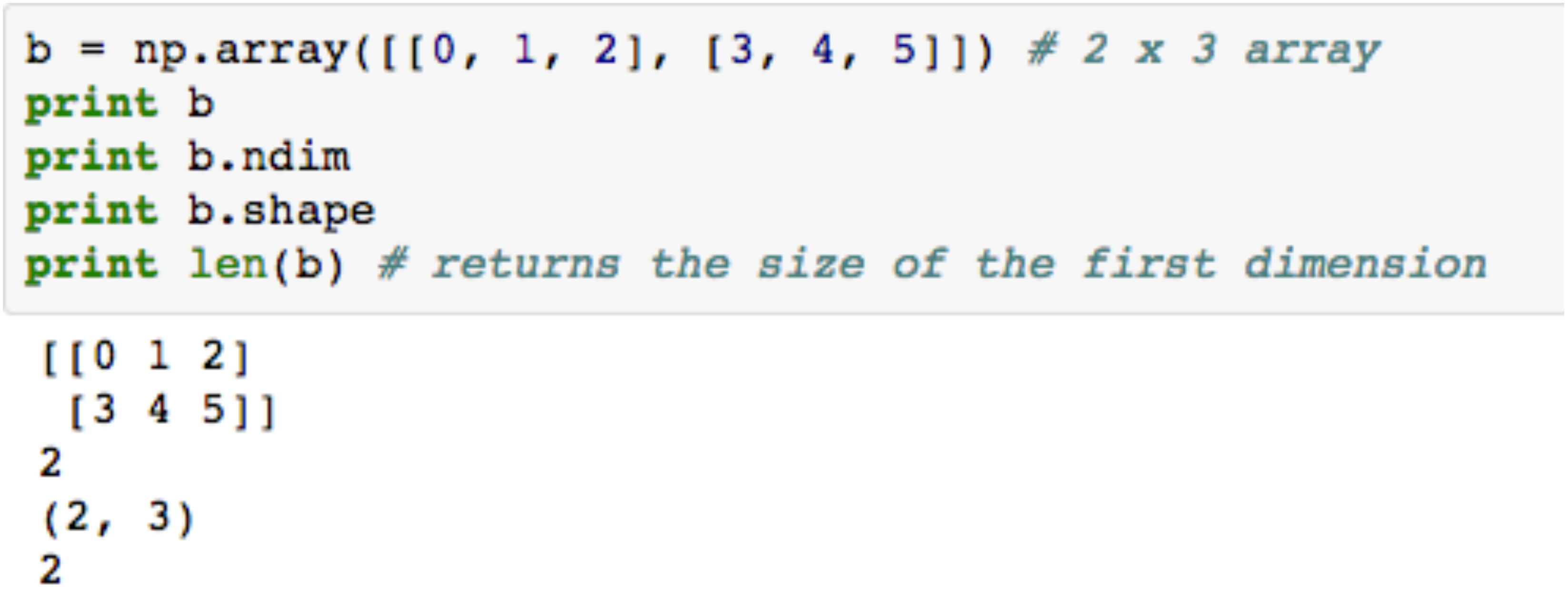
Array size



```
print a
print a.shape
print len(a)
print a.size
print a.ndim
```

```
[0 1 2 3 4 5 6 7 8 9]
(10,)
10
10
1
```

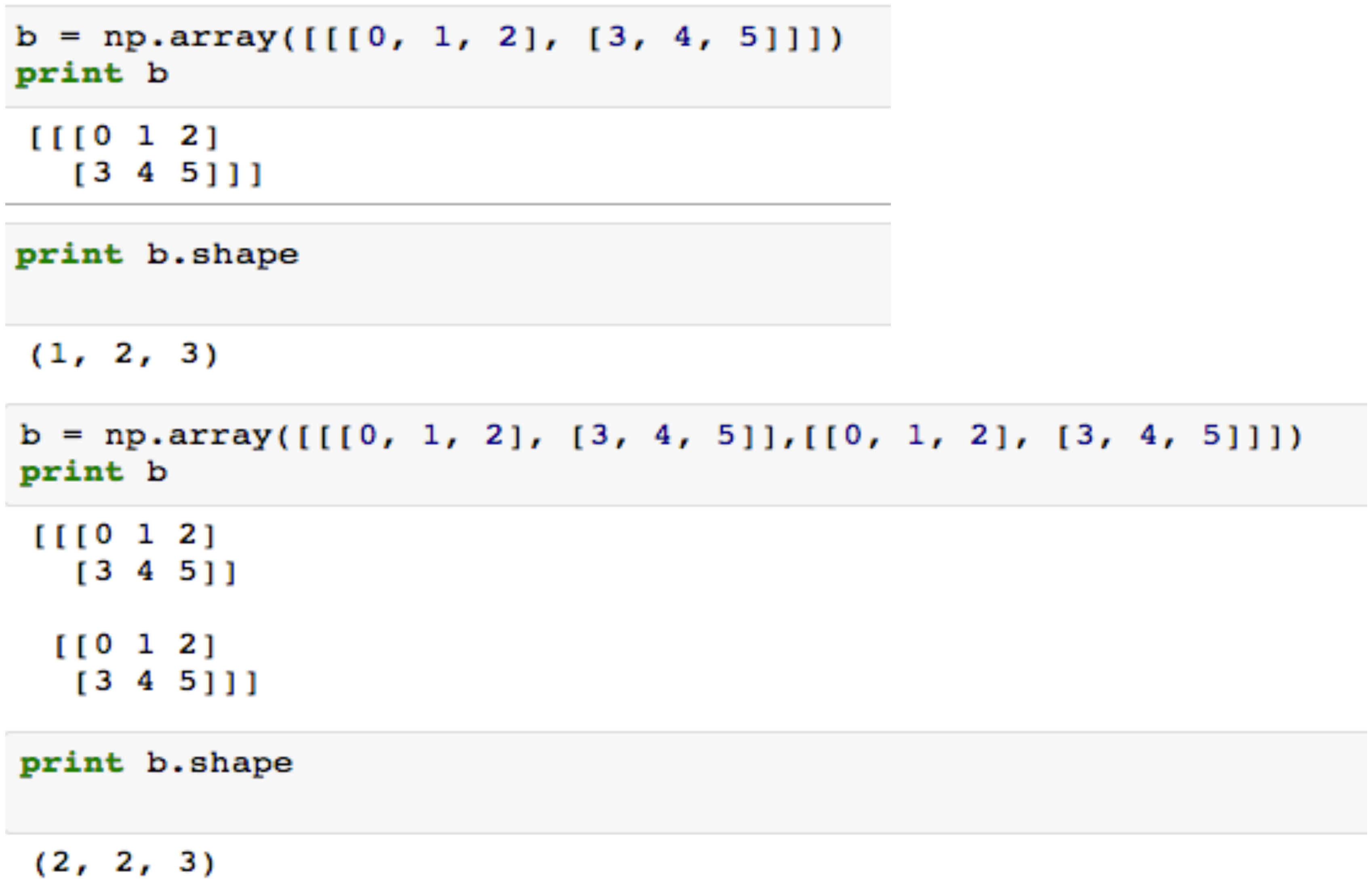
2 dimensional array



```
b = np.array([[0, 1, 2], [3, 4, 5]]) # 2 x 3 array
print b
print b.ndim
print b.shape
print len(b) # returns the size of the first dimension
```

```
[[0 1 2]
 [3 4 5]]
2
(2, 3)
2
```

3 dimensional array



```
b = np.array([[[0, 1, 2], [3, 4, 5]]])
print b
```

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

```
print b.shape
```

```
(1, 2, 3)
```

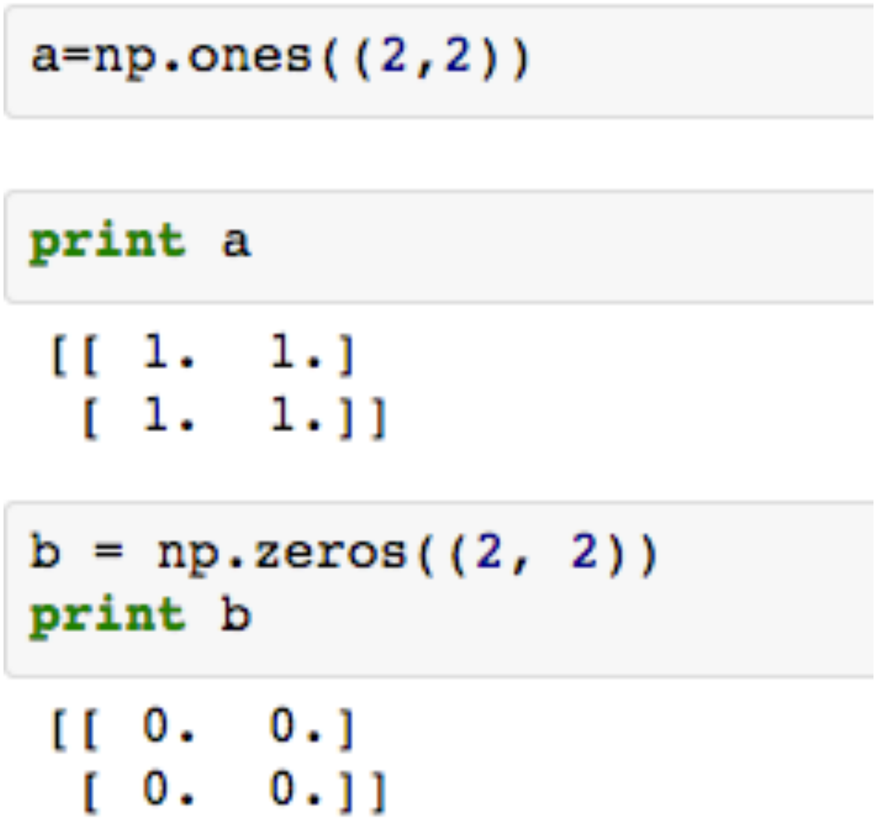
```
b = np.array([[[0, 1, 2], [3, 4, 5]],[[0, 1, 2], [3, 4, 5]]])
print b
```

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

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

```
print b.shape
```

```
(2, 2, 3)
```

Array initialization



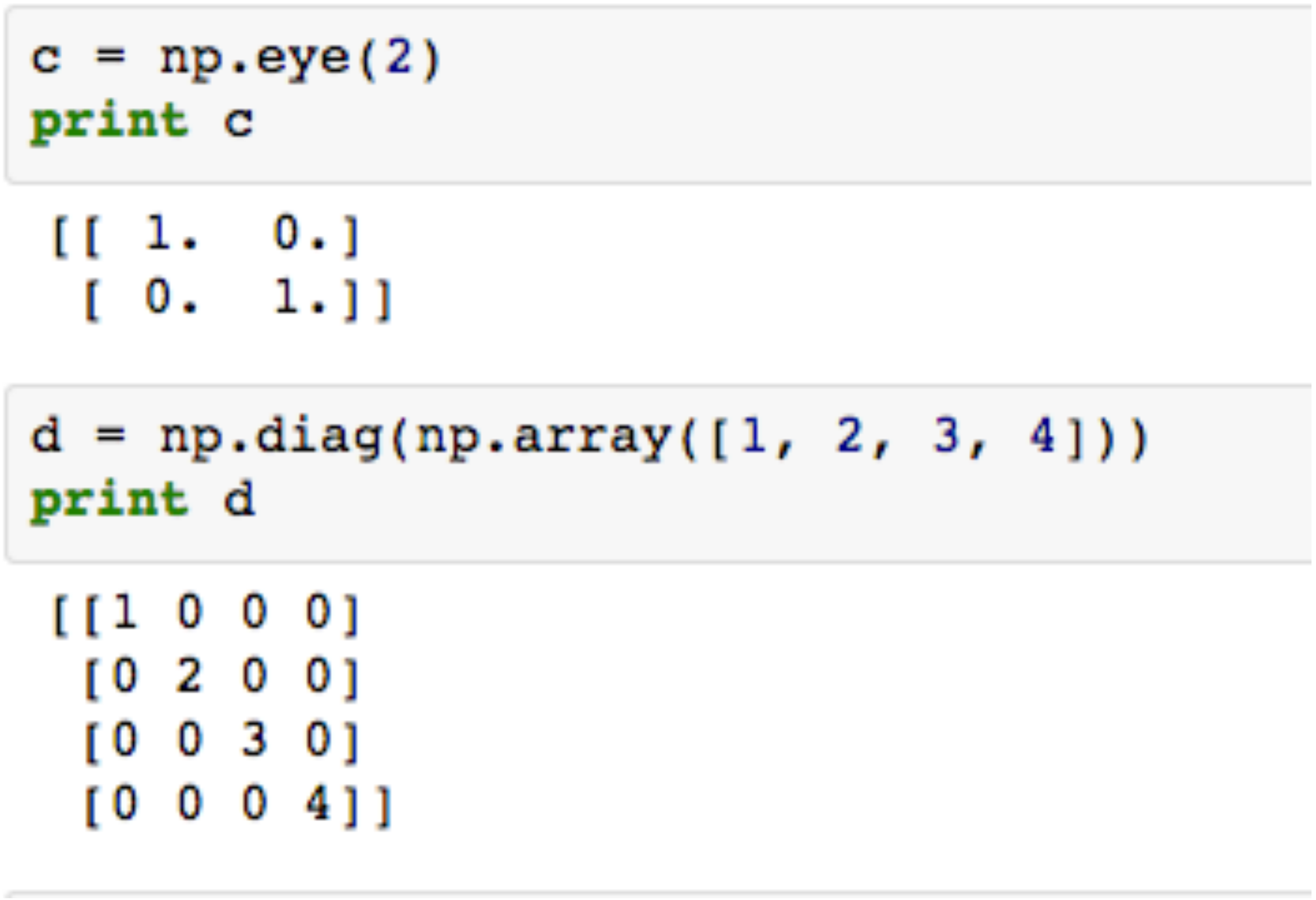
```
a=np.ones((2,2))
```

```
print a
```

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

```
b = np.zeros((2, 2))
print b
```

```
[[ 0.   0.]
 [ 0.   0.]]
```



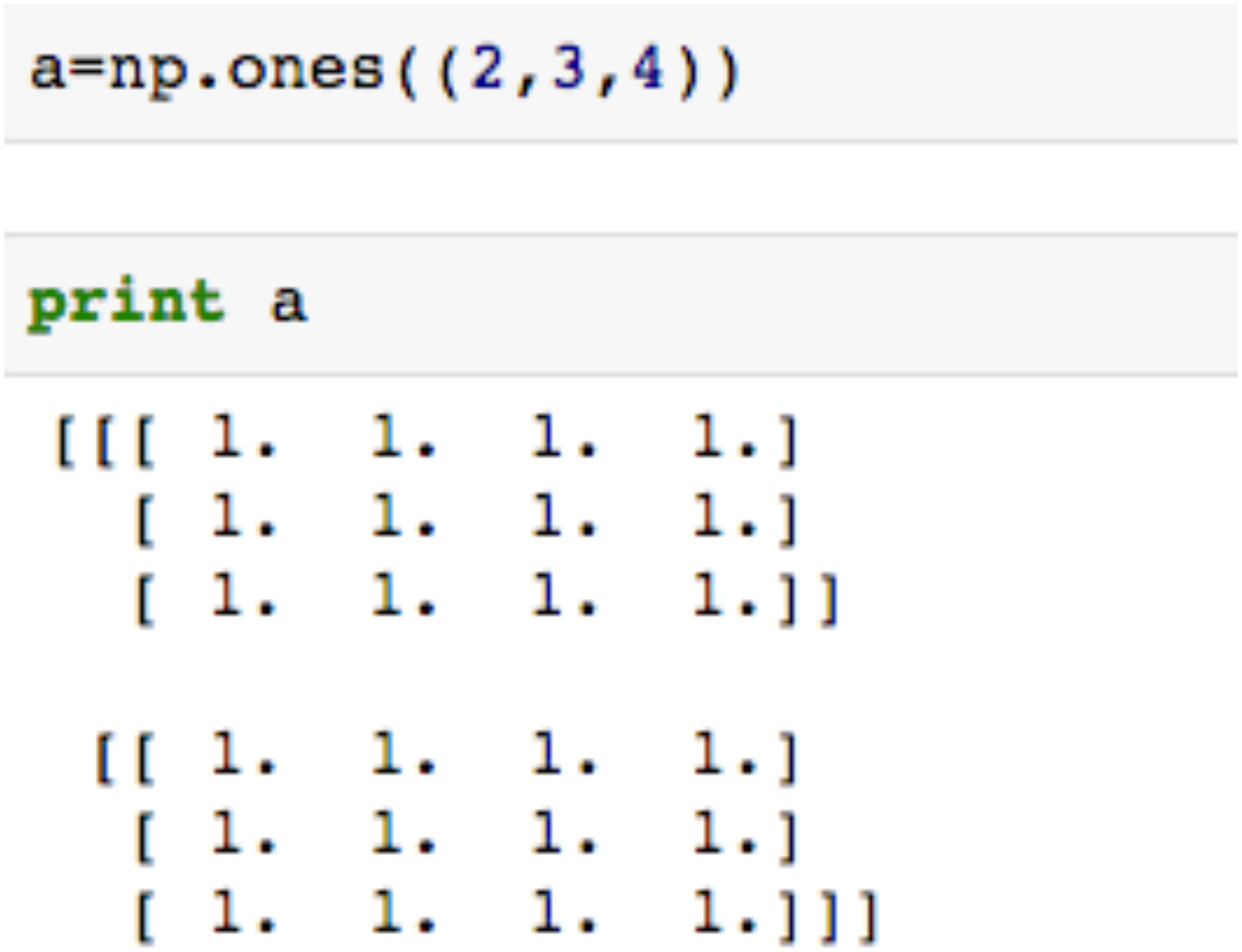
```
c = np.eye(2)
print c
```

```
[[ 1.  0.]
 [ 0.  1.]]
```

```
d = np.diag(np.array([1, 2, 3, 4]))
print d
```

```
[[1 0 0 0]
 [0 2 0 0]
 [0 0 3 0]
 [0 0 0 4]]
```

3 dimensional array



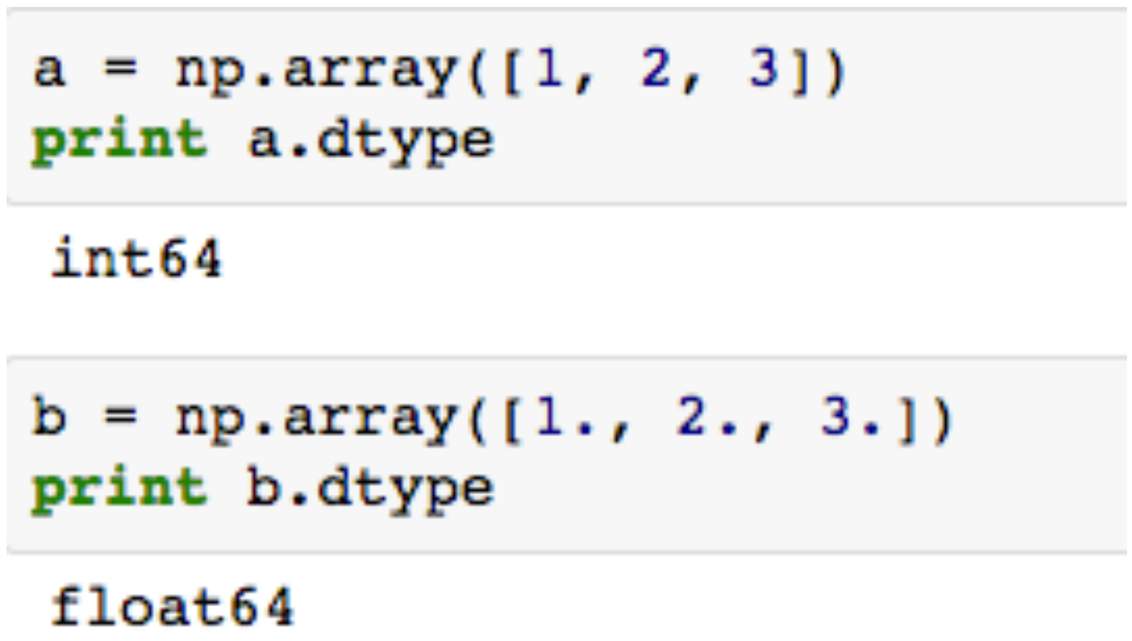
```
a=np.ones((2,3,4))
```

```
print a
```

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

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

Data type

Different data-types allow us to store data more compactly in memory, but most of the time we simply work with floating point numbers.



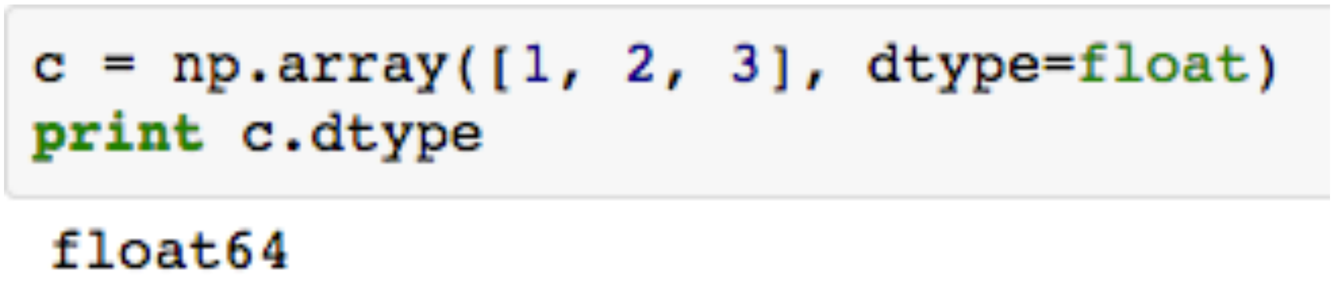
```
a = np.array([1, 2, 3])
print a.dtype
```

```
int64
```

```
b = np.array([1., 2., 3.])
print b.dtype
```

```
float64
```

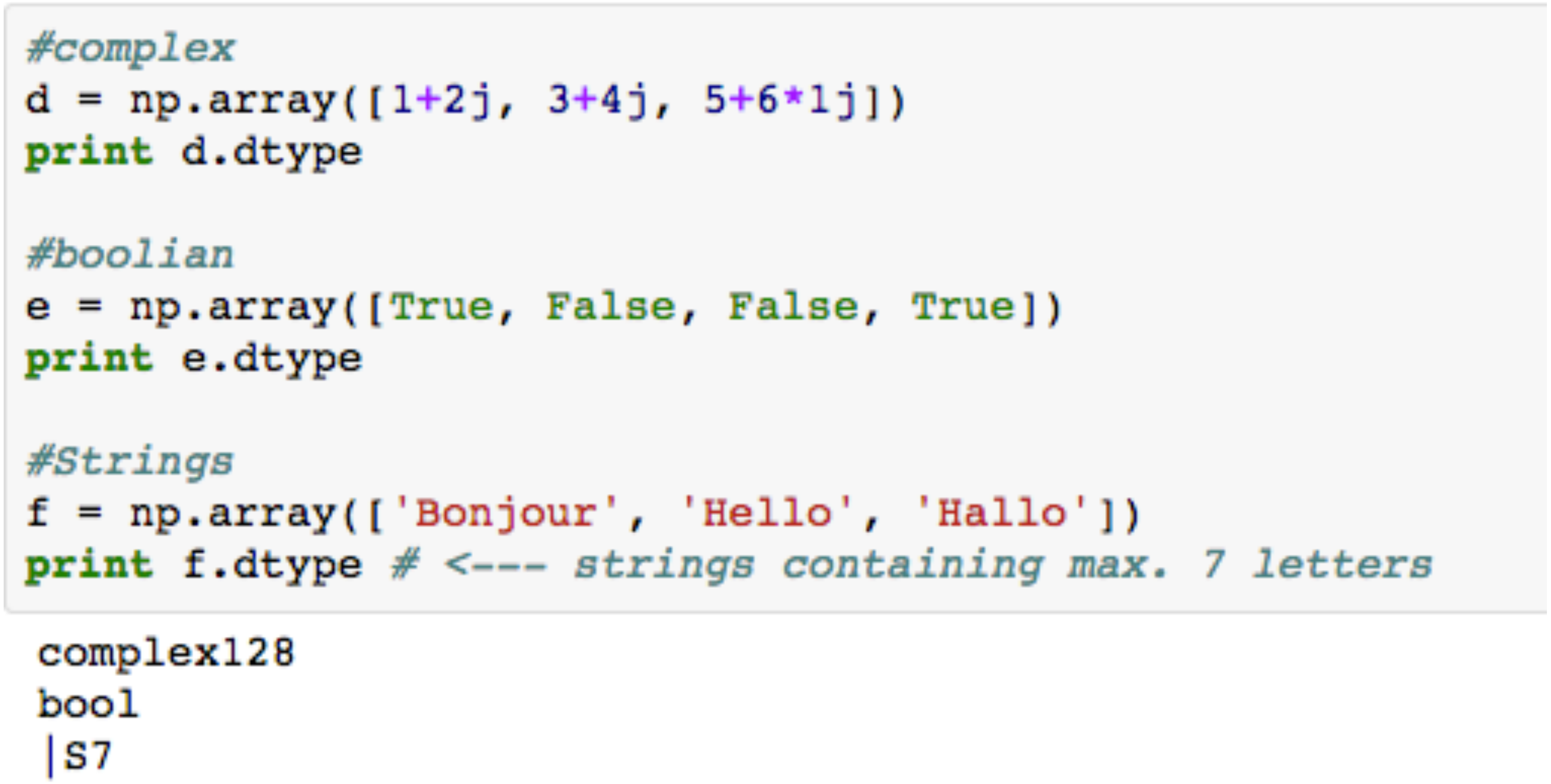
we can explicitly specify data



```
c = np.array([1, 2, 3], dtype=float)
print c.dtype
```

```
float64
```

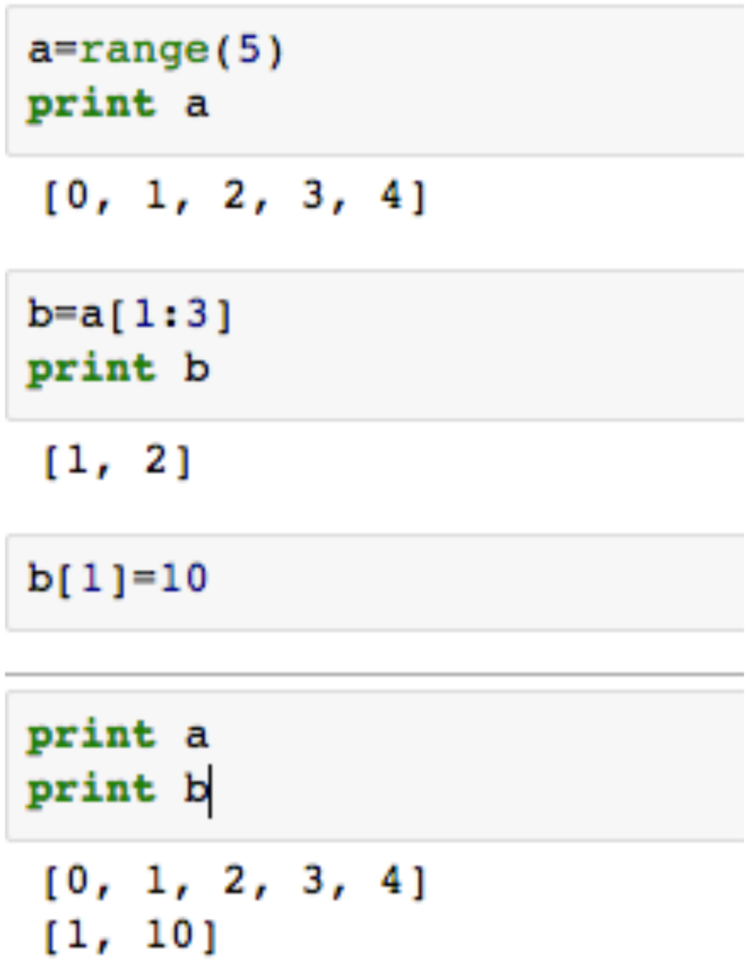
Other data types



```
#complex
d = np.array([1+2j, 3+4j, 5+6*1j])
print d.dtype

#boolian
e = np.array([True, False, False, True])
print e.dtype

#Strings
f = np.array(['Bonjour', 'Hello', 'Hallo'])
print f.dtype # <--- strings containing max. 7 letters
```

```
complex128
bool
|S7
```

Slices in list vs array



```
a=range(5)
print a
```

```
[0, 1, 2, 3, 4]
```

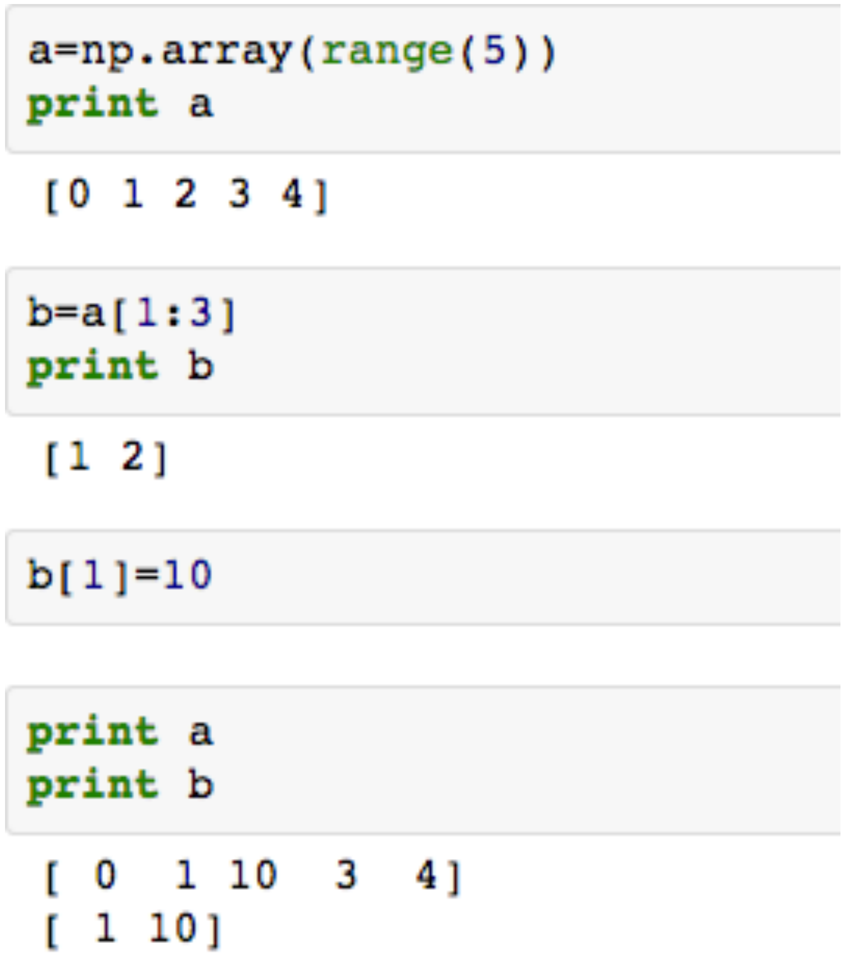
```
b=a[1:3]
print b
```

```
[1, 2]
```

```
b[1]=10
```

```
print a
print b
```

```
[0, 1, 2, 3, 4]
[1, 10]
```



```
a=np.array(range(5))
print a
```

```
[0 1 2 3 4]
```

```
b=a[1:3]
print b
```

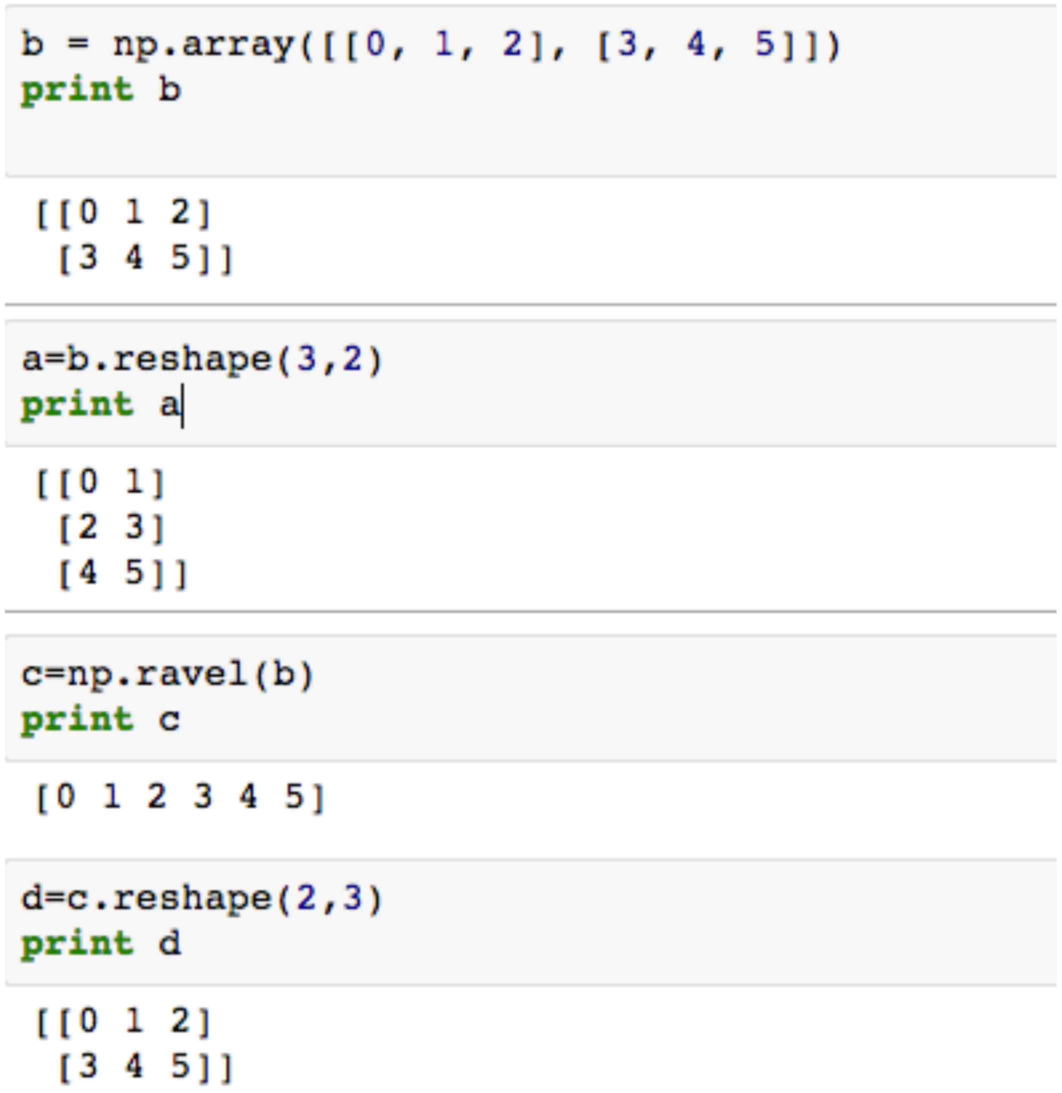
```
[1 2]
```

```
b[1]=10
```

```
print a
print b
```

```
[ 0  1 10  3  4]
[ 1 10]
```

reshape



```
b = np.array([[0, 1, 2], [3, 4, 5]])
print b
```

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

```
a=b.reshape(3,2)
print a
```

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

```
c=np.ravel(b)
print c
```

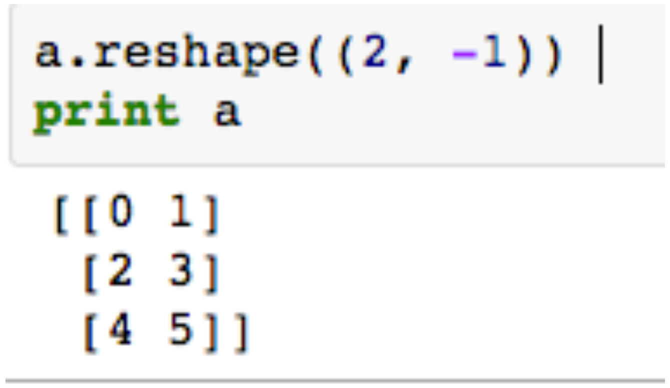
```
[0 1 2 3 4 5]
```

```
d=c.reshape(2,3)
print d
```

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

Ravel: return 1-D array of input

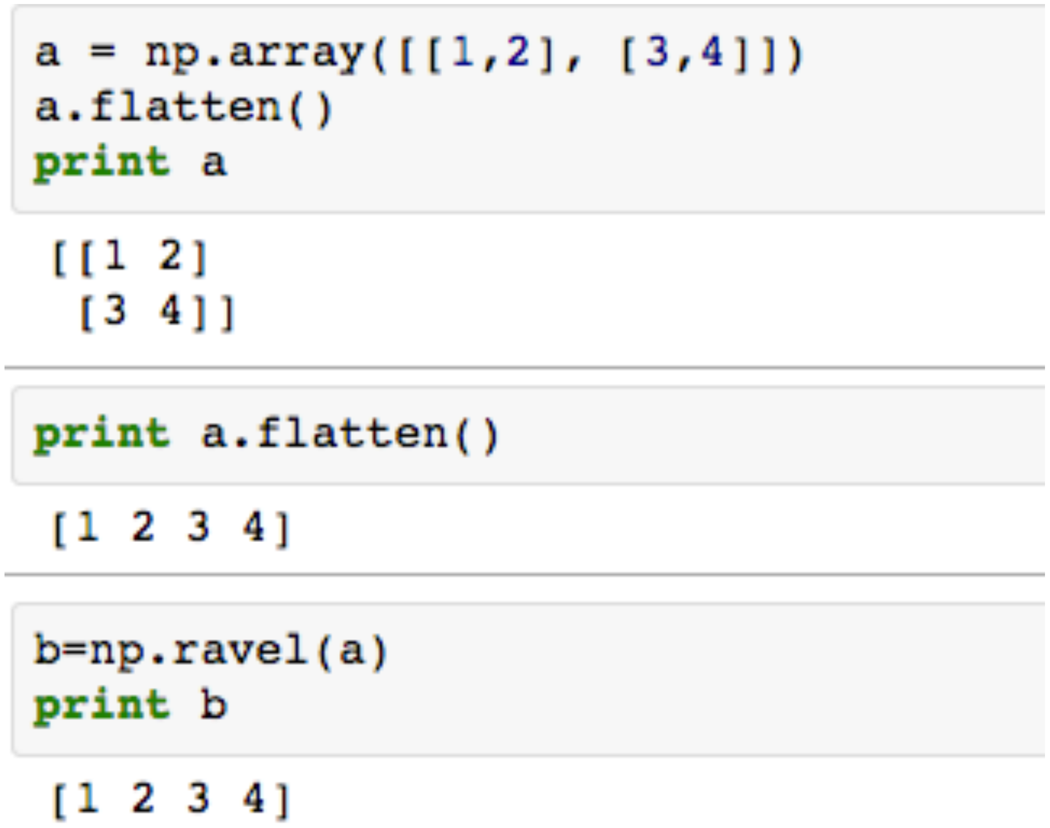
unspecified (-1) value is inferred



```
a.reshape((2, -1))
print a
```

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

Ravel vs Flatten



```
a = np.array([[1,2], [3,4]])
a.flatten()
print a
```

```
[[1 2]
 [3 4]]
```

```
print a.flatten()
```

```
[1 2 3 4]
```

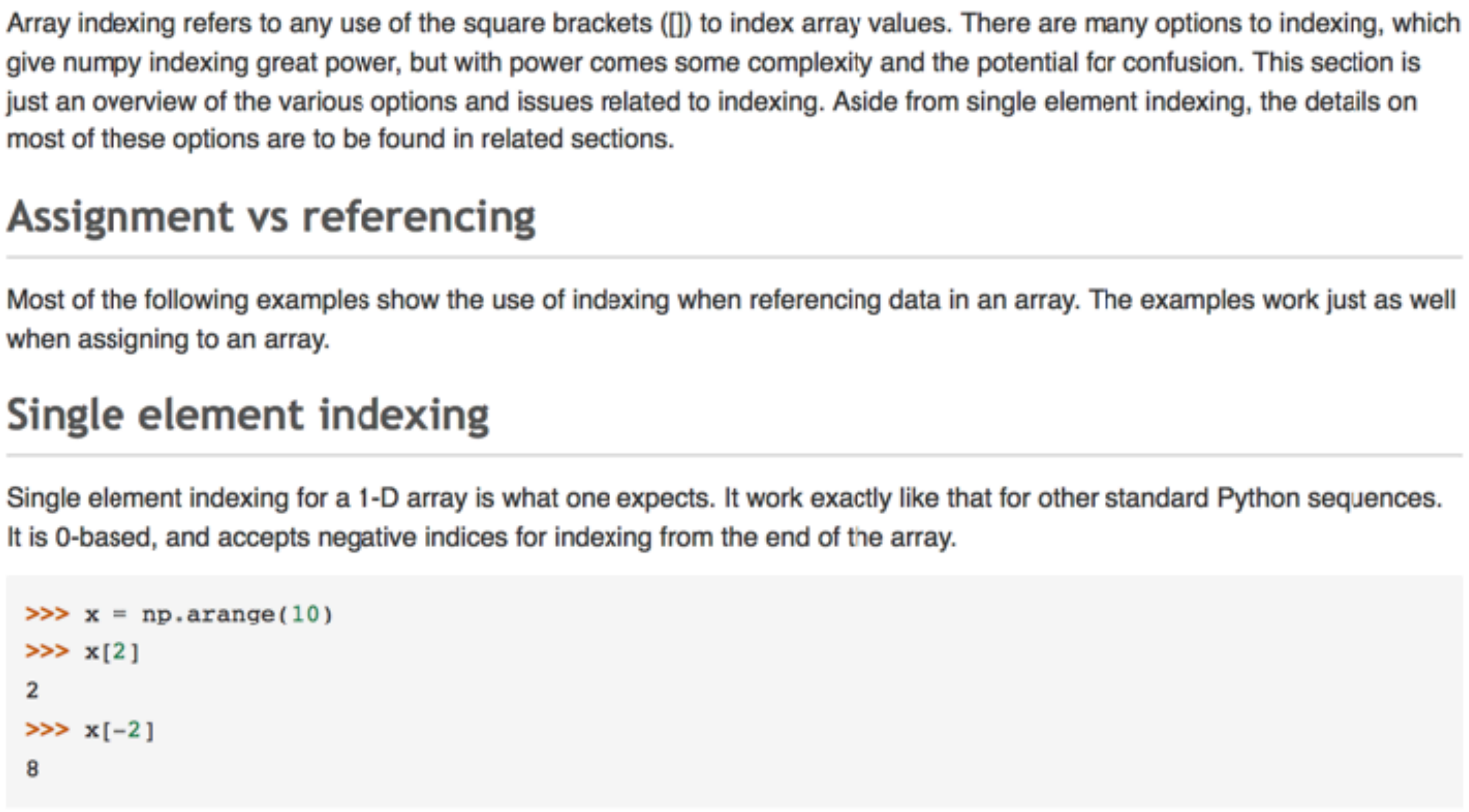
```
b=np.ravel(a)
print b
```

```
[1 2 3 4]
```

Flatten always returns a copy

Ravel returns a view

Indexing



Array indexing refers to any use of the square brackets ([]) to index array values. There are many options to indexing, which give numpy indexing great power, but with power comes some complexity and the potential for confusion. This section is just an overview of the various options and issues related to indexing. Aside from single element indexing, the details on most of these options are to be found in related sections.

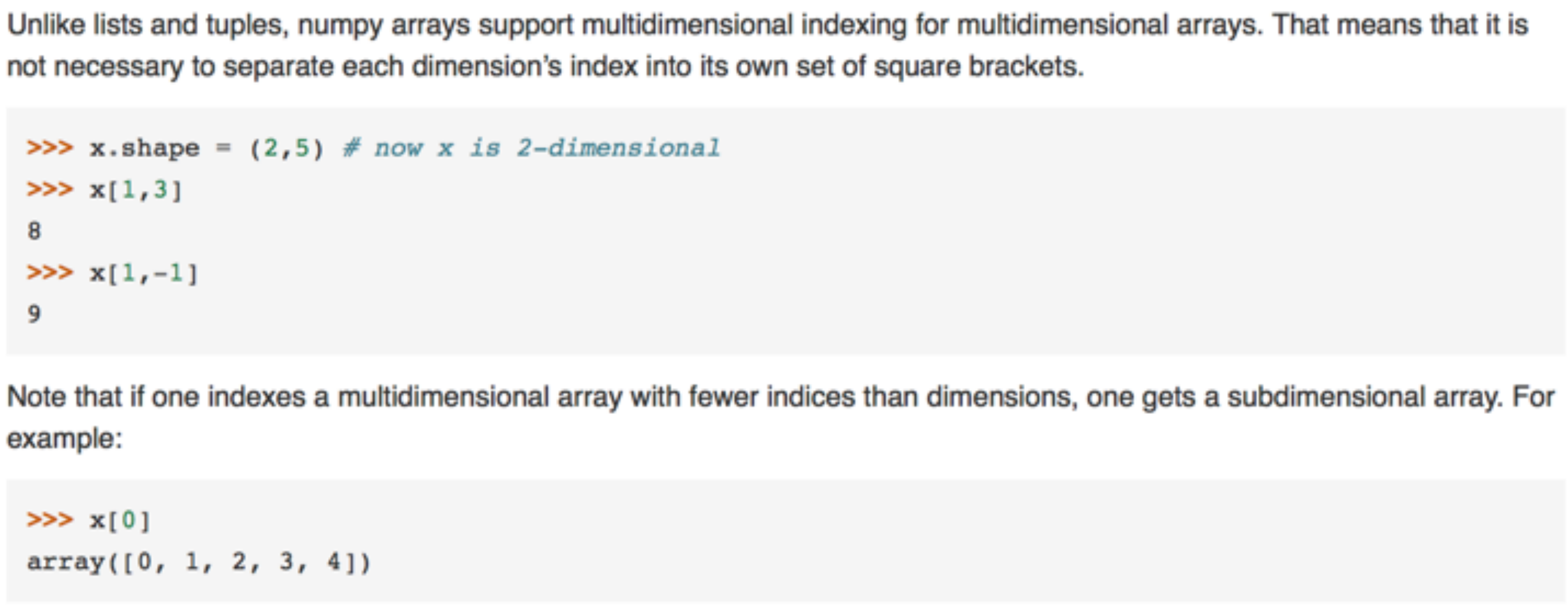
Assignment vs referencing

Most of the following examples show the use of indexing when referencing data in an array. The examples work just as well when assigning to an array.

Single element indexing

Single element indexing for a 1-D array is what one expects. It work exactly like that for other standard Python sequences. It is 0-based, and accepts negative indices for indexing from the end of the array.

```
>>> x = np.arange(10)
>>> x[2]
2
>>> x[-2]
8
```


Unlike lists and tuples, numpy arrays support multidimensional indexing for multidimensional arrays. That means that it is not necessary to separate each dimension's index into its own set of square brackets.

```
>>> x.shape = (2,5) # now x is 2-dimensional
>>> x[1,3]
8
>>> x[1,-1]
9
```

Note that if one indexes a multidimensional array with fewer indices than dimensions, one gets a subdimensional array. For example:

```
>>> x[0]
array([0, 1, 2, 3, 4])
```

That is, each index specified selects the array corresponding to the rest of the dimensions selected. In the above example, choosing 0 means that the remaining dimension of length 5 is being left unspecified, and that what is returned is an array of that dimensionality and size. It must be noted that the returned array is not a copy of the original, but points to the same values in memory as does the original array. In this case, the 1-D array at the first position (0) is returned. So using a single index on the returned array, results in a single element being returned. That is:

```
>>> x[0][2]
2
```

So note that `x[0,2] = x[0][2]` though the second case is more inefficient as a new temporary array is created after the first index that is subsequently indexed by 2.

```
>>> x = np.arange(10)
>>> x[2:5]
array([2, 3, 4])
>>> x[:-7]
array([0, 1, 2])
>>> x[1:7:2]
array([1, 3, 5])
>>> y = np.arange(35).reshape(5,7)
>>> y[1:5:2,::3]
array([[ 7, 10, 13],
       [21, 24, 27]])
```

Index arrays

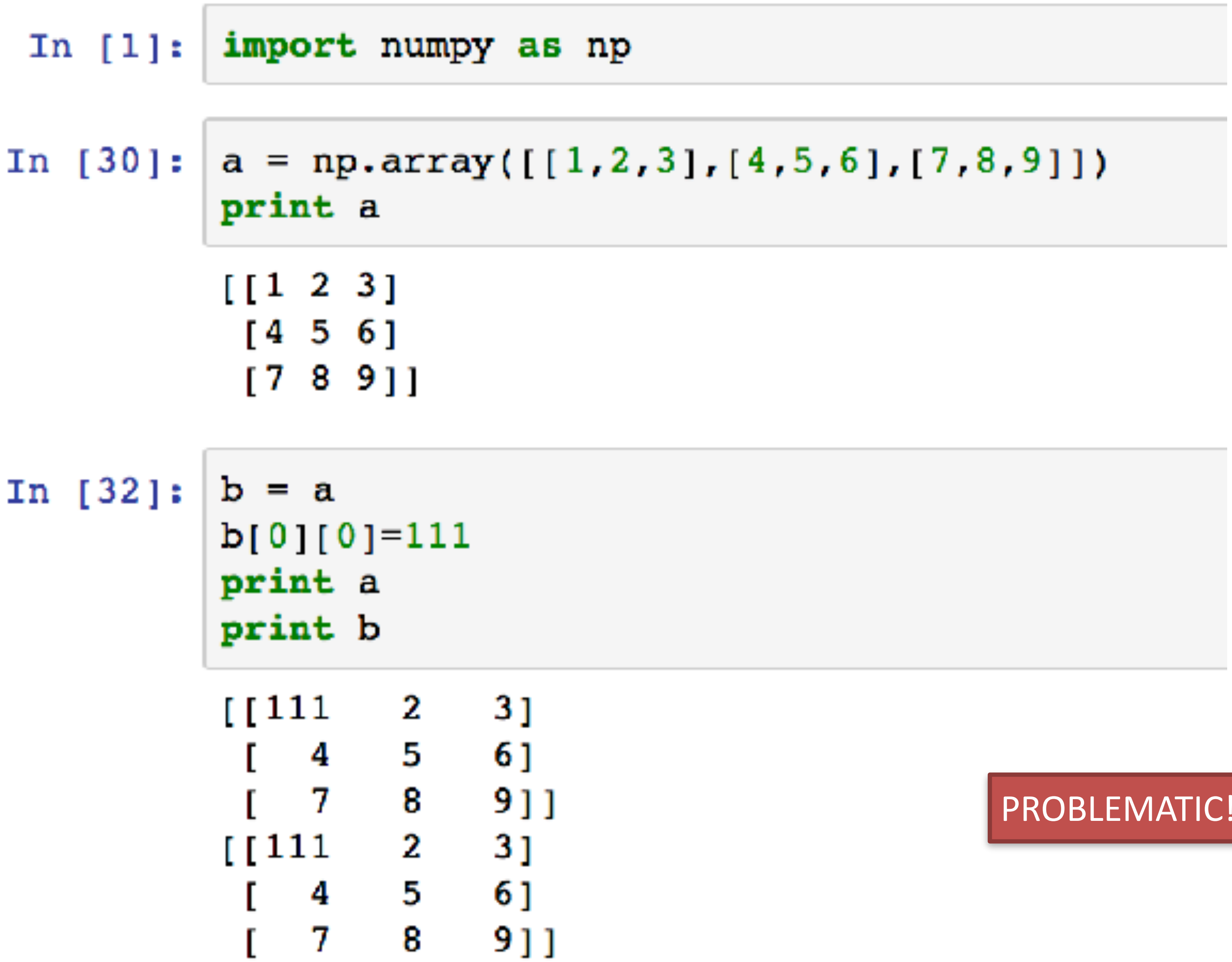
NumPy arrays may be indexed with other arrays (or any other sequence- like object that can be converted to an array, such as lists, with the exception of tuples; see the end of this document for why this is). The use of index arrays ranges from simple, straightforward cases to complex, hard-to-understand cases. For all cases of index arrays, what is returned is a copy of the original data, not a view as one gets for slices.

Index arrays must be of integer type. Each value in the array indicates which value in the array to use in place of the index. To illustrate:

```
>>> x = np.arange(10,1,-1)
>>> x
array([10,  9,  8,  7,  6,  5,  4,  3,  2])
>>> x[np.array([3, 3, 1, 8])]
array([7, 7, 9, 2])
```

```
>>> a
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> b = a < 6
>>> b
array([ True,  True,  True,  True,  True,  True, False, False,
False, False], dtype=bool)
>>> c = a[b]
>>> c
array([0, 1, 2, 3, 4, 5])
```

Assignment



```
In [1]: import numpy as np
```

```
In [30]: a = np.array([[1,2,3],[4,5,6],[7,8,9]])
         print a
```

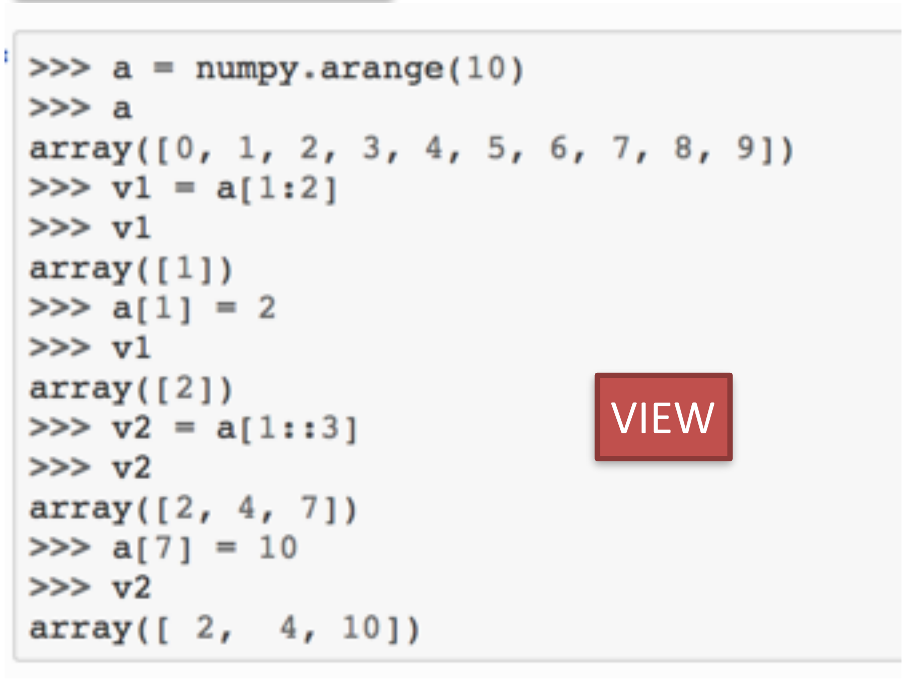
```
[[1 2 3]
 [4 5 6]
 [7 8 9]]
```

```
In [32]: b = a
         b[0][0]=111
         print a
         print b
```

```
[[111   2   3]
 [  4   5   6]
 [  7   8   9]]
[[111   2   3]
 [  4   5   6]
 [  7   8   9]]
```

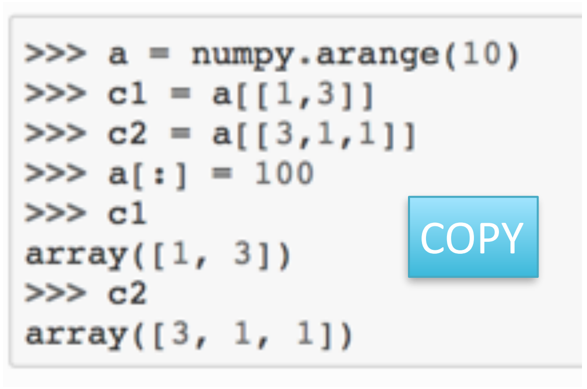
PROBLEMATIC!

views versus copy



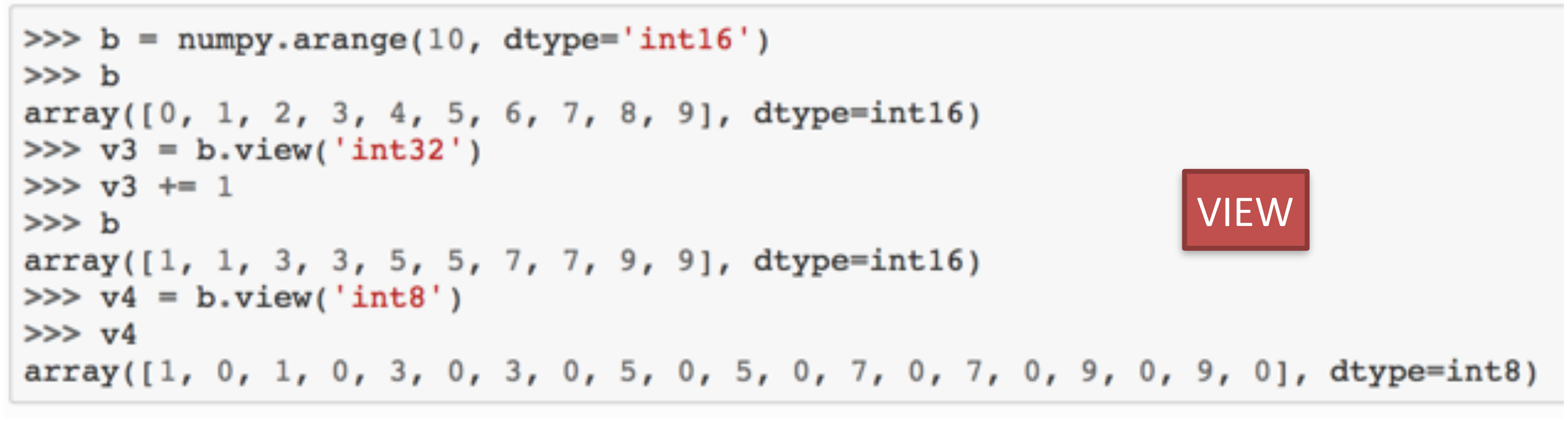
```
>>> a = numpy.arange(10)
>>> a
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> v1 = a[1:2]
>>> v1
array([1])
>>> a[1] = 2
>>> v1
array([2])
>>> v2 = a[1::3]
>>> v2
array([2, 4, 7])
>>> a[7] = 10
>>> v2
array([ 2,  4, 10])
```

VIEW



```
>>> a = numpy.arange(10)
>>> c1 = a[[1,3]]
>>> c2 = a[[3,1,1]]
>>> a[:] = 100
>>> c1
array([1, 3])
>>> c2
array([3, 1, 1])
```

COPY



```
>>> b = numpy.arange(10, dtype='int16')
>>> b
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9], dtype=int16)
>>> v3 = b.view('int32')
>>> v3 += 1
>>> b
array([1, 1, 3, 3, 5, 5, 7, 7, 9, 9], dtype=int16)
>>> v4 = b.view('int8')
>>> v4
array([1, 0, 1, 0, 3, 0, 3, 0, 5, 0, 5, 0, 7, 0, 7, 0, 9, 0, 9, 0], dtype=int8)
```

VIEW

http://scipy-cookbook.readthedocs.io/items/ViewsVsCopies.html

But fancy indexing does seem to return views sometimes, doesn't it?

Many users get fooled and think that fancy indexing returns views instead of copies when they use this idiom:

In [ ]:
```
>>> a = numpy.arange(10)
>>> a[[1,2]] = 100
>>> a
array([  0, 100, 100,   3,   4,   5,   6,   7,   8,   9])
```

So, it seems that a<1,2> is actually a *view* because elements 1 and 2 have been updated. However, if we try this step by step, it won't work:

In [ ]:
```
>>> a = numpy.arange(10)
>>> c1 = a[[1,2]]
>>> c1[:] = 100
>>> a
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> c1
array([100, 100])
```

In [ ]:
```
>>> a = numpy.arange(10)
>>> c1 = a[[1,2]]
>>> c1[:] = 100
>>> a
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> c1
array([100, 100])
```

What happens here is that, in the first idiom (), the python interpreter translate it to:

In [ ]:
```
a.__setitem__([1,2], 100)
```

i.e. there is not need to create neither a view or a copy because the method can be evaluated *inplace* (i.e. no new object creation is involved).

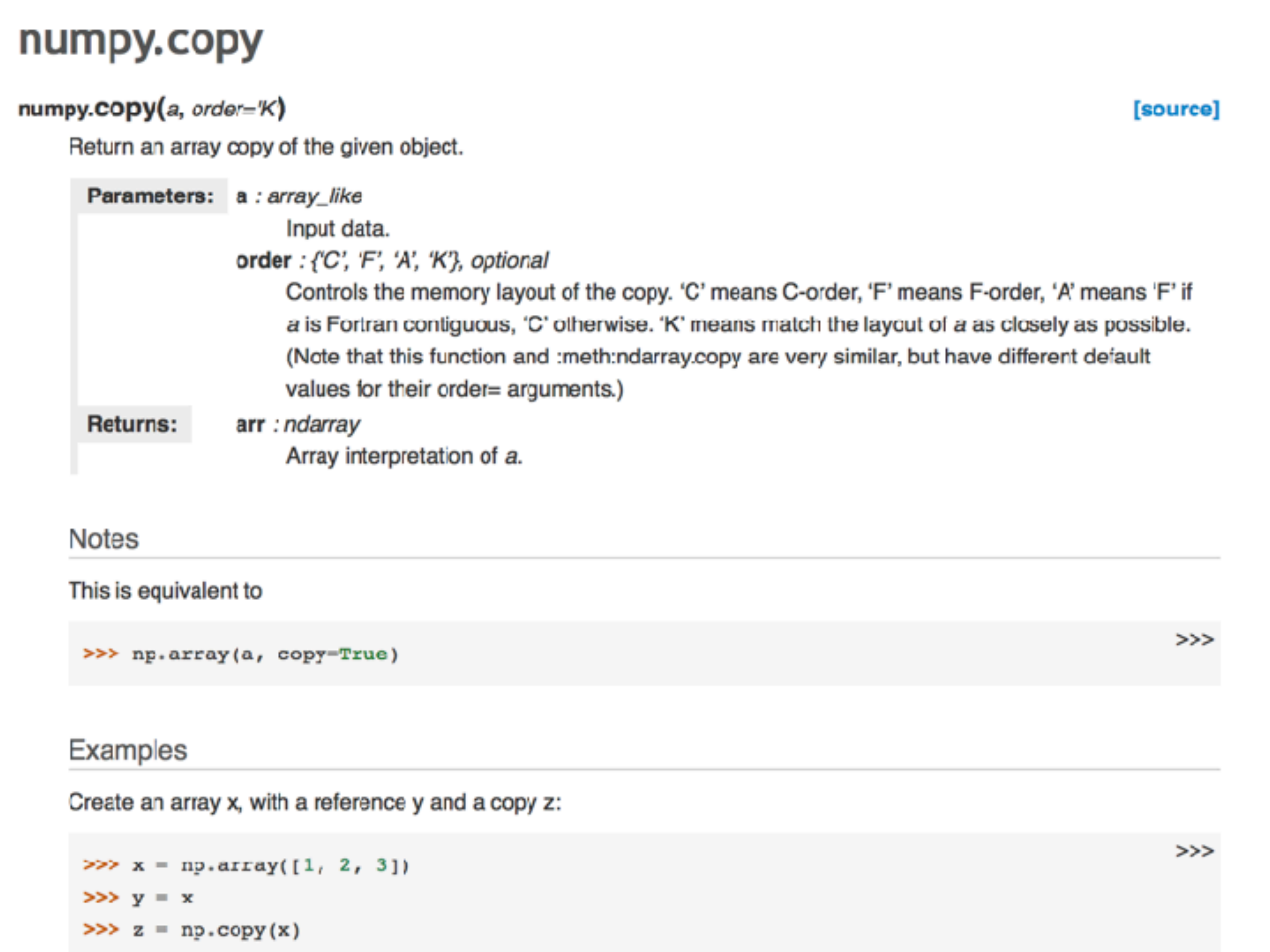
However, the second idiom () is translated to:

In [ ]:
```
c1 = a.__getitem__([1,2])
c1.__setitem__(slice(None, None, None), 100)  # [:] translates into slice(None,
None, None)
```

Read/Study these these sections

https://docs.scipy.org/doc/numpy-1.13.0/user/basics.indexing.html

http://scipy-cookbook.readthedocs.io/items/ViewsVsCopies.html



numpy.copy

numpy.copy(*a*, *order='K'*) [source]

Return an array copy of the given object.

Parameters: **a** : *array_like*

Input data.

order : *{'C', 'F', 'A', 'K'}, optional*

Controls the memory layout of the copy. 'C' means C-order, 'F' means F-order, 'A' means 'F' if *a* is Fortran contiguous, 'C' otherwise. 'K' means match the layout of *a* as closely as possible. (Note that this function and :meth:ndarray.copy are very similar, but have different default values for their order= arguments.)

Returns: **arr** : *ndarray*

Array interpretation of *a*.

Notes

This is equivalent to

```
>>> np.array(a, copy=True)
```

Examples

Create an array x, with a reference y and a copy z:

```
>>> x = np.array([1, 2, 3])
>>> y = x
>>> z = np.copy(x)
```

Notes

This is equivalent to

```
>>> np.array(a, copy=True)
```

Examples

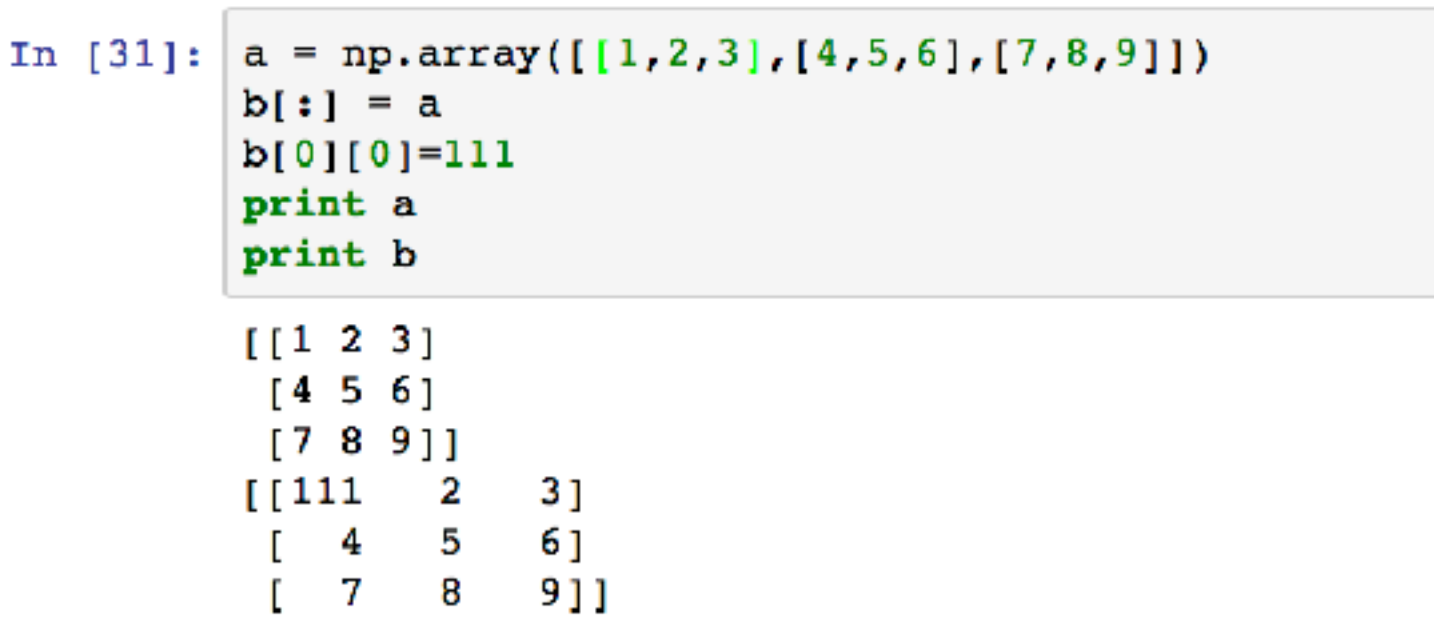
Create an array x, with a reference y and a copy z:

```
>>> x = np.array([1, 2, 3])
>>> y = x
>>> z = np.copy(x)
```

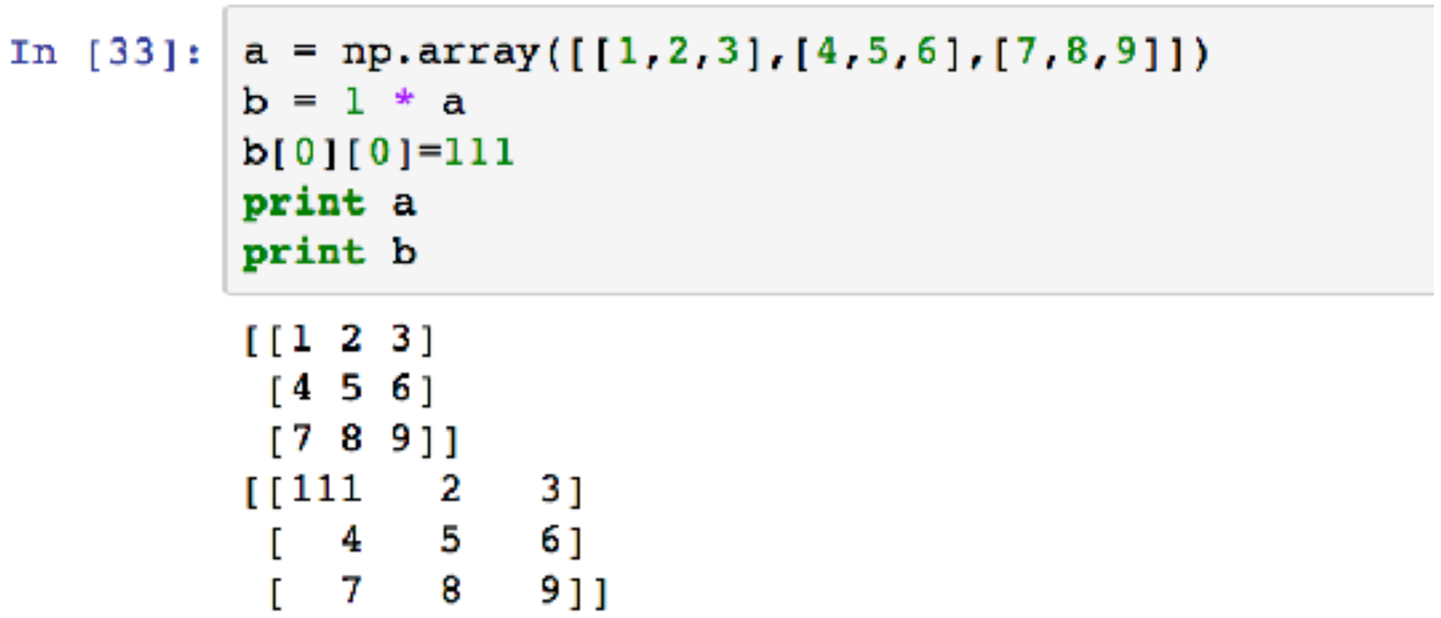
Note that, when we modify x, y changes, but not z:

```
>>> x[0] = 10
>>> x[0] == y[0]
True
>>> x[0] == z[0]
False
```

Assignment: TWO POSSIBLE SOLUTIONS



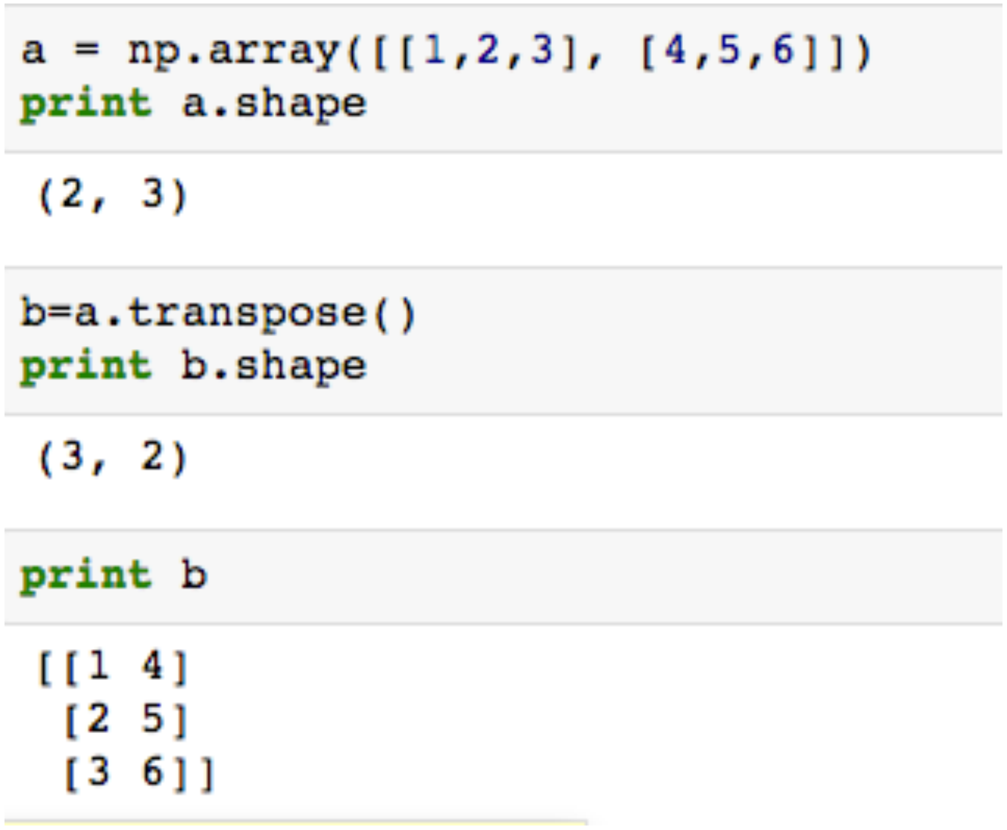
```
In [31]: a = np.array([[1,2,3],[4,5,6],[7,8,9]])
         b[:] = a
         b[0][0]=111
         print a
         print b

         [[1 2 3]
          [4 5 6]
          [7 8 9]]
         [[111   2   3]
          [  4   5   6]
          [  7   8   9]]
```



```
In [33]: a = np.array([[1,2,3],[4,5,6],[7,8,9]])
         b = 1 * a
         b[0][0]=111
         print a
         print b

         [[1 2 3]
          [4 5 6]
          [7 8 9]]
         [[111   2   3]
          [  4   5   6]
          [  7   8   9]]
```

Transpose for dimension shuffling

- If **A** is an $m \times n$ matrix then $\mathbf{A}^T$ is an *n x m* matrix



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

```
(2, 3)
```

```
b=a.transpose()
print b.shape
```

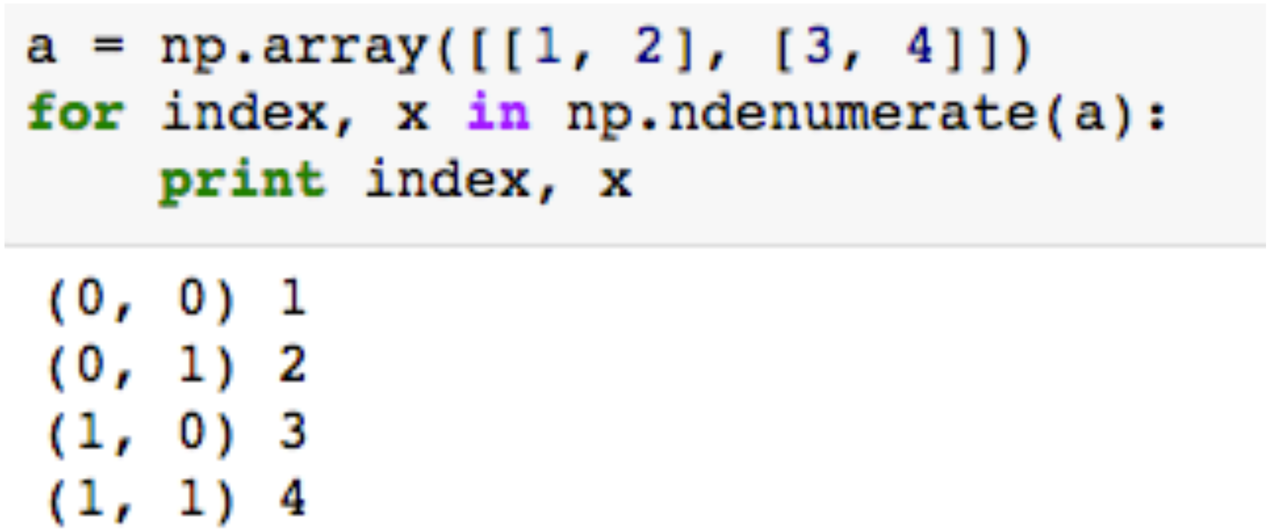
```
(3, 2)
```

```
print b
```

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

ndenumerate

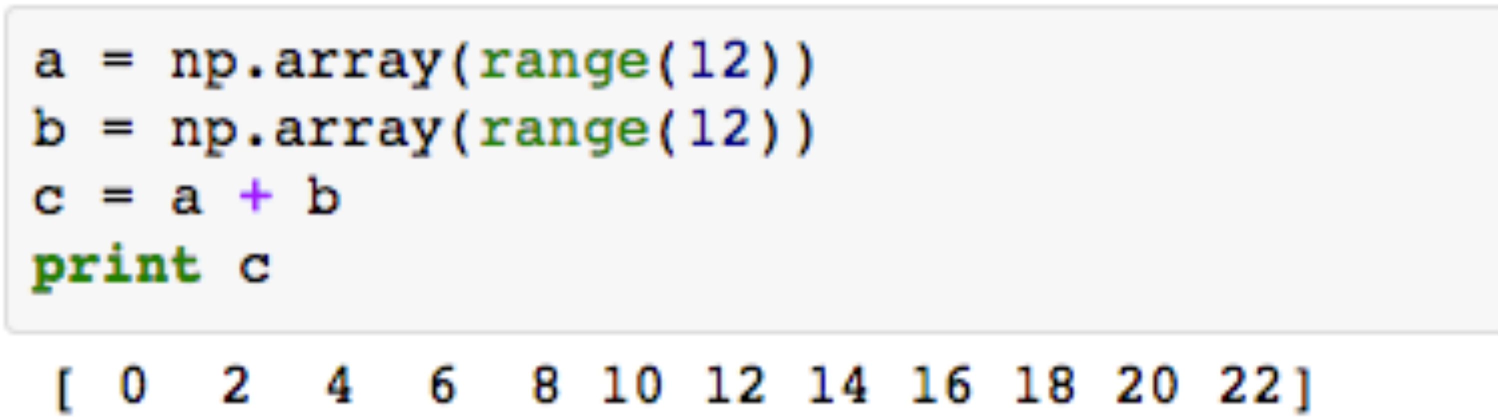
- Multidimensional index iterator.
- Return an iterator yielding pairs of array coordinates and values.



```python
a = np.array([[1, 2], [3, 4]])
for index, x in np.ndenumerate(a):
    print index, x
```

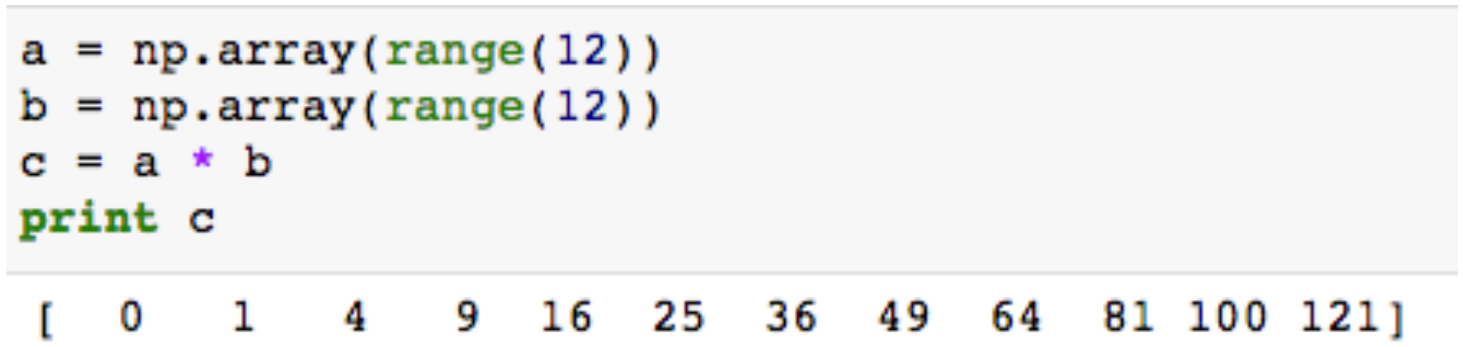
```
(0, 0) 1
(0, 1) 2
(1, 0) 3
(1, 1) 4
```

Adding and multiplying element wise



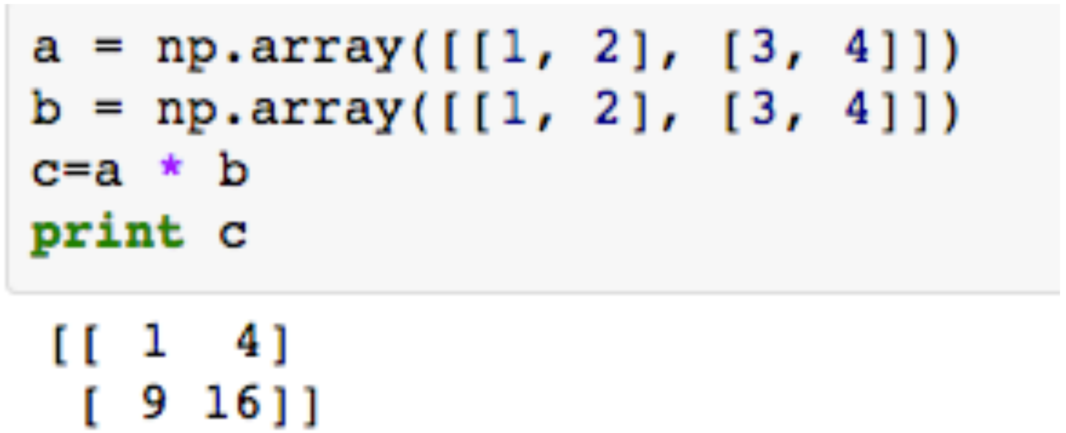
```
a = np.array(range(12))
b = np.array(range(12))
c = a + b
print c
```

```
[ 0  2  4  6  8 10 12 14 16 18 20 22]
```



```
a = np.array(range(12))
b = np.array(range(12))
c = a * b
print c
```

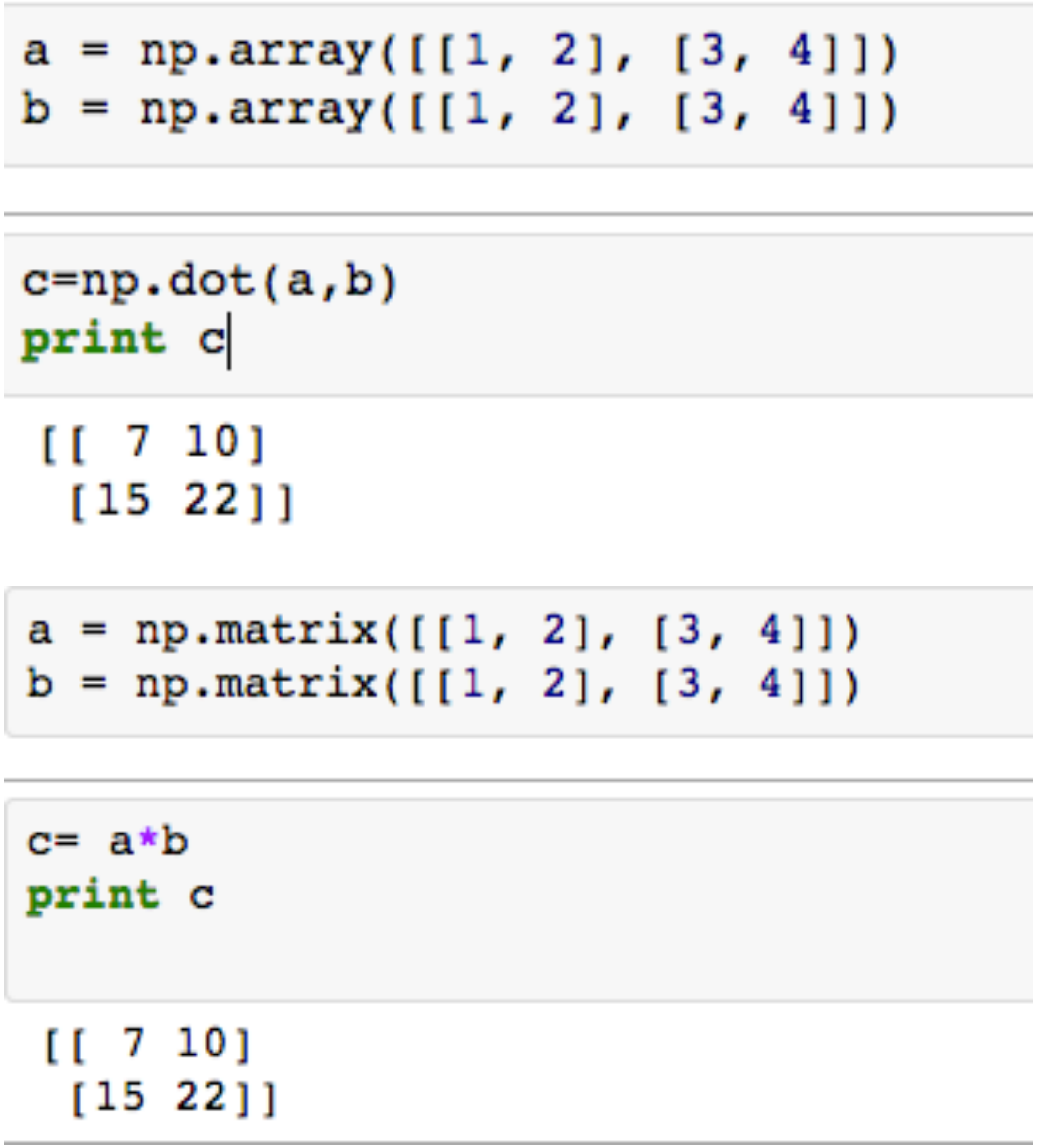
```
[  0   1   4   9  16  25  36  49  64  81 100 121]
```



```
a = np.array([[1, 2], [3, 4]])
b = np.array([[1, 2], [3, 4]])
c=a * b
print c
```

```
[[ 1  4]
 [ 9 16]]
```

Matrix multiplication



```
a = np.array([[1, 2], [3, 4]])
b = np.array([[1, 2], [3, 4]])
```

array

```
c=np.dot(a,b)
print c
```

```
[[ 7 10]
 [15 22]]
```

matrix

```
a = np.matrix([[1, 2], [3, 4]])
b = np.matrix([[1, 2], [3, 4]])
```

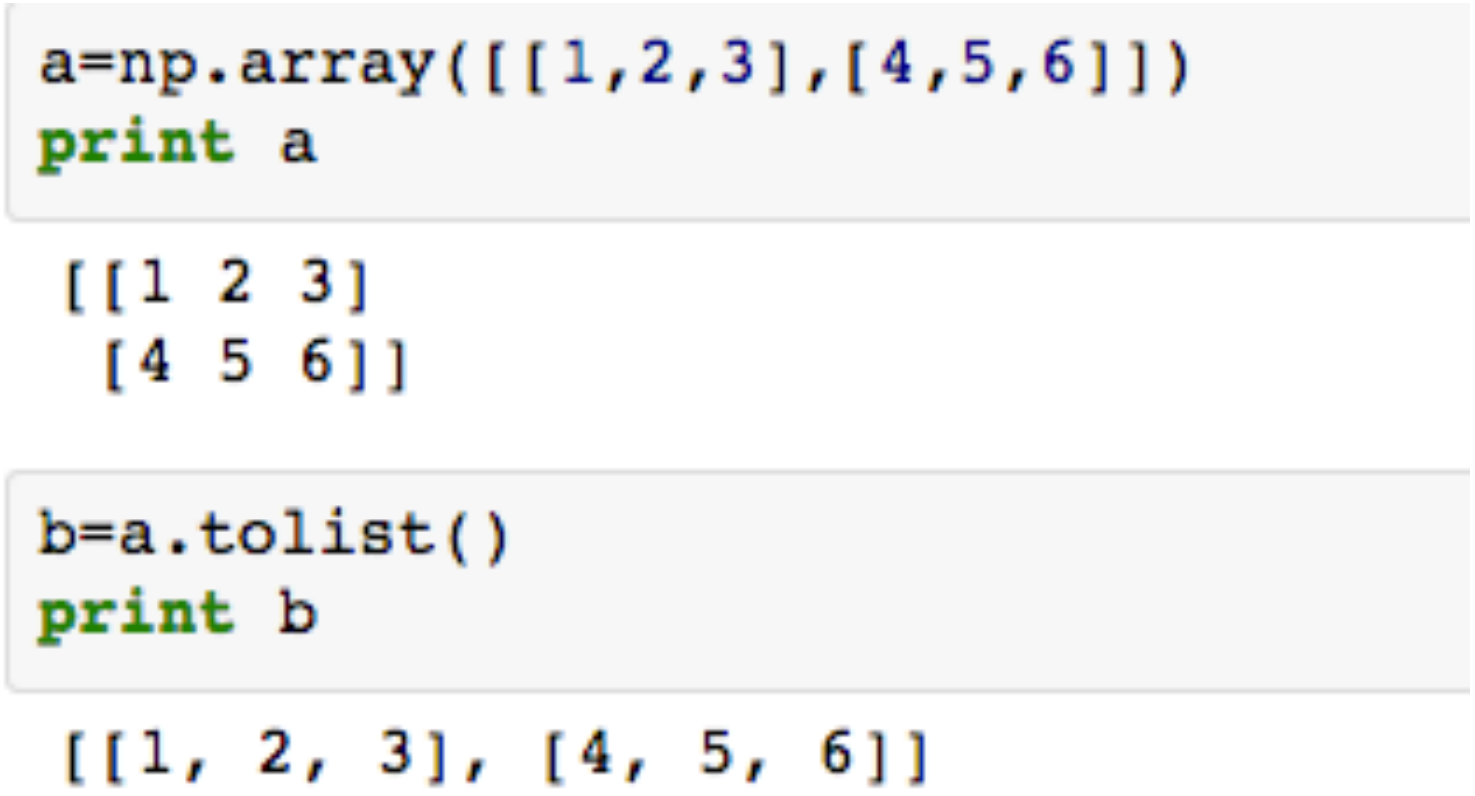
```
c= a*b
print c
```

```
[[ 7 10]
 [15 22]]
```

Many operations work with arrays

- abs, cos, sin, ...
- accumulate, all
- append, arange, argsort, array_split, matrix,
- asmatrix (not copied)
- average, copy, cross,delete
- linear algebra: diagonal, dot, eye, fill, fix, flat (iterator), flatten, indices, inner, insert, item, linspace, mat, maximum, ndim, outer, pinv, repeat, reshape, shape, swapaxis, tile, tolist, transpose, zeros

Converting numpy array to python list



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

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

```
b=a.tolist()
print b
```

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

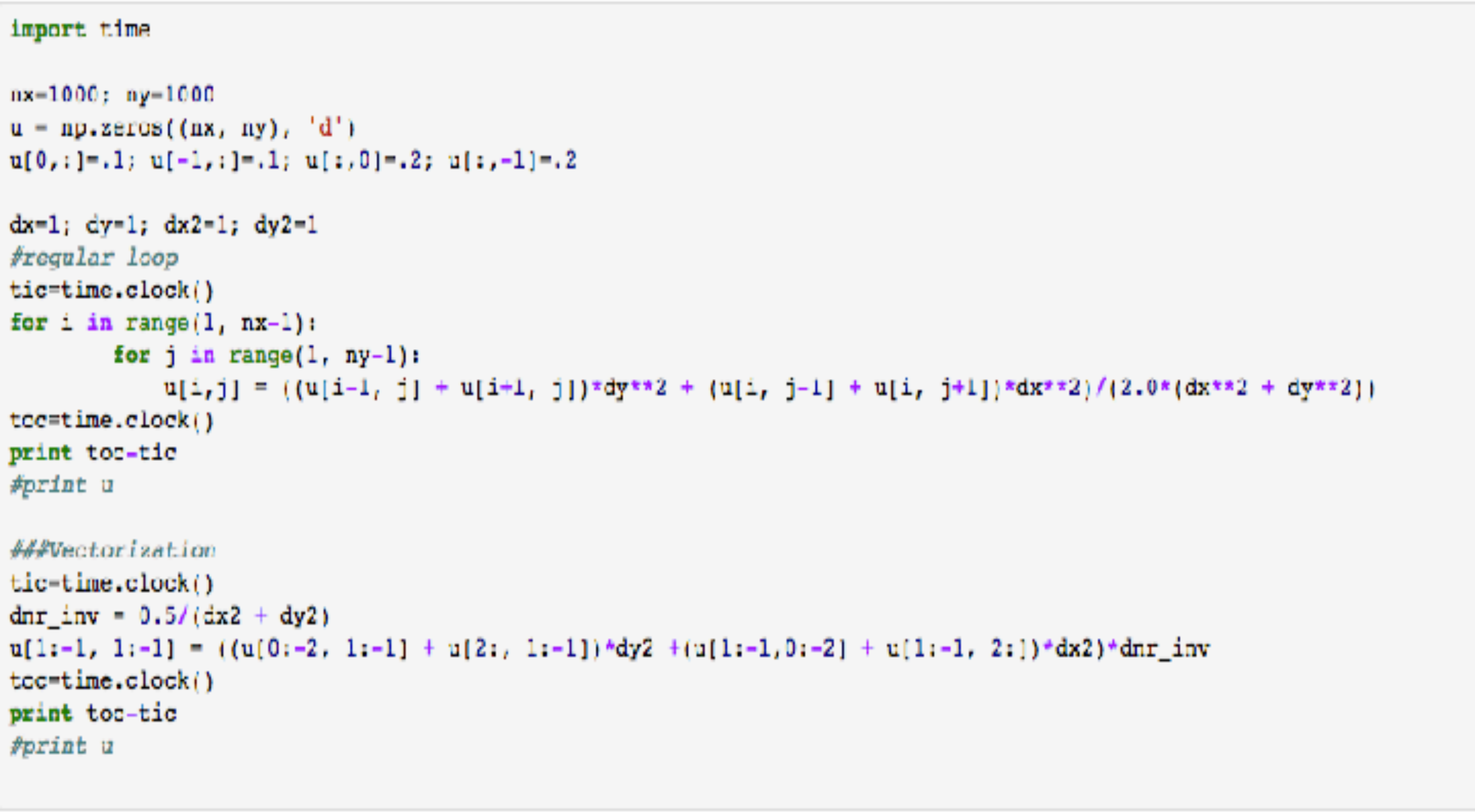
Regular loop vs vectorization

Example : 2D Lapacian equation

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} = \psi_{xx} + \psi_{yy} = 0$$

Numerical solution using finite difference

$$T_{ij} = \frac{\gamma_y^2(T_{i-1,j} + T_{i+1,j} + r_x(T_{i+1,j} - T_{i-1,j})) + \gamma_x^2(T_{i,j-1} + T_{i,j+1} + r_y(T_{i,j+1} - T_{i,j-1}))}{2(\gamma_x^2 + \gamma_y^2)}$$



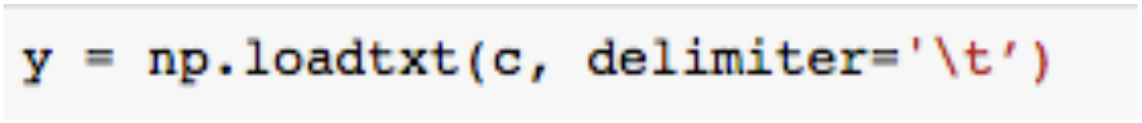
```
import time

nx=1000; ny=1000
u = np.zeros((nx, ny), 'd')
u[0,:]=.1; u[-1,:]=.1; u[:,0]=.2; u[:,-1]=.2

dx=1; dy=1; dx2=1; dy2=1
#regular loop
tic=time.clock()
for i in range(1, nx-1):
        for j in range(1, ny-1):
            u[i,j] = ((u[i-1, j] + u[i+1, j])*dy**2 + (u[i, j-1] + u[i, j+1])*dx**2)/(2.0*(dx**2 + dy**2))
toc=time.clock()
print toc-tic
#print u

###Vectorization
tic=time.clock()
dnr_inv = 0.5/(dx2 + dy2)
u[1:-1, 1:-1] = ((u[0:-2, 1:-1] + u[2:, 1:-1])*dy2 +(u[1:-1,0:-2] + u[1:-1, 2:])*dx2)*dnr_inv
toc=time.clock()
print toc-tic
#print u
```

comparison

	N=10	N=100	N=1000
loop	0.000897000000002	0.106809	6.922471
Vectorization	0.000724000000002	0.00067	0.023252

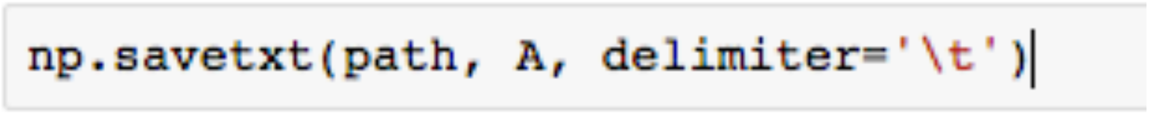
Read and Write files

- Loadtxt : Construct an array from data in a text or binary file.



```
y = np.loadtxt(c, delimiter='\t')
```

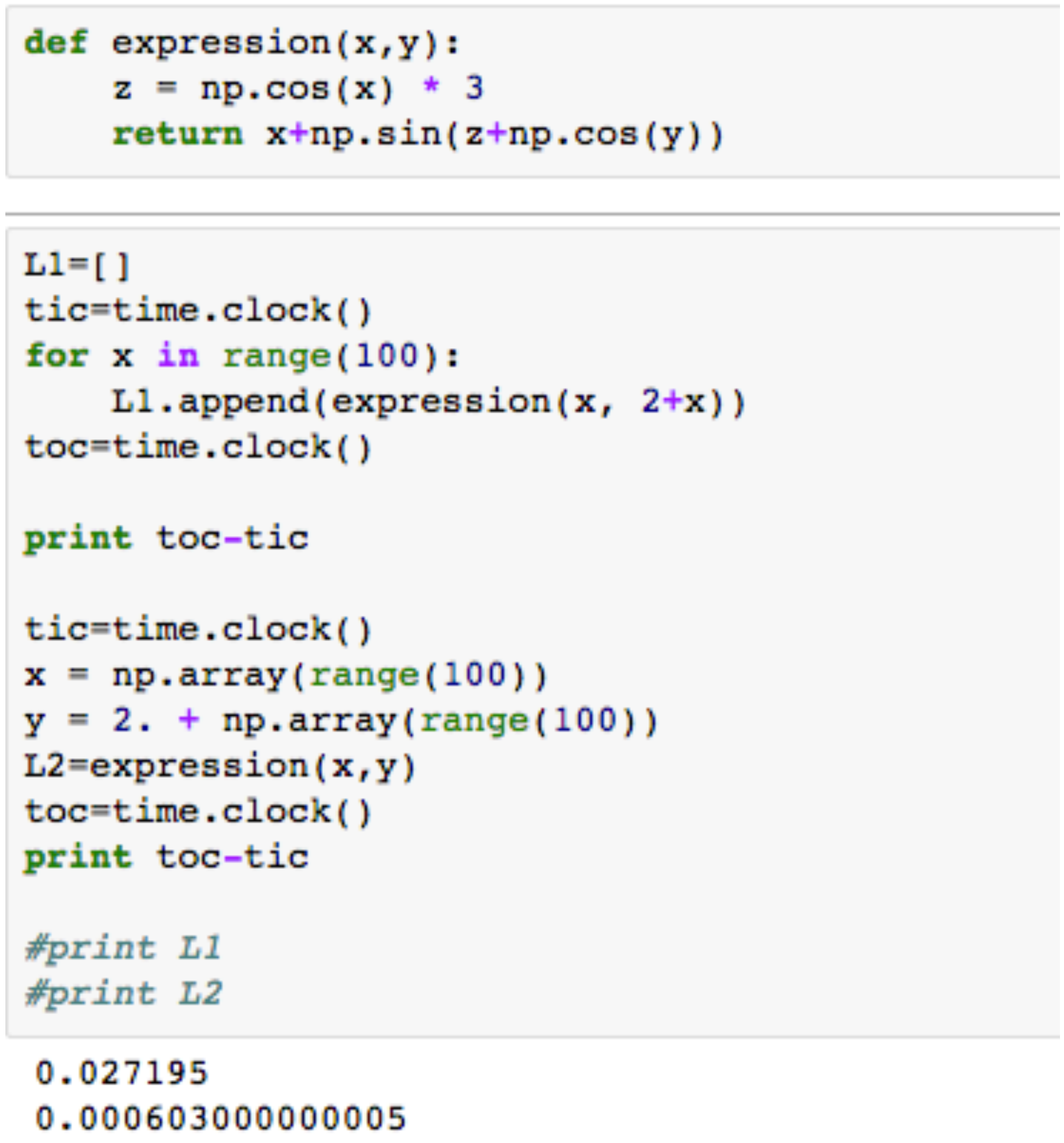
- Savetxt: save as delimitated text



```
np.savetxt(path, A, delimiter='\t')
```

Functions

- Functions with scalar arguments
  - scalar: float, int
- Functions with array arguments
  - automatically speedup



```python
def expression(x,y):
    z = np.cos(x) * 3
    return x+np.sin(z+np.cos(y))
```

```python
L1=[]
tic=time.clock()
for x in range(100):
    L1.append(expression(x, 2+x))
toc=time.clock()

print toc-tic

tic=time.clock()
x = np.array(range(100))
y = 2. + np.array(range(100))
L2=expression(x,y)
toc=time.clock()
print toc-tic

#print L1
#print L2
```

```
0.027195
0.00603000000005
```