NumPy: creating and manipulating numerical data

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Chapters contents

The numpy array object

What are Numpy and numpy arrays

Python has built-in:

- containers: lists (costless insertion and append), dictionnaries (fast lookup)
- high-level number objects: integers, floating point

Numpy is:

- extension package to Python for multidimensional arrays
- closer to hardware (efficiency)
- designed for scientific computation (convenience)

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

For example:

An array containing:

- discretized time of an experiment/simulation
- signal recorded by a measurement device
- pixels of an image
- ...

Why it is useful: Memory-efficient and fast container for numerical operations.

```
In [1]: l = range(1000)

In [2]: %timeit [i**2 for i in l]
1000 loops, best of 3: 403 us per loop

In [3]: a = np.arange(1000)

In [4]: %timeit a**2
100000 loops, best of 3: 12.7 us per loop
```

Reference documentation

- On the web: http://docs.scipy.org/
- Interactive help:

```
>>> help(np.array)
array(object, dtype=None, copy=True, order=None, subok=False, ndmin=0)
```

```
    Create an array.

    Parameters
    ----------
    object : array_like
    ...

    Examples
    --------
    >>> np.array([1, 2, 3])
    array([1, 2, 3])
    ...
```

- Looking for something:

```
>>> np.lookfor('create array') 
    Search results for 'create array'
    ---------------------------------
    numpy.array
        Create an array.
    numpy.memmap
         Create a memory-map to an array stored in a *binary* file on
    disk.
    ...
```

```
>>> help(np.lookfor)             
    ...
```

Creating arrays

1-D:

```
>>> a = np.array([0, 1, 2, 3])
>>> a
array([0, 1, 2, 3])
>>> a.ndim
1
>>> a.shape
(4,)
>>> len(a)
4
```

2-D, 3-D, ...:

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

```
2

>>> c = np.array([[[1], [2]], [[3], [4]]])
>>> c
array([[[1],
        [2]],

       [[3],
        [4]]])
>>> c.shape
(2, 2, 1)
```

In practice, we rarely enter items one by one...

- Evenly spaced:

```
>>> import numpy as np
      >>> a = np.arange(10) # 0 .. n-1  (!)
      >>> a
      array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
      >>> b = np.arange(1, 9, 2) # start, end (exlusive), step
      >>> b
      array([1, 3, 5, 7])
```

or by number of points:

```
>>> c = np.linspace(0, 1, 6)   # start, end, num-points
      >>> c
      array([ 0. ,  0.2,  0.4,  0.6,  0.8,  1. ])
      >>> d = np.linspace(0, 1, 5, endpoint=False)
      >>> d
      array([ 0. ,  0.2,  0.4,  0.6,  0.8])
```

- Common arrays:

```
>>> a = np.ones((3, 3))  # reminder: (3, 3) is a tuple
      >>> a
      array([[ 1.,  1.,  1.],
             [ 1.,  1.,  1.],
             [ 1.,  1.,  1.]])
      >>> b = np.zeros((2, 2))
      >>> b
      array([[ 0.,  0.],
             [ 0.,  0.]])
      >>> c = np.eye(3)
      >>> c
      array([[ 1.,  0.,  0.],
             [ 0.,  1.,  0.],
             [ 0.,  0.,  1.]])
      >>> d = np.diag(np.array([1, 2, 3, 4]))
      >>> d
      array([[1, 0, 0, 0],
             [0, 2, 0, 0],
             [0, 0, 3, 0],
             [0, 0, 0, 4]])
```

- `np.random`: random numbers (Mersenne Twister PRNG):

```
>>> a = np.random.rand(4)       # uniform in [0, 1]
>>> a
array([ 0.58597729,  0.86110455,  0.9401114 ,  0.54264348])

>>> b = np.random.randn(4)      # Gaussian
>>> b
array([-2.56844807,  0.06798064, -0.36823781,  0.86966886])

>>> np.random.seed(1234)        # Setting the random seed
```

Exercise: Array creation

Create the following arrays (with correct data types):

```
[[ 1   1   1   1]
 [ 1   1   1   1]
 [ 1   1   1   2]
 [ 1   6   1   1]]

[[0. 0. 0. 0. 0.]
 [2. 0. 0. 0. 0.]
 [0. 3. 0. 0. 0.]
 [0. 0. 4. 0. 0.]
 [0. 0. 0. 5. 0.]
 [0. 0. 0. 0. 6.]]
```

Par on course: 3 statements for each

Exercise: Tiling for array creation

Skim through the documentation for `np.tile`, and use this function to construct the array:

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

Basic data types

You probably noted the `1` and `1.` above. These are different data types:

```
>>> a = np.array([1, 2, 3])
>>> a.dtype
dtype('int64')

>>> b = np.array([1., 2., 3.])
>>> b.dtype
dtype('float64')
```

Much of the time you don’t necessarily need to care, but remember they are there.

You can also choose which one you want:

```
>>> c = np.array([1, 2, 3], dtype=float)
      >>> c.dtype
      dtype('float64')
```

The **default** data type is floating point:

```
>>> a = np.ones((3, 3))
      >>> a.dtype
      dtype('float64')
```

There are also other types:

Complex	`>>> d = np.array([1+2j, 3+4j, 5+6*1j])`
	`>>> d.dtype`
	`dtype('complex128')`

Bool	`>>> e = np.array([True, False, False, True])`
	`>>> e.dtype`
	`dtype('bool')`

Strings	`>>> f = np.array(['Bonjour', 'Hello', 'Hallo',])`
	`>>> f.dtype`
	`dtype('S7')          # <--- strings containing max. 7 letters`

Much more: int32/int64...	

Basic visualization

Now that we have our first data arrays, we are going to visualize them.

Matplotlib is a 2D plotting package. We can import its functions as below:

```
>>> import matplotlib.pyplot as plt  # the tidy way
```

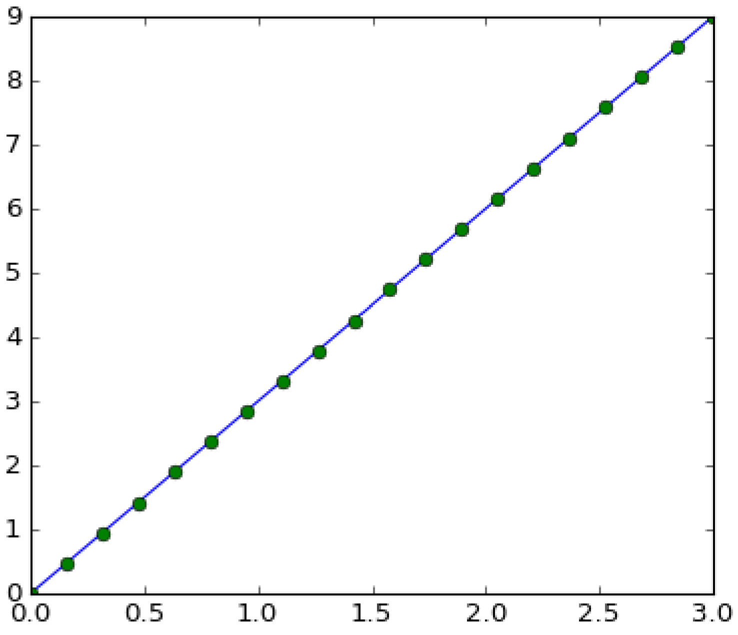
The recommended way of working is use `IPython`, started in `pylab` mode:

```
$ ipython -pylab
```

1D plotting

```
>>> x = np.linspace(0, 3, 20)
      >>> y = np.linspace(0, 9, 20)
      >>> plt.plot(x, y)       # line plot
      >>> plt.plot(x, y, 'o')  # dot plot
      >>> plt.show()           # <-- shows the plot (not needed with Ipython)
```

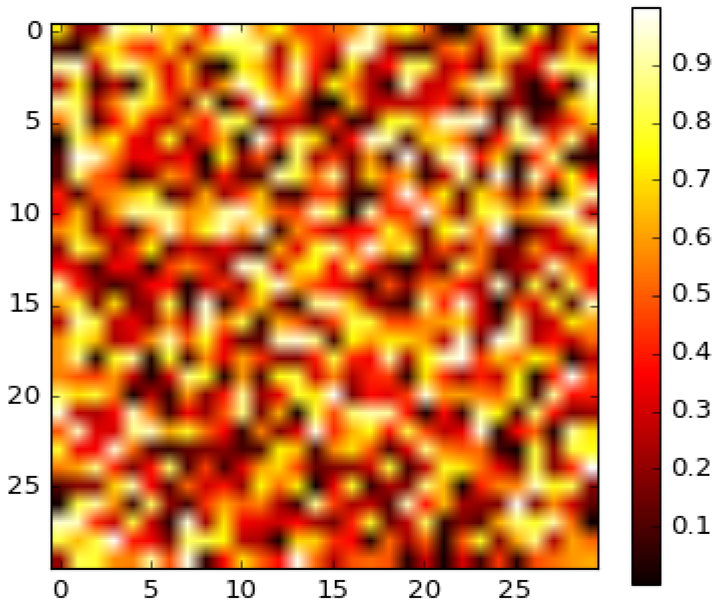
[source code, hires.png, pdf]



2D arrays (such as images)

```
>>> image = np.random.rand(30, 30)
      >>> plt.imshow(image, cmap=plt.cm.gray)
      >>> plt.colorbar()
      >>> plt.show()
```

[source code, hires.png, pdf]

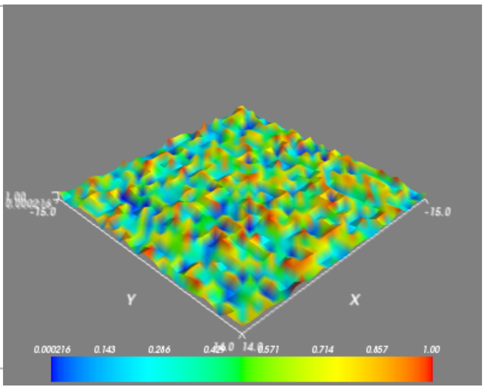


See also: More in the *matplotlib chapter*

3D plotting

For 3D visualization, we can use another package: **Mayavi**. A quick example: start with **relaunching iPython** with these options: **ipython -pylab -wthread** (or **ipython –pylab=wx** in IPython >= 0.10).

```
In [59]: from enthought.mayavi import mlab
      In [60]: mlab.figure()
      Out[60]: <enthought.mayavi.core.scene.
      Scene object at 0xcb2677c>
      In [61]: mlab.surf(image)
      Out[61]: <enthought.mayavi.modules.
      surface.Surface object at 0xd0862fc>
      In [62]: mlab.axes()
      Out[62]: <enthought.mayavi.modules.axes.
      Axes object at 0xd07892c>
```



The mayavi/mlab window that opens is interactive : by clicking on the left mouse button you can rotate the image, zoom with the mouse wheel, etc.

For more information on Mayavi : http://github.enthought.com/mayavi/mayavi

See also: More in the *Mayavi chapter*

Indexing and slicing

The items of an array can be accessed and assigned to the same way as other Python sequences (e.g. lists)

```
>>> a = np.arange(10)
      >>> a
      array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
      >>> a[0], a[2], a[-1]
      (0, 2, 9)
```

⚠ Indices begin at 0, like other Python sequences (and C/C++). In contrast, in Fortran or Matlab, indices begin at 1.

For multidimensional arrays, indexes are tuples of integers:

```
>>> a = np.diag(np.arange(3))
      >>> a
      array([[0, 0, 0],
             [0, 1, 0],
             [0, 0, 2]])
      >>> a[1, 1]
      1
      >>> a[2, 1] = 10 # third line, second column
      >>> a
      array([[ 0,  0,  0],
             [ 0,  1,  0],
             [ 0, 10,  2]])
```

```
    >>> a[1]
    array([0, 1, 0])
```

Note that:

- In 2D, the first dimension corresponds to rows, the second to columns.
- for multidimensional `a`, `a[0]` is interpreted by taking all elements in the unspecified dimensions.

Slicing Arrays, like other Python sequences can also be sliced:

```
>>> a = np.arange(10)
    >>> a
    array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
    >>> a[2:9:3] # [start:end:step]
    array([2, 5, 8])
```

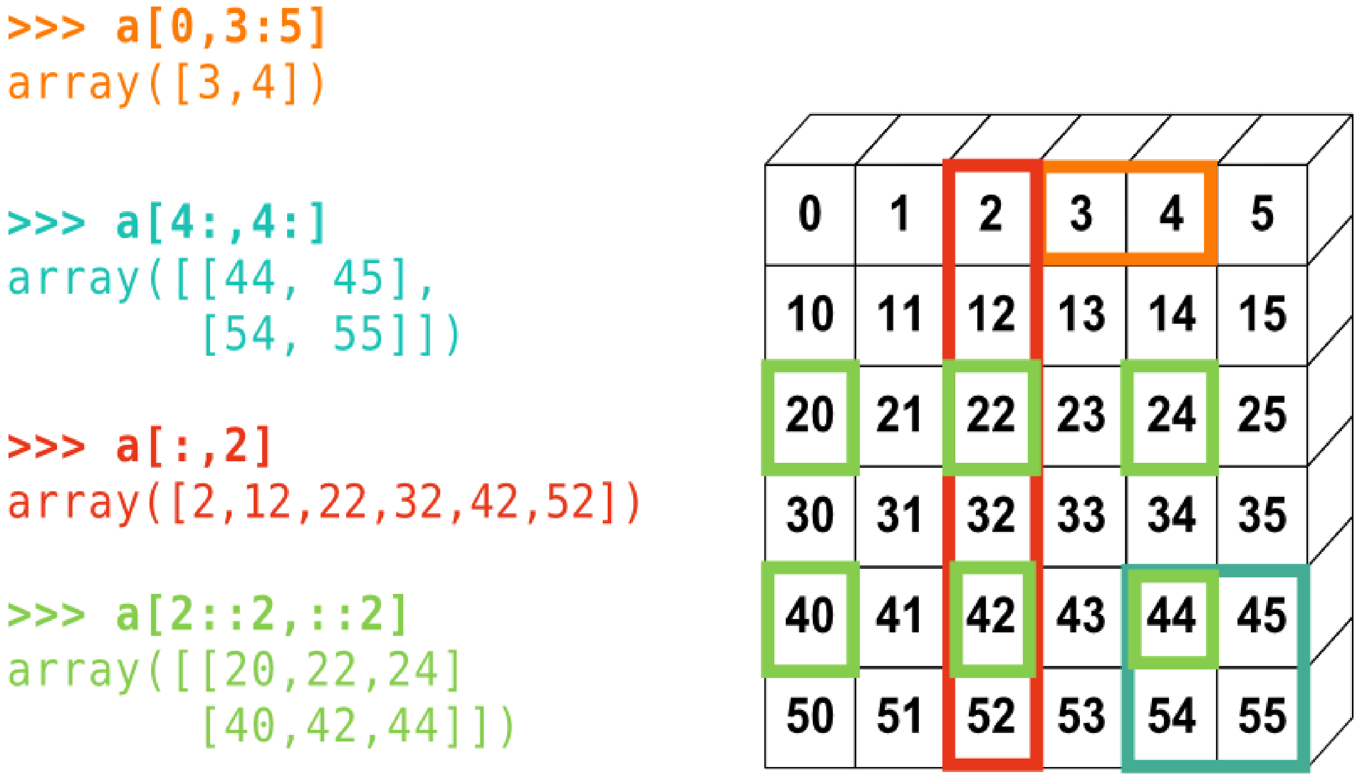
Note that the last index is not included!:

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

All three slice components are not required: by default, `start` is 0, `end` is the last and `step` is 1:

```
>>> a[1:3]
    array([1, 2])
    >>> a[::2]
    array([0, 2, 4, 6, 8])
    >>> a[3:]
    array([3, 4, 5, 6, 7, 8, 9])
```

A small illustrated summary of Numpy indexing and slicing...



```
>>> a[0,3:5]
array([3,4])

>>> a[4:,4:]
array([[44, 45],
       [54, 55]])

>>> a[:,2]
array([2,12,22,32,42,52])

>>> a[2::2,::2]
array([[20,22,24]
       [40,42,44]])
```

Copies and views

A slicing operation creates a **view** on the original array, which is just a way of accessing array data. Thus the original array is not copied in memory.

When modifying the view, the original array is modified as well:

```
>>> a = np.arange(10)
>>> a
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> b = a[::2]; b
array([0, 2, 4, 6, 8])
>>> b[0] = 12
>>> b
array([12,  2,  4,  6,  8])
>>> a   # (!)
array([12,  1,  2,  3,  4,  5,  6,  7,  8,  9])

>>> a = np.arange(10)
>>> b = a[::2].copy()  # force a copy
>>> b[0] = 12
>>> a
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

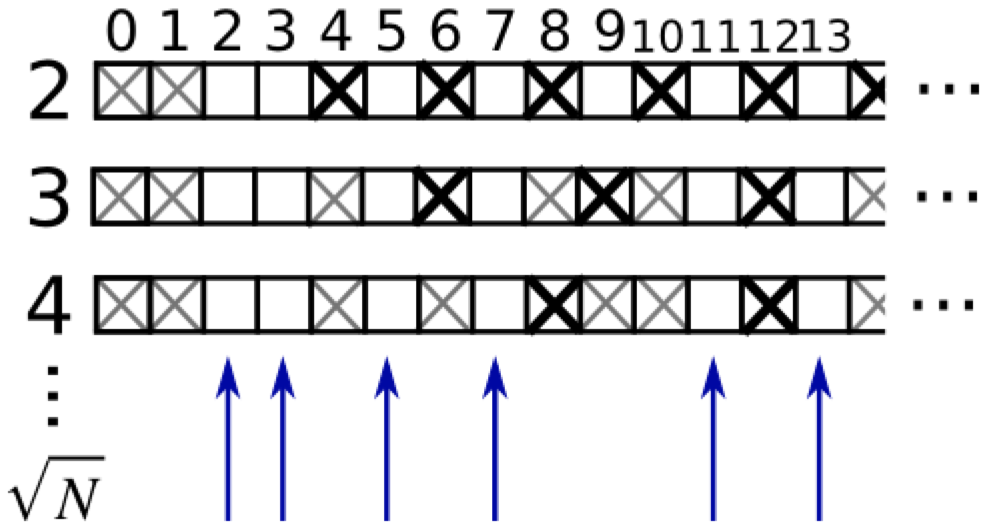
This behavior can be surprising at first sight... but it allows to save both memory and time.

The transpose is a view

As a result, a matrix cannot be made symmetric in-place:

```
>>> a = np.ones((100, 100))
>>> a += a.T
>>> a
array([[ 2.,  2.,  2., ...,  2.,  2.,  2.],
       [ 2.,  2.,  2., ...,  2.,  2.,  2.],
       [ 2.,  2.,  2., ...,  2.,  2.,  2.],
       ...,
       [ 3.,  3.,  3., ...,  2.,  2.,  2.],
       [ 3.,  3.,  3., ...,  2.,  2.,  2.],
       [ 3.,  3.,  3., ...,  2.,  2.,  2.]])
```

Worked example: Prime number sieve



Compute prime numbers in 0–99, with a sieve

- Construct a shape (100,) boolean array `is_prime`, filled with True in the beginning:

```
>>> is_prime = np.ones((100,), dtype=bool)
```

- Cross out 0 and 1 which are not primes:

```
>>> is_prime[:2] = 0
```

- For each integer `j` starting from 2, cross out its higher multiples:

```
>>> N_max = int(np.sqrt(len(is_prime)))
      >>> for j in range(2, N_max):
      ...     is_prime[2*j::j] = False
```

- Skim through `help(np.nonzero)`, and print the prime numbers
- Follow-up:
    - Move the above code into a script file named `prime_sieve.py`
    - Run it to check it works
    - Convert the simple sieve to the sieve of Eratosthenes:

        1. Skip `j` which are already known to not be primes
        2. The first number to cross out is j^2

Fancy indexing

Numpy arrays can be indexed with slices, but also with boolean or integer arrays (**masks**). This method is called *fancy indexing*. It creates **copies not view**.

Using boolean masks

```
>>> np.random.seed(3)
      >>> a = np.random.random_integers(0, 20, 15)
      >>> a
      array([10,  3,  8,  0, 19, 10, 11,  9, 10,  6,  0, 20, 12,  7, 14])
      >>> (a % 3 == 0)
      array([False,  True, False,  True, False, False, False,  True, False,
              True,  True, False,  True, False, False], dtype=bool)
      >>> mask = (a % 3 == 0)
      >>> extract_from_a = a[mask] # or,  a[a%3==0]
      >>> extract_from_a           # extract a sub-array with the mask
      array([ 3,  0,  9,  6,  0, 12])
```

Indexing with a mask can be very useful to assign a new value to a sub-array:

```
>>> a[a % 3 == 0] = -1
>>> a
array([10, -1,  8, -1, 19, 10, 11, -1, 10, -1, -1, 20, -1,  7, 14])
```

Indexing with an array of integers

```
>>> a = np.arange(10)
>>> a[::2] += 3 # to avoid having always the same np.arange(10)...
>>> a
array([ 3,  1,  5,  3,  7,  5,  9,  7, 11,  9])
>>> a[[2, 5, 1, 8]] # or, a[np.array([2, 5, 1, 8])]
array([ 5,  5,  1, 11])
```

Indexing can be done with an array of integers, where the same index is repeated several time:

```
>>> a[[2, 3, 2, 4, 2]]  # note: [2, 3, 2, 4, 2] is a Python list
array([5, 3, 5, 7, 5])
```

New values can be assigned with this kind of indexing:

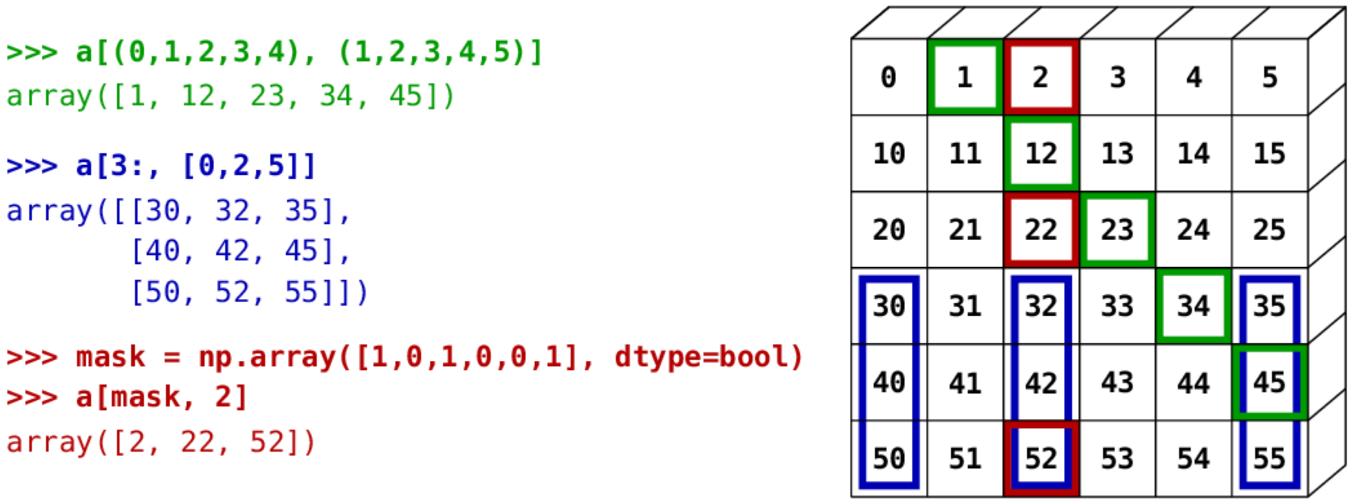
```
>>> a[[9, 7]] = -10
>>> a
array([  3,   1,   5,   3,   7,   5,   9, -10,  11, -10])
>>> a[[2, 3, 2, 4, 2]] += 1
>>> a
array([  3,   1,   6,   4,   8,   5,   9, -10,  11, -10])
```

When a new array is created by indexing with an array of integers, the new array has the same shape than the array of integers:

```
>>> a = np.arange(10)
>>> idx = np.array([[3, 4], [9, 7]])
>>> a[idx]
array([[3, 4],
       [9, 7]])
>>> b = np.arange(10)

>>> a = np.arange(12).reshape(3, 4)
>>> a
array([[ 0,  1,  2,  3],
       [ 4,  5,  6,  7],
       [ 8,  9, 10, 11]])
>>> i = np.array([0, 1, 1, 2])
>>> j = np.array([2, 1, 3, 3])
>>> a[i, j]
array([ 2,  5,  7, 11])

>>> i = np.array([[0, 1], [1, 2]])
>>> j = np.array([[2, 1], [3, 3]])
>>> i
array([[0, 1],
       [1, 2]])
>>> j
array([[2, 1],
       [3, 3]])
>>> a[i, j]
array([[ 2,  5],
       [ 7, 11]])
```



```
>>> a[(0,1,2,3,4), (1,2,3,4,5)]
array([1, 12, 23, 34, 45])

>>> a[3:, [0,2,5]]
array([[30, 32, 35],
       [40, 42, 45],
       [50, 52, 55]])

>>> mask = np.array([1,0,1,0,0,1], dtype=bool)
>>> a[mask, 2]
array([2, 22, 52])
```

We can even use fancy indexing and broadcasting at the same time:

```
>>> a = np.arange(12).reshape(3,4)
    >>> a
    array([[ 0,  1,  2,  3],
           [ 4,  5,  6,  7],
           [ 8,  9, 10, 11]])
    >>> i = np.array([[0, 1], [1, 2]])
    >>> a[i, 2] # same as a[i, 2*np.ones((2,2), dtype=int)]
    array([[ 2,  6],
           [ 6, 10]])
```

Numerical operations on arrays

Elementwise operations

With scalars:

```
>>> a = np.array([1, 2, 3, 4])
>>> a + 1
array([2, 3, 4, 5])
>>> 2**a
array([ 2,  4,  8, 16])
```

All arithmetic operates elementwise:

```
>>> b = np.ones(4) + 1
>>> a - b
array([-1.,  0.,  1.,  2.])
>>> a * b
array([ 2.,  4.,  6.,  8.])
```

```
>>> j = np.arange(5)
>>> 2**(j + 1) - j
array([ 2,  3,  6, 13, 28])
```

Array multiplication is not matrix multiplication:

```
>>> c = np.ones((3, 3))
>>> c * c                   # NOT matrix multiplication!
array([[ 1.,  1.,  1.],
       [ 1.,  1.,  1.],
       [ 1.,  1.,  1.]])
```

Note: Matrix multiplication:

```
>>> c.dot(c)
array([[ 3.,  3.,  3.],
       [ 3.,  3.,  3.],
       [ 3.,  3.,  3.]])
```

Comparisons:

```
>>> a = np.array([1, 2, 3, 4])
>>> b = np.array([4, 2, 2, 4])
>>> a == b
array([False,  True, False,  True], dtype=bool)
>>> a > b
array([False, False,  True, False], dtype=bool)
```

Logical operations:

```
>>> a = np.array([1, 1, 0, 0], dtype=bool)
>>> b = np.array([1, 0, 1, 0], dtype=bool)
>>> np.logical_or(a, b)
array([ True,  True,  True, False], dtype=bool)
>>> np.logical_and(a, b)
array([ True, False, False, False], dtype=bool)
```

Note: For arrays: "`np.logical_and`" and "`np.logical_or`" for logical operations, not "`and`" and "`or`".

Shape mismatches:

```
>>> a
array([1, 2, 3, 4])
>>> a + np.array([1, 2])
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: shape mismatch: objects cannot be broadcast to a single
shape
```

‘Broadcast’? We’ll return to that later.

Transposition:

```
>>> a = np.triu(np.ones((3, 3)), 1)   # see help(np.triu)
>>> a
array([[ 0.,  1.,  1.],
    [ 0.,  0.,  1.],
    [ 0.,  0.,  0.]])
>>> a.T
array([[ 0.,  0.,  0.],
       [ 1.,  0.,  0.],
       [ 1.,  1.,  0.]])
```

Note: Linear algebra
The sub-module `np.linalg` implements basic linear algebra, such as eigenvalue decomposition, solving linear systems... However, it is not garantied to be compiled using efficient routines, and thus we recommend to use `scipy.linalg`, as detailed in section *Linear algebra operations: scipy.linalg*

Exercice

Generate arrays `[2**0, 2**1, 2**2, 2**3, 2**4]` and `a_j = 2^(3*j) - j`

Basic reductions

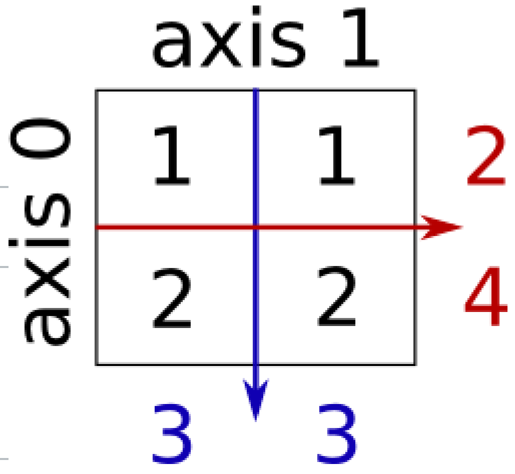
Computing sums:

```
>>> x = np.array([1, 2, 3, 4])
>>> np.sum(x)
10
>>> x.sum()
10
```

Sum by rows and by columns:

```
>>> x = np.array([[1, 1], [2, 2]])
>>> x
array([[1, 1],
    [2, 2]])
>>> x.sum(axis=0)   # columns (first dimension)
array([3, 3])
>>> x[:, 0].sum(), x[:, 1].sum()
(3, 3)
```

```
>>> x.sum(axis=1)    # rows (second dimension)
array([2, 4])
>>> x[0, :].sum(), x[1, :].sum()
(2, 4)
```



Same idea in higher dimensions:

```
>>> x = np.random.rand(2, 2, 2)
>>> x.sum(axis=2)[0, 1]
1.1600112273698793
>>> x[0, 1, :].sum()
1.1600112273698793
```

Other reductions — works the same way (and take `axis=`)

- Statistics:

```
>>> x = np.array([1, 2, 3, 1])
>>> y = np.array([[1, 2, 3], [5, 6, 1]])
>>> x.mean()
1.75
>>> np.median(x)
1.5
>>> np.median(y, axis=-1) # last axis
array([ 2.,  5.])
```

```
>>> x.std()          # full population standard dev.
0.82915619758884995
```

- Extrema:

```
>>> x = np.array([1, 3, 2])
>>> x.min()
1
>>> x.max()
3
```

```
>>> x.argmin()  # index of minimum
0
>>> x.argmax()  # index of maximum
1
```

- Logical operations:

```
>>> np.all([True, True, False])
False
>>> np.any([True, True, False])
True
```

Note: Can be used for array comparisons:

```
>>> a = np.zeros((100, 100))
>>> np.any(a != 0)
False
```

```
>>> np.all(a == a)
True
```

```
>>> a = np.array([1, 2, 3, 2])
>>> b = np.array([2, 2, 3, 2])
>>> c = np.array([6, 4, 4, 5])
>>> ((a <= b) & (b <= c)).all()
True
```

- ... and many more (best to learn as you go).

Example: data statistics

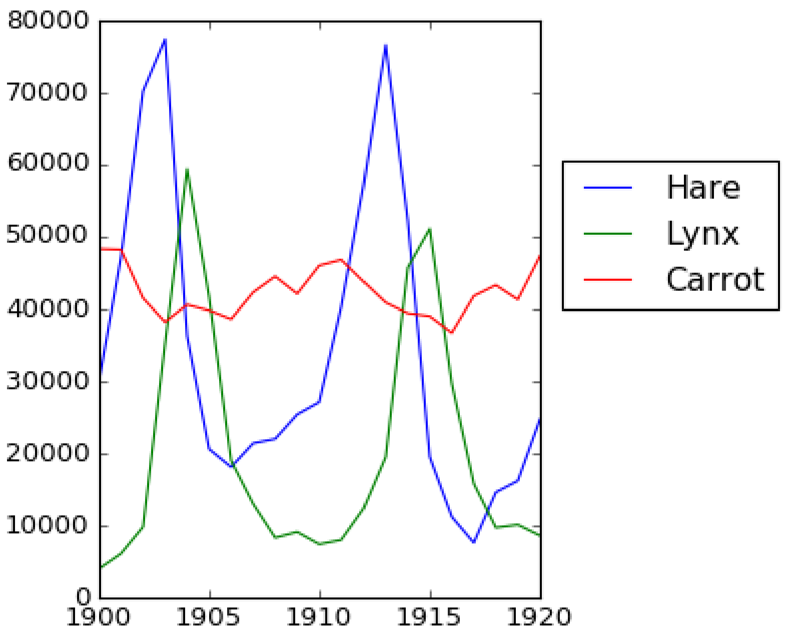
Data in `populations.txt` describes the populations of hares and lynxes (and carrots) in northern Canada during 20 years.

We can first plot the data:

```
>>> data = np.loadtxt('../../data/populations.txt')
>>> year, hares, lynxes, carrots = data.T  # trick: columns to variables

>>> plt.axes([0.2, 0.1, 0.5, 0.8])
>>> plt.plot(year, hares, year, lynxes, year, carrots)
>>> plt.legend(('Hare', 'Lynx', 'Carrot'), loc=(1.05, 0.5))
>>> plt.show()
```

[source code, hires.png, pdf]



The mean populations over time:

```
>>> populations = data[:, 1:]
>>> populations.mean(axis=0)
array([ 34080.95238095,  20166.66666667,  42400.        ])
```

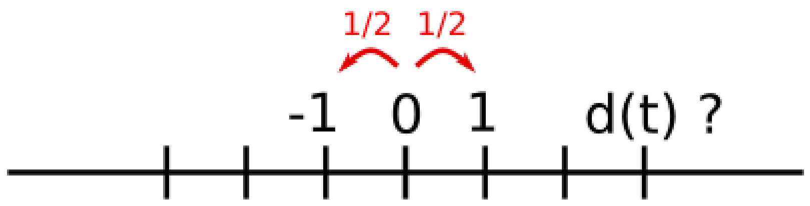
The sample standard deviations:

```
>>> populations.std(axis=0)
    array([ 20897.90645809,  16254.59153691,   3322.50622558])
```

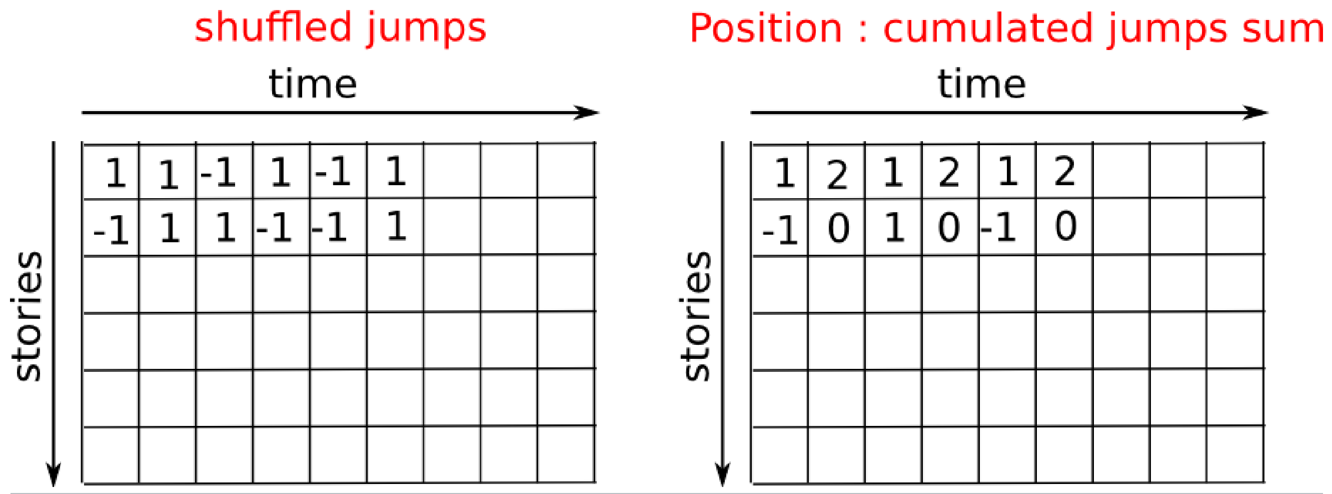
Which species has the highest population each year?

```
>>> np.argmax(populations, axis=1)
    array([2, 2, 0, 0, 1, 1, 2, 2, 2, 2, 2, 2, 0, 0, 0, 1, 2, 2, 2, 2,
    2])
```

Example: diffusion simulation using a random walk algorithm



What is the typical distance from the origin of a random walker after `t` left or right jumps?



```
>>> n_stories = 1000 # number of walkers
    >>> t_max = 200       # time during which we follow the walker
```

We randomly choose all the steps 1 or -1 of the walk

```
>>> t = np.arange(t_max)
    >>> steps = 2 * np.random.random_integers(0, 1, (n_stories, t_max)) -
    1
    >>> np.unique(steps) # Verification: all steps are 1 or -1
    array([-1,  1])
```

We build the walks by summing steps along the time

```
>>> positions = np.cumsum(steps, axis=1) # axis = 1: dimension of time
    >>> sq_distance = positions**2
```

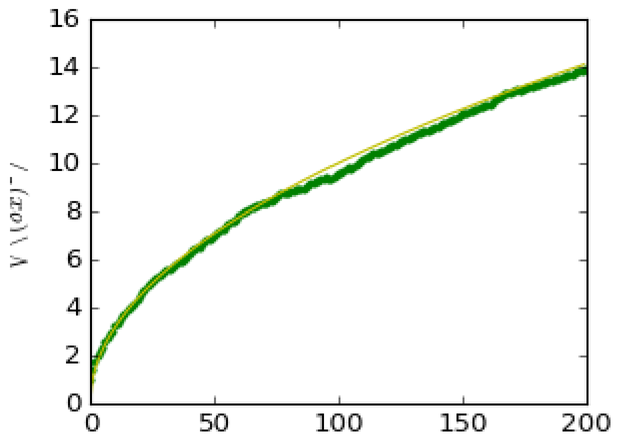
We get the mean in the axis of the stories

```
>>> mean_sq_distance = np.mean(sq_distance, axis=0)
```

Plot the results:

```
>>> plt.figure(figsize=(4, 3))
>>> plt.plot(t, np.sqrt(mean_sq_distance), 'g.', t, np.sqrt(t), 'y-')
>>> plt.xlabel(r"$t$")
>>> plt.ylabel(r"$\sqrt{\langle (\delta x)^2 \rangle}$")
>>> plt.show()
```

[source code, hires.png, pdf]



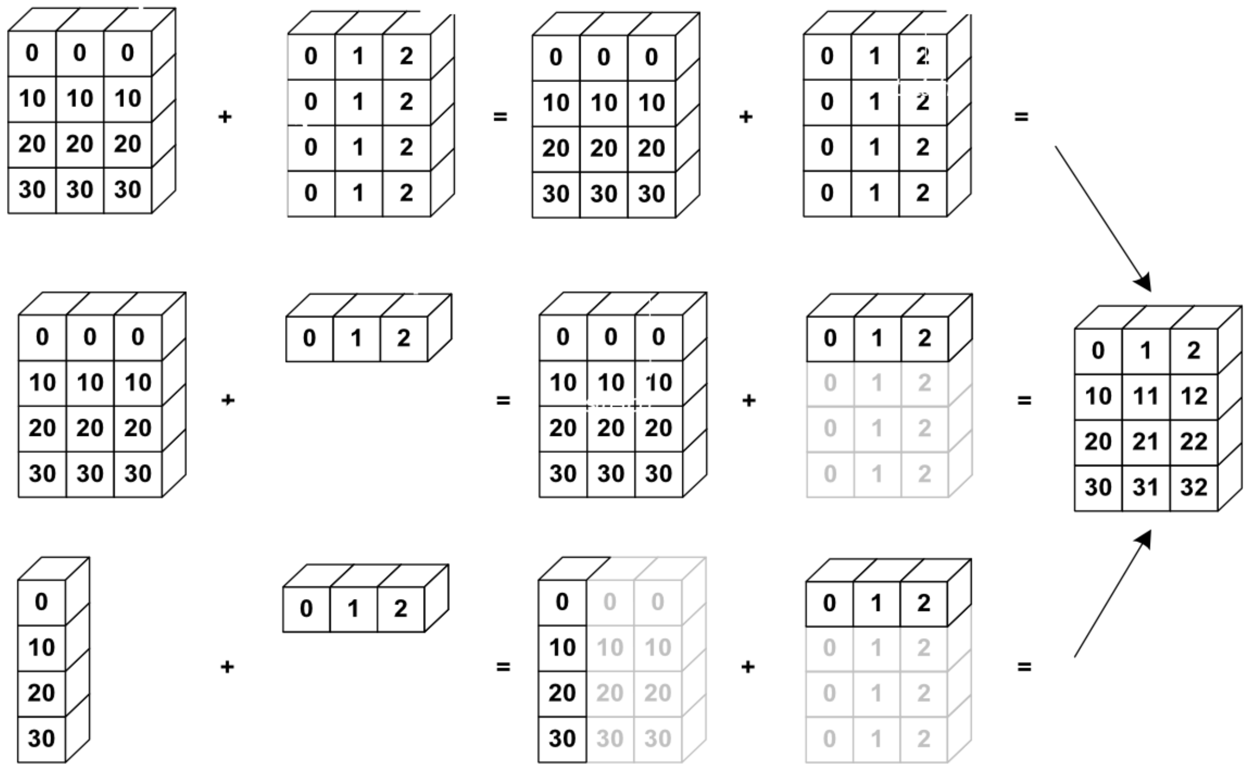
The RMS distance grows as the square root of the time!

Broadcasting

- Basic operations on `numpy` arrays (addition, etc.) are elementwise
- This works on arrays of the same size.

> **Nevertheless**, It’s also possible to do operations on arrays of different sizes if *Numpy* can transform these arrays so that they all have the same size: this conversion is called **broadcasting**.

The image below gives an example of broadcasting:



Let’s verify:

```
>>> a = np.tile(np.arange(0, 40, 10), (3, 1)).T
>>> a
array([[ 0,  0,  0],
       [10, 10, 10],
       [20, 20, 20],
       [30, 30, 30]])
>>> b = np.array([0, 1, 2])
>>> a + b
array([[ 0,  1,  2],
       [10, 11, 12],
       [20, 21, 22],
       [30, 31, 32]])
```

An useful trick:

```
>>> a = np.arange(0, 40, 10)
>>> a.shape
(4,)
>>> a = a[:, np.newaxis]  # adds a new axis -> 2D array
>>> a.shape
(4, 1)
>>> a
array([[ 0],
       [10],
       [20],
       [30]])
```

```
    >>> a + b
    array([[ 0,  1,  2],
           [10, 11, 12],
           [20, 21, 22],
           [30, 31, 32]])
```

We have already used broadcasting without knowing it!:

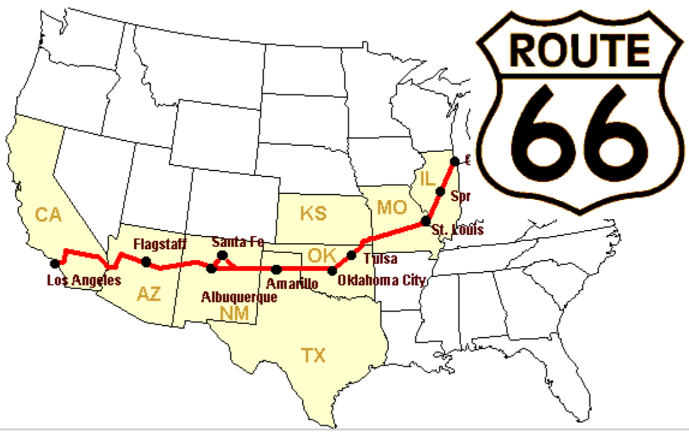
```
>>> a = np.ones((4, 5))
    >>> a[0] = 2  # we assign an array of dimension 0 to an array of
    dimension 1
    array([[ 2.,  2.,  2.,  2.,  2.],
           [ 1.,  1.,  1.,  1.,  1.],
           [ 1.,  1.,  1.,  1.,  1.],
           [ 1.,  1.,  1.,  1.,  1.]])
```

Broadcasting seems a bit magical, but it is actually quite natural to use it when we want to solve a problem whose output data is an array with more dimensions than input data.

Example

Let’s construct an array of distances (in miles) between cities of Route 66: Chicago, Springfield, Saint-Louis, Tulsa, Oklahoma City, Amarillo, Santa Fe, Albuquerque, Flagstaff and Los Angeles.

```
>>> mileposts = np.array([0, 198, 303, 736, 871, 1175, 1475, 1544,
    ...        1913, 2448])
    >>> distance_array = np.abs(mileposts - mileposts[:, np.newaxis])
    >>> distance_array
    array([[   0,  198,  303,  736,  871, 1175, 1475, 1544, 1913, 2448],
           [ 198,    0,  105,  538,  673,  977, 1277, 1346, 1715, 2250],
           [ 303,  105,    0,  433,  568,  872, 1172, 1241, 1610, 2145],
           [ 736,  538,  433,    0,  135,  439,  739,  808, 1177, 1712],
           [ 871,  673,  568,  135,    0,  304,  604,  673, 1042, 1577],
           [1175,  977,  872,  439,  304,    0,  300,  369,  738, 1273],
           [1475, 1277, 1172,  739,  604,  300,    0,   69,  438,  973],
           [1544, 1346, 1241,  808,  673,  369,   69,    0,  369,  904],
           [1913, 1715, 1610, 1177, 1042,  738,  438,  369,    0,  535],
           [2448, 2250, 2145, 1712, 1577, 1273,  973,  904,  535,    0]])
```



Good practices

- Explicit variable names (no need of a comment to explain what is in the variable)
- Style: spaces after commas, around `=`, etc.

A certain number of rules for writing "beautiful" code (and, more importantly, using the same conventions as everybody else!) are given in the Style Guide for Python Code and the Docstring Conventions page (to manage help strings).

- Except some rare cases, variable names and comments in English.

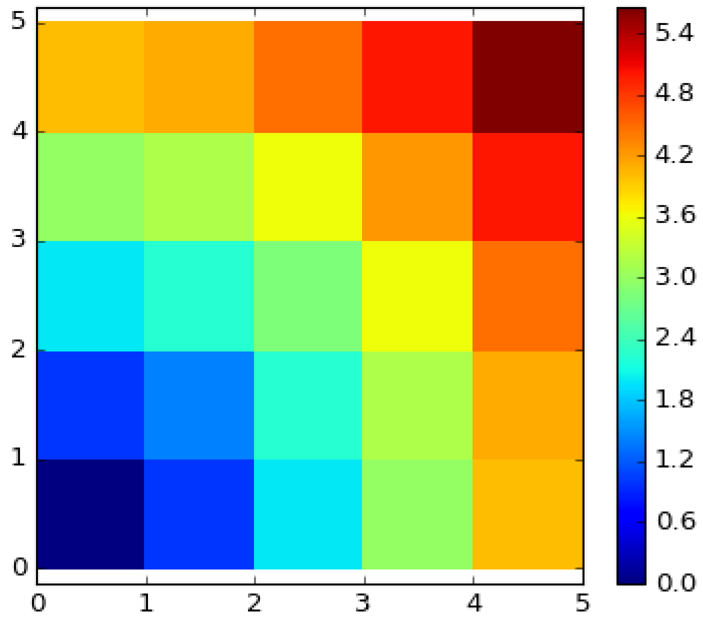
A lot of grid-based or network-based problems can also use broadcasting. For instance, if we want to compute the distance from the origin of points on a 10x10 grid, we can do:

```
>>> x, y = np.arange(5), np.arange(5)
      >>> distance = np.sqrt(x ** 2 + y[:, np.newaxis] ** 2)
      >>> distance
      array([[ 0.        ,  1.        ,  2.        ,  3.        ,
      4.        ],
              [ 1.        ,  1.41421356,  2.23606798,  3.16227766,
      4.12310563],
              [ 2.        ,  2.23606798,  2.82842712,  3.60555128,
      4.47213595],
              [ 3.        ,  3.16227766,  3.60555128,  4.24264069,
      5.        ],
              [ 4.        ,  4.12310563,  4.47213595,  5.        ,
      5.65685425]])
```

Or in color:

```
>>> plt.pcolor(distance)
      >>> plt.colorbar()
      >>> plt.axis('equal')
      >>> plt.show()   # <-- again, not needed in interactive Python
```

[source code, hires.png, pdf]



Remark : the `numpy.ogrid` function allows to directly create vectors x and y of the previous example, with two "significant dimensions":

```
>>> x, y = np.ogrid[0:5, 0:5]
>>> x, y
(array([[0],
        [1],
        [2],
        [3],
        [4]]), array([[0, 1, 2, 3, 4]]))
>>> x.shape, y.shape
((5, 1), (1, 5))
>>> distance = np.sqrt(x ** 2 + y ** 2)
```

So, `np.ogrid` is very useful as soon as we have to handle computations on a grid. On the other hand, `np.mgrid` directly provides matrices full of indices for cases where we can't (or don't want to) benefit from broadcasting:

```
>>> x, y = np.mgrid[0:4, 0:4]
>>> x
array([[0, 0, 0, 0],
       [1, 1, 1, 1],
       [2, 2, 2, 2],
       [3, 3, 3, 3]])
>>> y
array([[0, 1, 2, 3],
       [0, 1, 2, 3],
       [0, 1, 2, 3],
       [0, 1, 2, 3]])
```

However, in practice, this is rarely needed!

Array shape manipulation

Flattening

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

Higher dimensions: last dimensions ravel out "first".

Reshaping

The inverse operation to flattening:

```
>>> a.shape
(2, 3)
>>> b = a.ravel()
>>> b.reshape((2, 3))
```

```
array([[1, 2, 3],
       [4, 5, 6]])
```

Creating an array with a different shape, from another array:

```
>>> a = np.arange(36)
>>> b = a.reshape((6, 6))
>>> b
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],
       [30, 31, 32, 33, 34, 35]])
```

Or,

```
>>> b = a.reshape((6, -1))    # unspecified (-1) value is inferred
```

Views and copies

`ndarray.reshape` **may** return a view (cf `help(np.reshape)`)), not a copy:

```
>>> b[0,0] = 99
>>> a
array([99,  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, 30, 31, 32,
33,
       34, 35])
```

Beware!

```
>>> a = np.zeros((3,2))
>>> b = a.T.reshape(3*2)
>>> b[0] = 9
>>> a
array([[ 0.,  0.],
       [ 0.,  0.],
       [ 0.,  0.]])
```

To understand, see “Under the hood” below.

Dimension shuffling

```
>>> a = np.arange(4*3*2).reshape(4, 3, 2)
>>> a.shape
(4, 3, 2)
>>> a[0,2,1]
5
>>> b = a.transpose(1, 2, 0)
>>> b.shape
(3, 2, 4)
>>> b[2,1,0]
5
```

Also creates a view:

```
>>> b[2,1,0] = -1
      >>> a[0,2,1]
      -1
```

Resizing

Size of an array can be changed with `ndarray.resize`:

```
>>> a = np.arange(4)
      >>> a.resize((8,))
      >>> a
      array([0, 1, 2, 3, 0, 0, 0, 0])
```

However, it must not be referred to somewhere else:

```
>>> b = a
      >>> a.resize((4,))
      ...
      ValueError: cannot resize an array references or is referenced
      by another array in this way.  Use the resize function
```

Some examples of real-world use cases

Case 2.a: Calling (legacy) Fortran code

Shape-preserving functions with elementwise non-Python routines. For instance, Fortran

```
! 2_a_fortran_module.f90
      subroutine some_function(n, a, b)
        integer :: n
        double precision, dimension(n), intent(in) :: a
        double precision, dimension(n), intent(out) :: b
        b = a + 1
      end subroutine some_function
```

```
f2py -c -m fortran_module 2_a_fortran_module.f90
```

```
import numpy as np
      import fortran_module

      def some_function(input):
          """
          Call a Fortran routine, and preserve input shape
          """
          input = np.asarray(input)
          # fortran_module.some_function() takes 1-D arrays!
          output = fortran_module.some_function(input.ravel())
          return output.reshape(input.shape)

      print some_function(np.array([1, 2, 3]))
      print some_function(np.array([[1, 2], [3, 4]]))

      # ->
      # [ 2.  3.  4.]
      # [[ 2.  3.]
      #  [ 4.  5.]]
```

Case 2.b: Block matrices and vectors (and tensors)

Vector space: quantum level $\bigotimes$ spin

$$\check{\psi} = \begin{pmatrix} \hat{\psi}_1 \\ \hat{\psi}_2 \end{pmatrix}, \qquad \hat{\psi}_1 = \begin{pmatrix} \psi_{1\uparrow} \\ \psi_{1\downarrow} \end{pmatrix} \qquad \hat{\psi}_2 = \begin{pmatrix} \psi_{2\uparrow} \\ \psi_{2\downarrow} \end{pmatrix}$$

In short: for **block matrices and vectors**, it can be useful to preserve the **block structure**.

In Numpy:

```
>>> psi = np.zeros((2, 2))   # dimensions: level, spin
      >>> psi[0,1] # <-- psi_{1,downarrow}
```

Linear operators on such block vectors have similar block structure:

$$\check{H} = \begin{pmatrix} \hat{h}_{11} & \hat{V} \\ \hat{V}^\dagger & \hat{h}_{22} \end{pmatrix}, \qquad \hat{h}_{11} = \begin{pmatrix} \epsilon_{1,\uparrow} & 0 \\ 0 & \epsilon_{1,\downarrow} \end{pmatrix}, \qquad \ldots$$

```
>>> H = np.zeros((2, 2, 2, 2)) # dimensions: level1, level2, spin1, spin2
      >>> h_11 = H[0,0,:,:]
      >>> V = H[0,1]
```

Doing the matrix product: get rid of the block structure, do the 4x4 matrix product, then put it back

$$\check{H}\check{\psi}$$

```
>>> def mdot(operator, psi):
      ...     return operator.transpose(0, 2, 1, 3).reshape(4, 4).dot(
      ...                 psi.reshape(4)).reshape(2, 2)
```

I.e., reorder dimensions first to `level1, spin1, level2, spin2` and then reshape => correct matrix product.

Sorting data

Sorting along an axis:

```
>>> a = np.array([[4, 3, 5], [1, 2, 1]])
      >>> b = np.sort(a, axis=1)
      >>> b
      array([[3, 4, 5],
             [1, 1, 2]])
```

Note: Sorts each row separately!

In-place sort:

```
>>> a.sort(axis=1)
      >>> a
      array([[3, 4, 5],
             [1, 1, 2]])
```

Sorting with fancy indexing:

```
>>> a = np.array([4, 3, 1, 2])
      >>> j = np.argsort(a)
      array([2, 3, 1, 0])
      >>> a[j]
      array([1, 2, 3, 4])
```

Finding minima and maxima:

```
>>> a = np.array([4, 3, 1, 2])
      >>> j_max = np.argmax(a)
      >>> j_min = np.argmin(a)
      >>> j_max, j_min
      (0, 2)
```

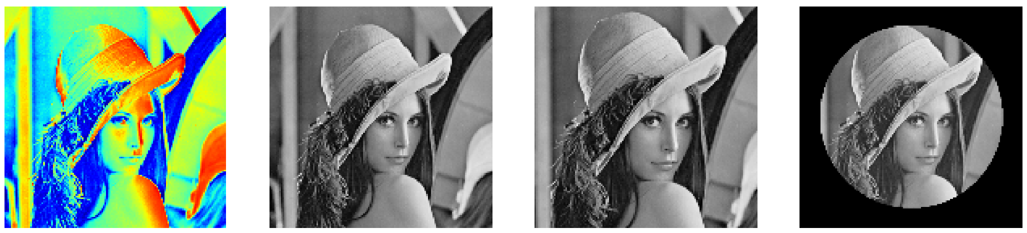
Some excercices

Worked example: Framing Lena

Let's do some manipulations on numpy arrays by starting with the famous image of Lena (http://www.cs.cmu.edu/~chuck/lennapg/). `scipy` provides a 2D array of this image with the `scipy.lena` function:

```
>>> from scipy import misc
      >>> lena = misc.lena()
```

Here are a few images we will be able to obtain with our manipulations: use different colormaps, crop the image, change some parts of the image.



- Let's use the imshow function of pylab to display the image.

```
In [3]: import pylab as plt
      In [4]: lena = misc.lena()
      In [5]: plt.imshow(lena)
```

- Lena is then displayed in false colors. A colormap must be specified for her to be displayed in grey.

```
In [6]: plt.imshow(lena, cmap=plt.cm.gray)
```

- Create an array of the image with a narrower centering : for example, remove 30 pixels from all the borders of the image. To check the result, display this new array with `imshow`.

  ```
  In [9]: crop_lena = lena[30:-30,30:-30]
  ```

- We will now frame Lena's face with a black locket. For this, we need to create a mask corresponding to the pixels we want to be black. The mask is defined by this condition `(y-256)**2 + (x-256)**2`

  ```
  In [15]: y, x = np.ogrid[0:512,0:512] # x and y indices of pixels
        In [16]: y.shape, x.shape
        Out[16]: ((512, 1), (1, 512))
        In [17]: centerx, centery = (256, 256) # center of the image
        In [18]: mask = ((y - centery)**2 + (x - centerx)**2) > 230**2 #
        circle
  ```

  then we assign the value 0 to the pixels of the image corresponding to the mask. The syntax is extremely simple and intuitive:

  ```
  In [19]: lena[mask] = 0
        In [20]: plt.imshow(lena)
        Out[20]: <matplotlib.image.AxesImage object at 0xa36534c>
  ```

- Follow-up: copy all instructions of this exercise in a script called `lena_locket.py` then execute this script in IPython with `%run lena_locket.py`.

  Change the circle to an ellipsoid.

Exercise: Array manipulations

1. Form the 2-D array (without typing it in explicitly):

   ```
   1   6 11
   2   7 12
   3   8 13
   4   9 14
   5  10 15
   ```

   and generate a new array containing its 2nd and 4th rows.
2. Divide each column of the array:

   ```
   >>> a = np.arange(25).reshape(5, 5)
   ```

   elementwise with the array `b = np.array([1., 5, 10, 15, 20])`. (Hint: `np.newaxis`).
3. Harder one: Generate a 10 x 3 array of random numbers (in range [0,1]). For each row, pick the number closest to 0.5.
   - Use `abs` and `argsort` to find the column `j` closest for each row.
   - Use fancy indexing to extract the numbers. (Hint: `a[i,j]` – the array `i` must contain the row numbers corresponding to stuff in `j`.)

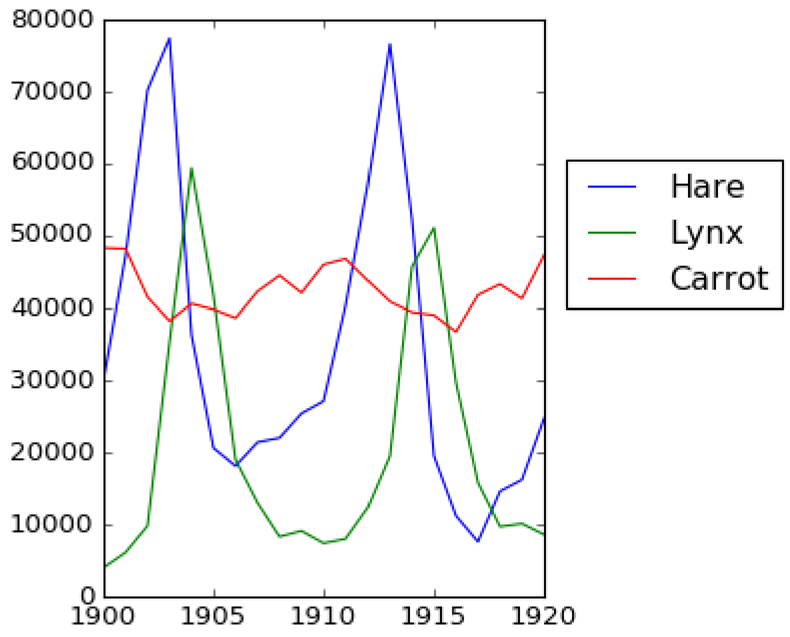
Exercise: Data statistics

The data in `populations.txt`:: describes the populations of hares and lynxes (and carrots) in northern Canada during 20 years:

```
>>> data = np.loadtxt('../../data/populations.txt')
      >>> year, hares, lynxes, carrots = data.T  # trick: columns to
      variables

      >>> plt.axes([0.2, 0.1, 0.5, 0.8])
      >>> plt.plot(year, hares, year, lynxes, year, carrots)
      >>> plt.legend(('Hare', 'Lynx', 'Carrot'), loc=(1.05, 0.5))
      >>> plt.show()
```

[source code, hires.png, pdf]



Computes and print, based on the data in `populations.txt`...

1. The mean and std of the populations of each species for the years in the period.
2. Which year each species had the largest population.
3. Which species has the largest population for each year. (Hint: `argsort` & fancy indexing of `np.array(['H', 'L', 'C'])`)
4. Which years any of the populations is above 50000. (Hint: comparisons and `np.any`)
5. The top 2 years for each species when they had the lowest populations. (Hint: `argsort`, fancy indexing)
6. Compare (plot) the change in hare population (see `help(np.gradient)`) and the number of lynxes. Check correlation (see `help(np.corrcoef)`).

... all without for-loops.

Exercise: Crude integral approximations

Write a function `f(a, b, c)` that returns $a^b - c$. Form a 24x12x6 array containing its values in parameter ranges `[0,1] x [0,1] x [0,1]`.

Approximate the 3-d integral

$$\int_0^1 \int_0^1 \int_0^1 (a^b - c) da\, db\, dc$$

over this volume with the mean. The exact result is: $\ln 2 - \frac{1}{2} \approx 0.1931\ldots$ — what is your relative error?

(Hints: use elementwise operations and broadcasting. You can make `np.ogrid` give a number of points in given range with `np.ogrid[0:1:20j]`.)

Reminder Python functions:

```
def f(a, b, c):
        return some_result
```

Exercise: Mandelbrot set

Write a script that computes the Mandelbrot fractal. The Mandelbrot iteration:

```
N_max = 50
      some_threshold = 50

      c = x + 1j*y

      for j in xrange(N_max):
          z = z**2 + c
```

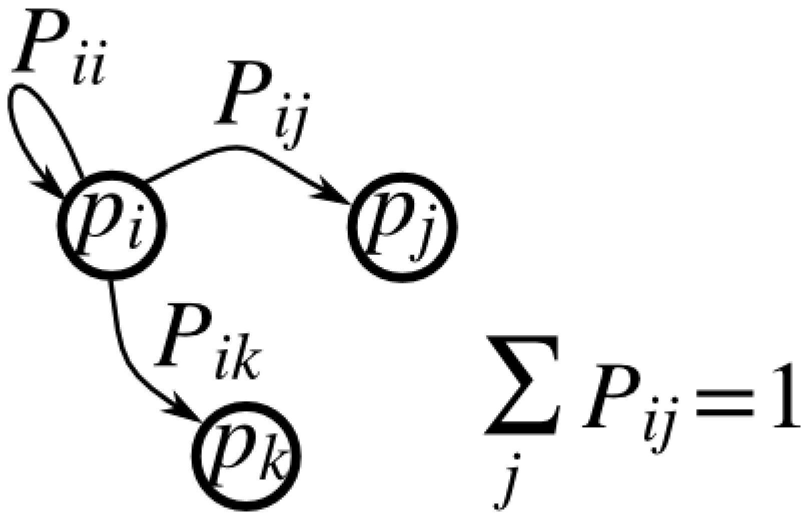
Point (x, y) belongs to the Mandelbrot set if $|c|$ < `some_threshold`.

Do this computation by:

1. Construct a grid of c = x + 1j*y values in range [-2, 1] x [-1.5, 1.5]
2. Do the iteration
3. Form the 2-d boolean mask indicating which points are in the set
4. Save the result to an image with:

```
>>> import matplotlib.pyplot as plt
      >>> plt.imshow(mask.T, extent=[-2, 1, -1.5, 1.5])
      >>> plt.gray()
      >>> plt.savefig('mandelbrot.png')
```

Exercise: Markov chain



Markov chain transition matrix `P`, and probability distribution on the states `p`:

1. `0 <= P[i,j] <= 1`: probability to go from state `i` to state `j`
2. Transition rule: $p_{new} = P^T p_{old}$
3. `all(sum(P, axis=1) == 1)`, `p.sum() == 1`: normalization

Write a script that works with 5 states, and:

- Constructs a random matrix, and normalizes each row so that it is a transition matrix.
- Starts from a random (normalized) probability distribution `p` and takes 50 steps => `p_50`
- Computes the stationary distribution: the eigenvector of `P.T` with eigenvalue 1 (numerically: closest to 1) => `p_stationary`

Remember to normalize the eigenvector — I didn't...

- Checks if `p_50` and `p_stationary` are equal to tolerance 1e-5

Toolbox: `np.random.rand`, `.dot()`, `np.linalg.eig`, reductions, `abs()`, `argmin`, comparisons, `all`, `np.linalg.norm`, etc.

Summary

What do you need to know to get started?

- Know how to create arrays : `array`, `arange`, `ones`, `zeros`.
- Know the shape of the array with `array.shape`, then use slicing to obtain different views of the array: `array[::2]`, etc. Adjust the shape of the array using `reshape` or flatten it with `ravel`.
- Obtain a subset of the elements of an array and/or modify their values with masks:

```
>>> a[a < 0] = 0
```

- Know miscellaneous operations on arrays, such as finding the mean or max (`array.max()`, `array.mean()`). No need to retain everything, but have the reflex to search in the documentation (online docs, `help()`, `lookfor()`)!!

- For advanced use: master the indexing with arrays of integers, as well as broadcasting. Know more Numpy functions to handle various array operations.

Advanced operations

Fourier transforms

Numpy contains 1-D, 2-D, and N-D fast discrete Fourier transform routines, which compute:

$$A_k = \sum_{m=0}^{n-1} a_m \exp\left\{-2\pi i \frac{mk}{n}\right\} \qquad k = 0, \ldots, n-1.$$

Full details of what for you can use such standard routines is beyond this tutorial. Neverheless, there they are, if you need them:

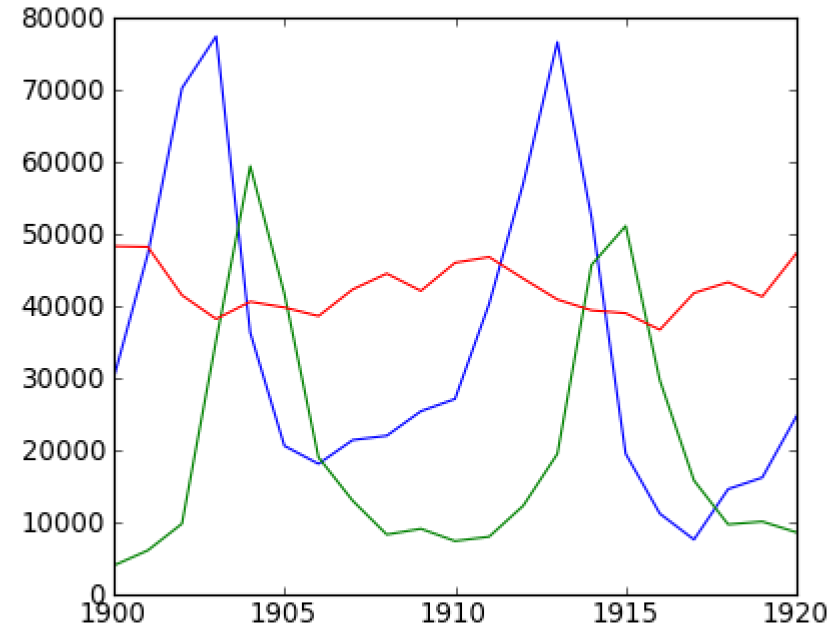
```
>>> a = np.exp(2j*np.pi*np.arange(10))
      >>> fa = np.fft.fft(a)
      >>> np.set_printoptions(suppress=True) # print small number as 0
      >>> fa
      array([ 10.-0.j,   0.+0.j,   0.+0.j,   0.+0.j,   0.+0.j,   0.+0.j,
              -0.+0.j,  -0.+0.j,  -0.+0.j,  -0.+0.j])
```

```
>>> a = np.exp(2j*np.pi*np.arange(3))
      >>> b = a[:,np.newaxis] + a[np.newaxis,:]
      >>> np.fft.fftn(b)
      array([[ 18.-0.j,   0.+0.j,  -0.+0.j],
             [  0.+0.j,   0.+0.j,   0.+0.j],
             [ -0.+0.j,   0.+0.j,   0.+0.j]])
```

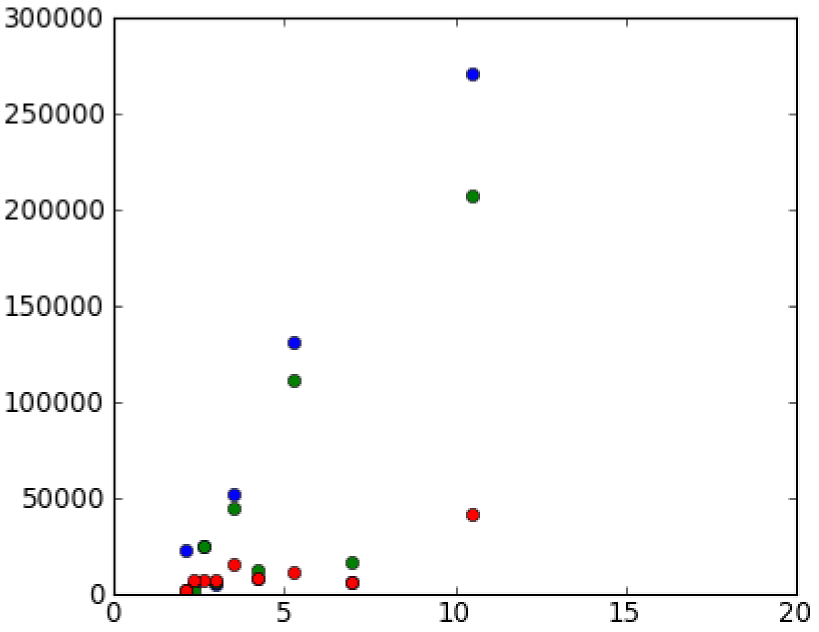
See `help(np.fft)` and `help(np.fft.fft)` for more. These functions in general take the `axes` argument, and you can additionally specify padding etc.

Worked example: Crude periodicity finding

[source code, hires.png, pdf]



[source code, hires.png, pdf]



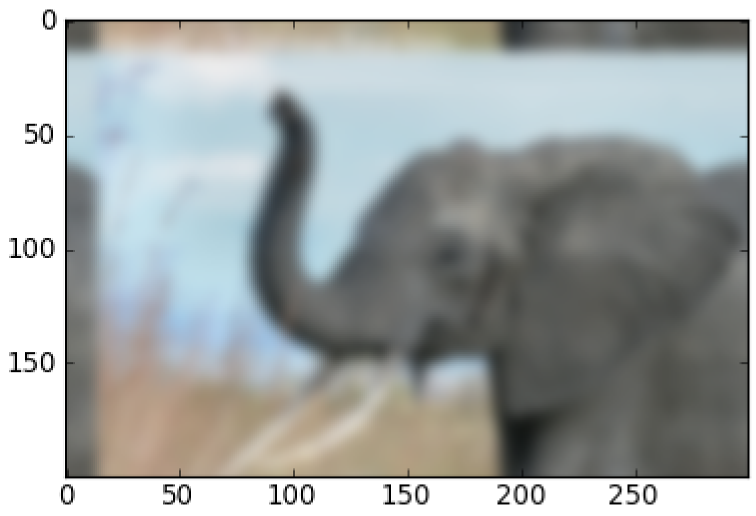
Worked example: Gaussian image blur

Convolution:

$$f_1(t) = \int dt'\, K(t - t') f_0(t')$$

$$\tilde{f}_1(\omega) = \tilde{K}(\omega) \tilde{f}_0(\omega)$$

[source code, hires.png, pdf]



Polynomials

Numpy also contains polynomials in different bases:

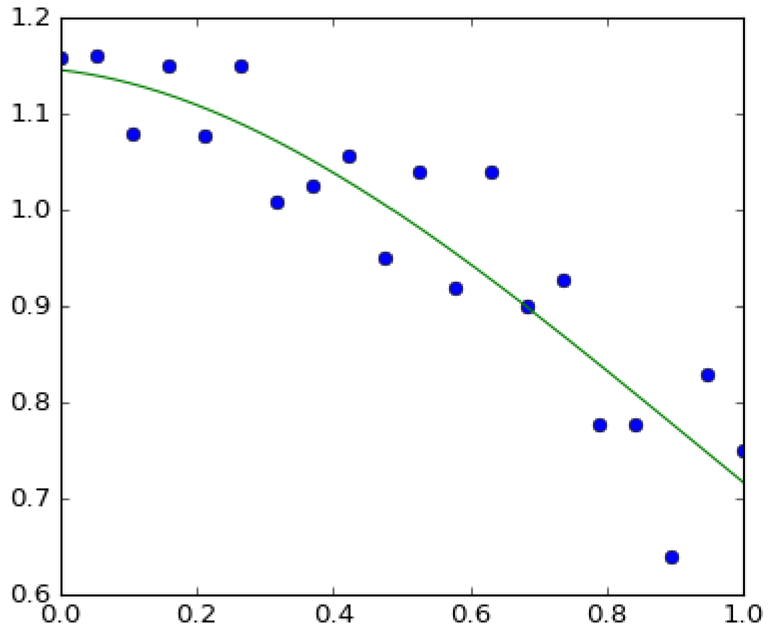
For example, $3x^2 + 2x - 1$

```
>>> p = np.poly1d([3, 2, -1])
>>> p(0)
-1
>>> p.roots
array([-1.        ,  0.33333333])
>>> p.order
2
```

```
>>> x = np.linspace(0, 1, 20)
>>> y = np.cos(x) + 0.3*np.random.rand(20)
>>> p = np.poly1d(np.polyfit(x, y, 3))
```

```
>>> t = np.linspace(0, 1, 200)
>>> plt.plot(x, y, 'o', t, p(t), '-')
>>> plt.show()
```

[source code, hires.png, pdf]



See http://docs.scipy.org/doc/numpy/reference/routines.polynomials.poly1d.html for more.

More polynomials (with more bases)

Numpy also has a more sophisticated polynomial interface, which supports e.g. the Chebyshev basis.

$$3x^2 + 2x - 1$$

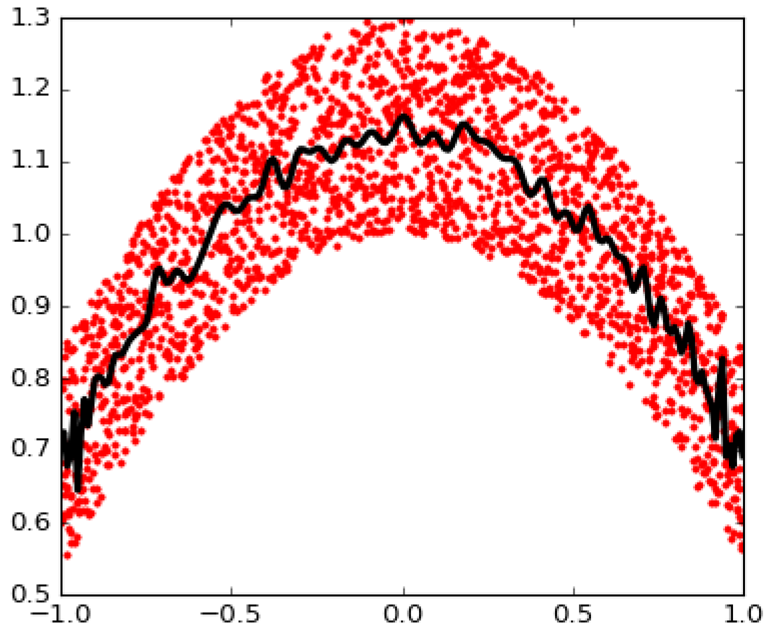
```
>>> p = np.polynomial.Polynomial([-1, 2, 3]) # coefs in different order!
    >>> p(0)
    -1.0
    >>> p.roots()
    array([-1.        ,  0.33333333])
    >>> p.order
    2
```

Example using polynomials in Chebyshev basis, for polynomials in range `[-1, 1]`:

```
>>> x = np.linspace(-1, 1, 2000)
    >>> y = np.cos(x) + 0.3*np.random.rand(2000)
    >>> p = np.polynomial.Chebyshev.fit(x, y, 90)
```

```
>>> t = np.linspace(-1, 1, 200)
    >>> plt.plot(x, y, 'r.')
    >>> plt.plot(t, p(t), 'k-', lw=3)
    >>> plt.show()
```

[source code, hires.png, pdf]



The Chebyshev polynomials have some advantages in interpolation.

Summary & Exercises

- There is a number of data types with different precisions. In some special cases you may need to care about this.
- Structured arrays contain data of a composite type. Lumping pieces of data together this way has various possible uses.
- Fourier transform routines are under `np.fft`
- Masked arrays can be used for missing data
- Polynomials are available in various bases

Loading data files

Text files

Example: `populations.txt`:

```
1900        30e3    4e3     51300
1901        47.2e3  6.1e3   48200
1902        70.2e3  9.8e3   41500
...
```

```
>>> data = np.loadtxt('populations.txt')    # if in current directory
>>> data
array([[  1900.,  30000.,   4000.,  51300.],
       [  1901.,  47200.,   6100.,  48200.],
       [  1902.,  70200.,   9800.,  41500.],
...

>>> np.savetxt('pop2.txt', data)
>>> data2 = np.loadtxt('pop2.txt')
```

Note: If you have a complicated text file, what you can try are:

- `np.genfromtxt`
- Using Python's I/O functions and e.g. regexps for parsing (Python is quite well suited for this)

Navigating the filesystem with *Ipython*

```
In [1]: pwd      # show current directory
'/home/user/stuff/2011-numpy-tutorial'
In [2]: cd ex
'/home/user/stuff/2011-numpy-tutorial/ex'
In [3]: ls
populations.txt  species.txt
```

Images

Using Matplotlib:

```
>>> img = plt.imread('../../data/elephant.png')
>>> img.shape, img.dtype
((200, 300, 3), dtype('float32'))
>>> plt.imshow(img)
>>> plt.savefig('plot.png')
>>> plt.show()

>>> plt.imsave('red_elephant', img[:,:,0], cmap=plt.cm.gray)
```

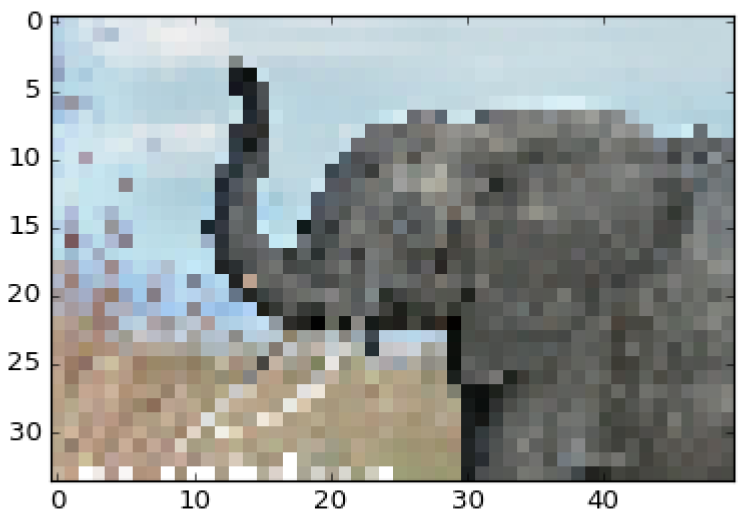
This saved only one channel (of RGB):

```
>>> plt.imshow(plt.imread('red_elephant.png'))
>>> plt.show()
```

Other libraries:

```
>>> from scipy.misc import imsave
>>> imsave('tiny_elephant.png', img[::6,::6])
>>> plt.imshow(plt.imread('tiny_elephant.png'), interpolation=
'nearest')
>>> plt.show()
```

[source code, hires.png, pdf]



Numpy's own format

Numpy has its own binary format, not portable but with efficient I/O:

```
>>> np.save('pop.npy', data)
       >>> data3 = np.load('pop.npy')
```

Well-known (& more obscure) file formats

- HDF5: h5py, PyTables
- NetCDF: `scipy.io.netcdf_file`, netcdf4-python, ...
- Matlab: `scipy.io.loadmat`, `scipy.io.savemat`
- MatrixMarket: `scipy.io.mmread`, `scipy.io.mmread`

... if somebody uses it, there's probably also a Python library for it.

Exercise: Text data files

Write a Python script that loads data from `populations.txt`:: and drop the last column and the first 5 rows. Save the smaller dataset to `pop2.txt`.

More elaborate arrays

More data types

Casting

“Bigger” type wins in mixed-type operations:

```
>>> np.array([1, 2, 3]) + 1.5
    array([ 2.5,  3.5,  4.5])
```

Assignment never changes the type!

```
>>> a = np.array([1, 2, 3])
    >>> a.dtype
    dtype('int64')
    >>> a[0] = 1.9     # <-- float is truncated to integer
    >>> a
    array([1, 2, 3])
```

Forced casts:

```
>>> a = np.array([1.7, 1.2, 1.6])
    >>> b = a.astype(int)  # <-- truncates to integer
    >>> b
    array([1, 1, 1])
```

Rounding:

```
>>> a = np.array([1.7, 1.2, 1.6])
    >>> b = np.around(a)
    >>> b                    # still floating-point
    array([ 2.,  1.,  2.])
    >>> c = np.around(a).astype(int)
    >>> c
    array([2, 1, 2])
```

Different data type sizes

Integers (signed):

`int8`	8 bits
`int16`	16 bits
`int32`	32 bits (same as `int` on 32-bit platform)
`int64`	64 bits (same as `int` on 64-bit platform)

```
>>> np.array([1], dtype=int).dtype
    dtype('int64')
    >>> np.iinfo(np.int32).max, 2**31 - 1
    (2147483647, 2147483647)
    >>> np.iinfo(np.int64).max, 2**63 - 1
    (9223372036854775807, 9223372036854775807L)
```

Unsigned integers:

`uint8`

	8 bits
`uint16`	16 bits
`uint32`	32 bits
`uint64`	64 bits

```
>>> np.iinfo(np.uint32).max, 2**32 - 1
      (2147483647, 2147483647)
      >>> np.iinfo(np.uint64).max, 2**64 - 1
      (9223372036854775807, 9223372036854775807L)
```

Floating-point numbers:

`float16`	16 bits
`float32`	32 bits
`float64`	64 bits (same as `float`)
`float96`	96 bits, platform-dependent (same as `np.longdouble`)
`float128`	128 bits, platform-dependent (same as `np.longdouble`)

```
>>> np.finfo(np.float32).eps
      1.1920929e-07
      >>>  np.finfo(np.float64).eps
      2.2204460492503131e-16
```

```
>>> np.float32(1e-8) + np.float32(1) == 1
      True
      >>> np.float64(1e-8) + np.float64(1) == 1
      False
```

Complex floating-point numbers:

`complex64`	two 32-bit floats
`complex128`	two 64-bit floats
`complex192`	two 96-bit floats, platform-dependent
`complex256`	two 128-bit floats, platform-dependent

Smaller data types

If you don't know you need special data types, then you probably don't.

Comparison on using `float32` instead of `float64`:

- Half the size in memory and on disk
- Half the memory bandwidth required (may be a bit faster in some operations)

```
In [1]: a = np.zeros((1e6,), dtype=np.float64)

        In [2]: b = np.zeros((1e6,), dtype=np.float32)

        In [3]: %timeit a*a
        1000 loops, best of 3: 1.78 ms per loop
```

```
In [4]: %timeit b*b
1000 loops, best of 3: 1.07 ms per loop
```

- But: bigger rounding errors — sometimes in surprising places (i.e., don't use them unless you really need them)

Structured data types

Composite data types

`sensor_code` (4-character string)
`position` (float)
`value` (float)

```
>>> samples = np.zeros((6,), dtype=[('sensor_code', 'S4'),
...                                 ('position', float), ('value',
float)])
>>> samples.ndim
1
>>> samples.shape
(6,)
>>> samples.dtype.names
('sensor_code', 'position', 'value')
```

```
>>> samples[:] = [('ALFA', 1, 0.35), ('BETA', 1, 0.11), ('TAU', 1, 0.39),
...               ('ALFA', 1.5, 0.35), ('ALFA', 2.1, 0.11), ('TAU',
1.2, 0.39)]
>>> samples
array([('ALFA', 1.0, 0.35), ('BETA', 1.0, 0.11), ('TAU', 1.0, 0.39),
       ('ALFA', 1.5, 0.35), ('ALFA', 2.1, 0.11), ('TAU', 1.2, 0.39)],
      dtype=[('sensor_code', '|S4'), ('position', '<f8'), ('value',
'<f8')])
```

Field access works by indexing with field names:

```
>>> samples['sensor_code']
array(['ALFA', 'BETA', 'TAU', 'ALFA', 'ALFA', 'TAU'],
      dtype='|S4')
>>> samples['value']
array([ 0.35,  0.11,  0.39,  0.35,  0.11,  0.39])
>>> samples[0]
('ALFA', 1.0, 0.35)
```

```
>>> samples[0]['sensor_code'] = 'TAU'
>>> samples[0]
('TAU', 1.0, 0.35)
```

Multiple fields at once:

```
>>> samples[['position', 'value']]
array([(1.0, 0.35), (1.0, 0.11), (1.0, 0.39), (1.5, 0.35), (2.1, 0.11),
          (1.2, 0.39)],
         dtype=[('position', '<f8'), ('value', '<f8')])
```

Fancy indexing works, as usually:

```
>>> samples[samples['sensor_code'] == 'ALFA']
    array([('ALFA', 1.0, 0.35), ('ALFA', 1.5, 0.35), ('ALFA', 2.1, 0.11)],
          dtype=[('sensor_code', '|S4'), ('position', '<f8'), ('value',
    '<f8')])
```

Note: There are a bunch of other syntaxes for constructing structured arrays, see here and here.

Masked arrays

Masked arrays are arrays that may have missing or invalid entries.

For example, suppose we have an array where the fourth entry is invalid:

```
>>> x = np.array([1, 2, 3, -99, 5])
```

One way to describe this is to create a masked array:

```
>>> mx = ma.masked_array(x, mask=[0, 0, 0, 1, 0])
    >>> mx
    masked_array(data = [1 2 3 -- 5],
                 mask = [False False False  True False],
           fill_value = 999999)
```

Masked mean ignores masked data:

```
>>> mx.mean()
    2.75
    >>> np.mean(mx)
    2.75
```

⚠ Not all Numpy functions respect masks, for instance `np.dot`, so check the return types.

The `masked_array` returns a **view** to the original array:

```
>>> mx[1] = 9
    >>> x
    array([  1,   9,   3, -99,   5])
```

The mask

You can modify the mask by assigning:

```
>>> mx[1] = np.ma.masked
    >>> mx
    masked_array(data = [1 -- 3 -- 5],
                mask = [False  True False  True False],
        fill_value = 999999)
```

The mask is cleared on assignment:

```
>>> mx[1] = 9
    >>> mx
    masked_array(data = [1 9 3 -- 5],
                 mask = [False False False  True False],
          fill_value = 999999)
```

The mask is also available directly:

```
>>> mx.mask
    array([False, False, False,  True, False], dtype=bool)
```

The masked entries can be filled with a given value to get an usual array back:

```
>>> x2 = mx.filled(-1)
    >>> x2
    array([ 1,  9,  3, -1,  5])
```

The mask can also be cleared:

```
>>> mx.mask = np.ma.nomask
    >>> mx
    masked_array(data = [1 9 3 -99 5],
                 mask = [False False False False False],
          fill_value = 999999)
```

Domain-aware functions

The masked array package also contains domain-aware functions:

```
>>> np.ma.log(np.array([1, 2, -1, -2, 3, -5]))
    masked_array(data = [0.0 0.69314718056 -- -- 1.09861228867 --],
                 mask = [False False  True  True False  True],
          fill_value = 1e+20)
```

Note: Streamlined and more seamless support for dealing with missing data in arrays is making its way into Numpy 1.7. Stay tuned!

Example: Masked statistics

Canadian rangers were distracted when counting hares and lynxes in 1903-1910 and 1917-1918, and got the numbers are wrong. (Carrot farmers stayed alert, though.) Compute the mean populations over time, ignoring the invalid numbers.

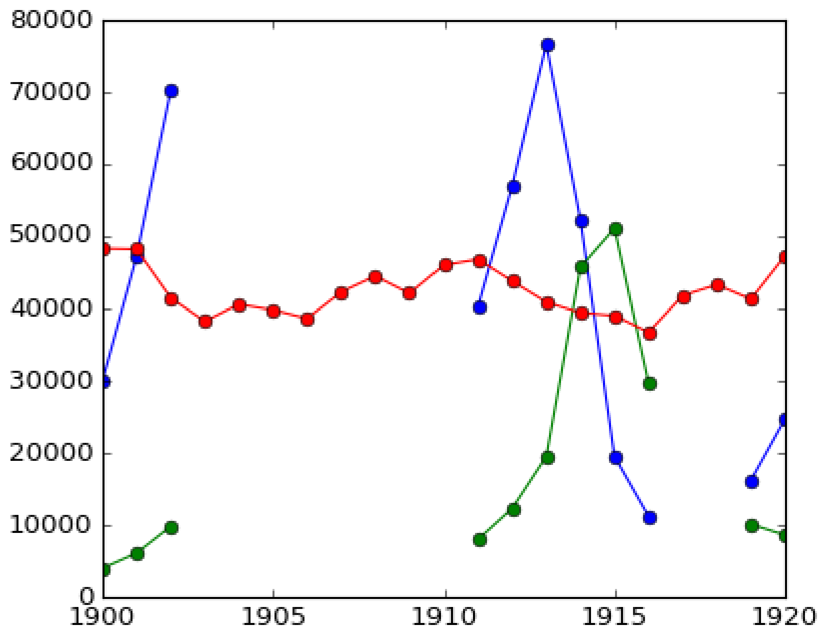
```
>>> data = np.loadtxt('../../data/populations.txt')
    >>> populations = np.ma.masked_array(data[:,1:])
    >>> year = data[:,0]
```

```
>>> bad_years = (((year >= 1903) & (year <= 1910))
    ...            | ((year >= 1917) & (year <= 1918)))
    >>> populations[bad_years,0] = np.ma.masked
    >>> populations[bad_years,1] = np.ma.masked
>>> populations.mean(axis=0)
    masked_array(data = [40472.7272727 18627.2727273 42400.0],
                 mask = [False False False],
          fill_value = 1e+20)
    >>> populations.std(axis=0)
    masked_array(data = [21087.656489 15625.7998142 3322.50622558],
                 mask = [False False False],
           fill_value = 1e+20)
```

Note that Matplotlib knows about masked arrays:

```
>>> plt.plot(year, populations, 'o-')
      >>> plt.show()
```

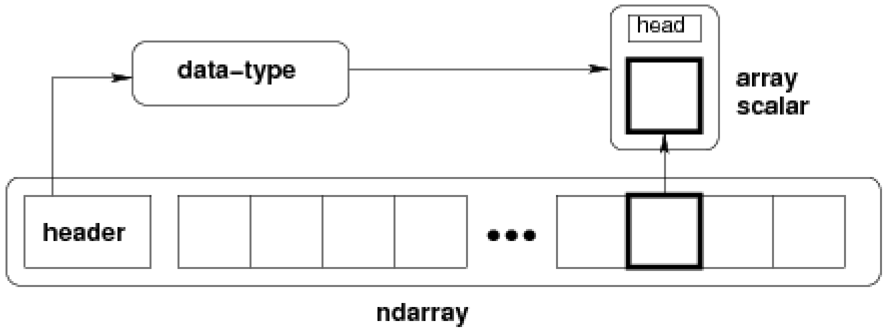
[source code, hires.png, pdf]



Under the hood: the memory layout of a numpy array

A numpy array is:

> block of memory + indexing scheme + data type descriptor
>
> - raw data
> - how to locate an element
> - how to interpret an element



Block of memory

```
>>> x = np.array([1, 2, 3, 4], dtype=np.int32)
>>> x.data
<read-write buffer for 0xa37bfd8, size 16, offset 0 at 0xa4eabe0>
>>> str(x.data)
'\x01\x00\x00\x00\x02\x00\x00\x00\x03\x00\x00\x00\x04\x00\x00\x00'
```

Memory address of the data:

```
>>> x.__array_interface__['data'][0]
159755776
```

Reminder: two `ndarrays` may share the same memory:

```
>>> x = np.array([1,2,3,4])
>>> y = x[:]
>>> x[0] = 9
>>> y
array([9, 2, 3, 4])
>>> y.base is x
True
```

Memory does not need to be owned by an `ndarray`:

```
>>> x = '\x01\x02\x03\x04'
>>> y = np.frombuffer(x, dtype=np.int8)
>>> y
array([1, 2, 3, 4], dtype=int8)
>>> y.data
<read-only buffer for 0xa588ba8, size 4, offset 0 at 0xa55cd60>
>>> y.base is x
True
```

```
>>> y.flags
  C_CONTIGUOUS : True
  F_CONTIGUOUS : True
  OWNDATA : False
  WRITEABLE : False
  ALIGNED : True
  UPDATEIFCOPY : False
```

The `owndata` and `writeable` flags indicate status of the memory block.

Indexing scheme: strides

The question

```
>>> x = np.array([[1, 2, 3],
                  [4, 5, 6],
                  [7, 8, 9]], dtype=np.int8)
>>> str(x.data)
'\x01\x02\x03\x04\x05\x06\x07\x08\x09'
```

At which byte in `x.data` does the item `x[1,2]` begin?

The answer (in Numpy)

- **strides**: the number of bytes to jump to find the next element
- 1 stride per dimension

```
>>> x.strides
(3, 1)
>>> byte_offset = 3*1 + 1*2   # to find x[1,2]
>>> x.data[byte_offset]
'\x06'
>>> x[1,2]
6
```

- simple, **flexible**

C and Fortran order

```
>>> x = np.array([[1, 2, 3],
                  [4, 5, 6],
                  [7, 8, 9]], dtype=np.int16, order='C')
>>> x.strides
(6, 2)
>>> str(x.data)
'\x01\x00\x02\x00\x03\x00\x04\x00\x05\x00\x06\x00\x07\x00\x08\x00\t\x00
'
```

- Need to jump 6 bytes to find the next row
- Need to jump 2 bytes to find the next column

```
>>> y = np.array(x, order='F')
>>> y.strides
(2, 6)
>>> str(y.data)
'\x01\x00\x04\x00\x07\x00\x02\x00\x05\x00\x08\x00\x03\x00\x06\x00\t\x00
'
```

- Need to jump 2 bytes to find the next row
- Need to jump 6 bytes to find the next column

- Similarly to higher dimensions:
  - C: last dimensions vary fastest (= smaller strides)
  - F: first dimensions vary fastest

$$\text{shape} = (d_1, d_2, ..., d_n)$$
$$\text{strides} = (s_1, s_2, ..., s_n)$$
$$s_j^C = d_{j+1} d_{j+2} ... d_n \times \text{itemsize}$$
$$s_j^F = d_1 d_2 ... d_{j-1} \times \text{itemsize}$$

Slicing

- *Everything* can be represented by changing only `shape`, `strides`, and possibly adjusting the `data` pointer!
- Never makes copies of the data

```
>>> x = np.array([1, 2, 3, 4, 5, 6], dtype=np.int32)
>>> y = x[::-1]
>>> y
array([6, 5, 4, 3, 2, 1])
>>> y.strides
(-4,)
```

```
>>> y = x[2:]
>>> y.__array_interface__['data'][0] - x.__array_interface__['data'][0]
8
```

```
>>> x = np.zeros((10, 10, 10), dtype=np.float)
>>> x.strides
(800, 80, 8)
>>> x[::2,::3,::4].strides
(1600, 240, 32)
```

- Similarly, transposes never make copies (it just swaps strides)

```
>>> x = np.zeros((10, 10, 10), dtype=np.float)
>>> x.strides
(800, 80, 8)
>>> x.T.strides
(8, 80, 800)
```

Reshaping

But: not all reshaping operations can be represented by playing with strides.

```
>>> a = np.arange(6, dtype=np.int8).reshape(3, 2)
>>> b = a.T
>>> b.strides
(1, 2)
```

So far, so good. However:

```
>>> str(a.data)
    '\x00\x01\x02\x03\x04\x05'
    >>> b
    array([[0, 2, 4],
           [1, 3, 5]], dtype=int8)
    >>> c = b.reshape(3*2)
    >>> c
    array([0, 2, 4, 1, 3, 5], dtype=int8)
```

Here, there is no way to represent the array `c` given one stride and the block of memory for `a`. Therefore, the `reshape` operation needs to make a copy here.

Summary

- Numpy array: block of memory + indexing scheme + data type description
- Indexing: strides

  `byte_position = np.sum(arr.strides * indices)`
- Various tricks can you do by playing with the strides (stuff for an advanced tutorial it is)