Introduction to NumPy

Original slides by:
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https://www.slideshare.net/PyData/introduction-to-numpy

What is NumPy

- NumPy is a Python C extension library for array-oriented computing
  - Efficient
  - In-memory
  - Contiguous (or Strided)
  - Homogeneous (but types can be algebraic)

- NumPy is suited to many applications
  - Image processing
  - Signal processing
  - Linear algebra
  - A plethora of others

Arrays – Numerical Python (Numpy)

- Lists ok for storing small amounts of one-dimensional data

```
>>> a = [1,3,5,7,9]
>>> print(a[2:4])
[5, 7]
>>> b = [[1, 3, 5, 7, 9], [2, 4, 6, 8, 10]]
>>> print(b[0])
[1, 3, 5, 7, 9]
>>> print(b[1][2:4])
[6, 8]
```

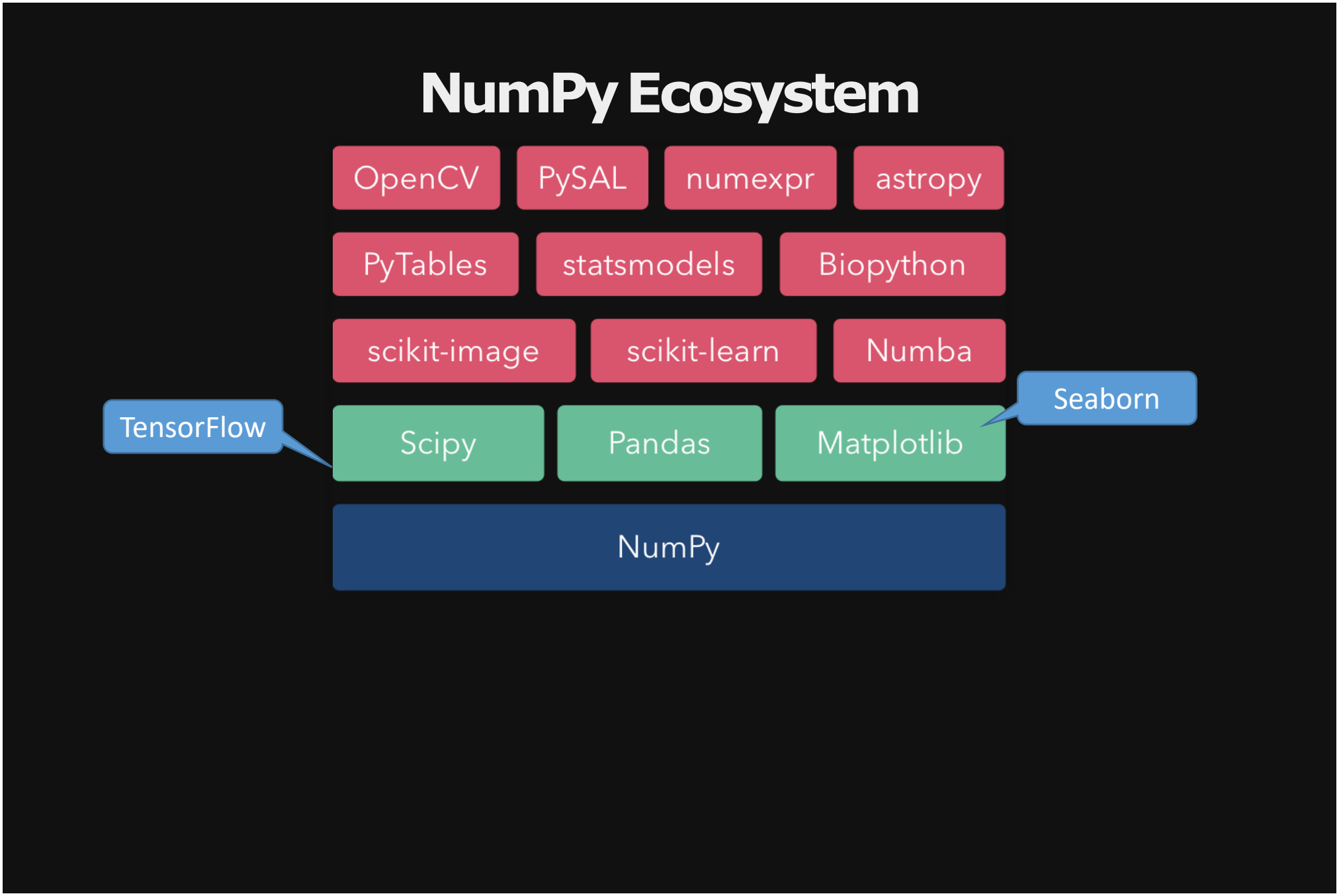
```
>>> a = [1,3,5,7,9]
>>> b = [3,5,6,7,9]
>>> c = a + b
>>> print c
[1, 3, 5, 7, 9, 3, 5, 6, 7, 9]
```

- But, can't use directly with arithmetical operators (+, -, *, /, …)
- Need efficient arrays with arithmetic and better multidimensional tools
- **Numpy**

```
>>> import numpy (as np)
```

- Similar to lists, but much more capable, except fixed size

NumPy is the foundation of the python scientific stack


NumPy Ecosystem
OpenCV
PySAL
numexpr
astropy
PyTables
statsmodels
Biopython
scikit-image
scikit-learn
Numba
TensorFlow
Scipy
Pandas
Matplotlib
Seaborn
NumPy

Numpy – Creating vectors

- From lists
  - numpy.array

```
# as vectors from lists
>>> a = numpy.array([1,3,5,7,9])
>>> b = numpy.array([3,5,6,7,9])
>>> c = a + b  # common operations element-wise (more later)
>>> print c
[4, 8, 11, 14, 18]

>>> type(c)
(<type 'numpy.ndarray'>)

>>> c.shape
(5,)
```

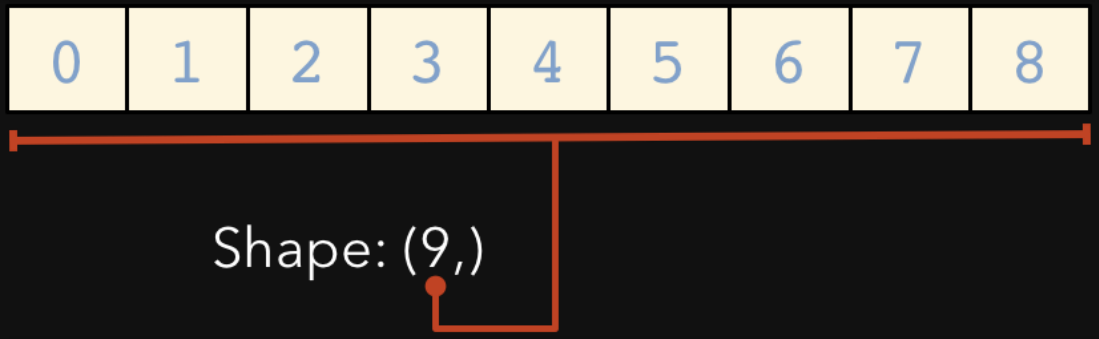
Numpy – Creating Arrays

```
>>> l = [[1, 2, 3], [3, 6, 9], [2, 4, 6]]  # create a list
>>> a = numpy.array(l)  # convert a list to an array
>>>print(a)
[[1 2 3]
 [3 6 9]
 [2 4 6]]
>>> a.shape
(3, 3)
>>> print(a.dtype)  # get type of an array
int64

# or directly as matrix
>>> M = array([[1, 2], [3, 4]])
>>> M.shape
(2,2)
>>> M.dtype
dtype('int64')
```

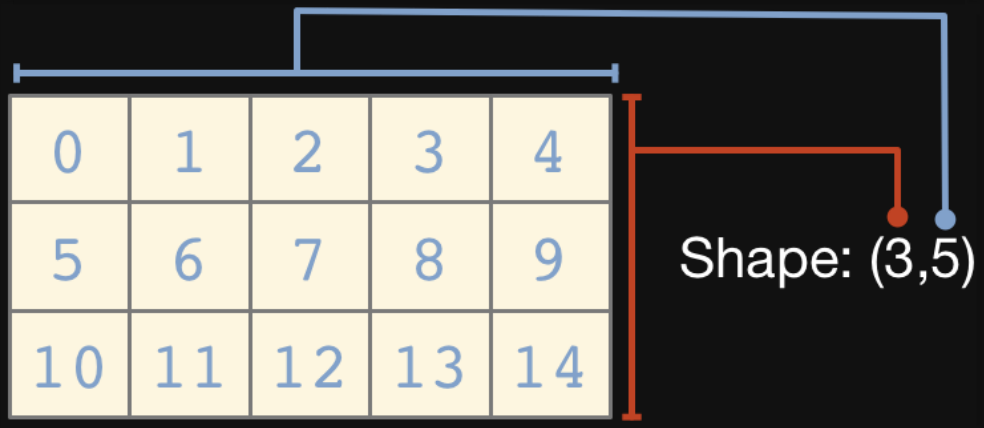
```
#only one type
>>> M[0,0] = "hello"
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: invalid literal for long() with base 10:
'hello'

>>> M = numpy.array([[1, 2], [3, 4]], dtype=complex)
>>> M
array([[ 1.+0.j,  2.+0.j],
       [ 3.+0.j,  4.+0.j]])
```

Array Shape

One dimensional arrays have a 1-tuple for their shape



...Two dimensional arrays have a 2-tuple

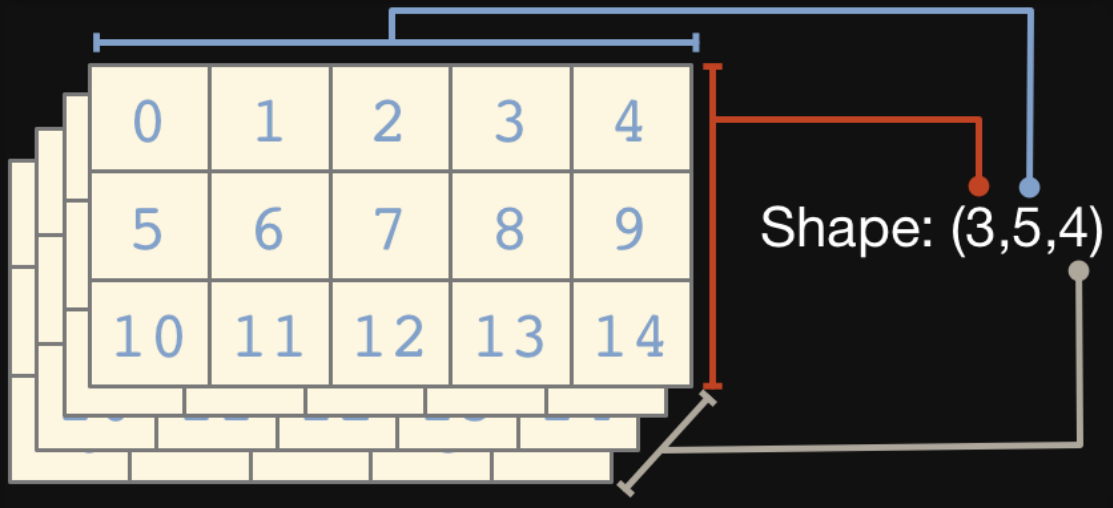


Shape must be maintained

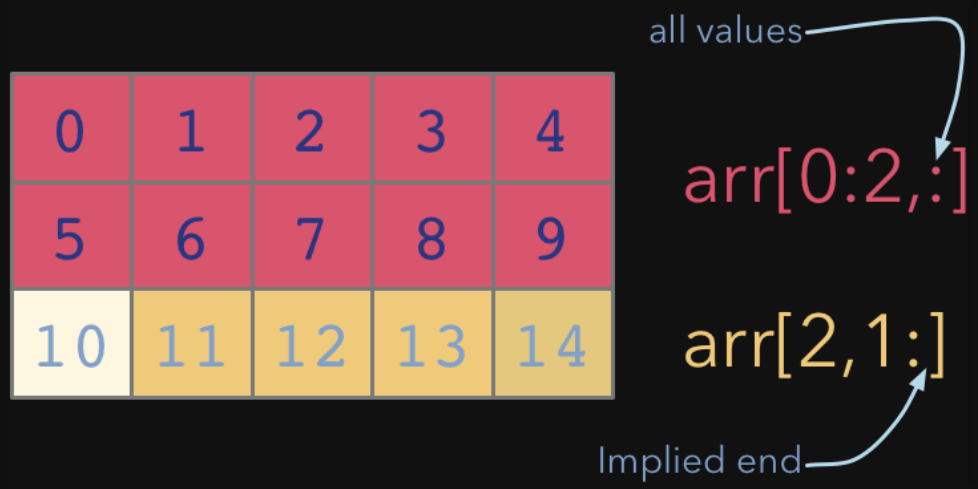
- A = np.array([[1,2,3], [4,5], [6]])
- A.shape #(3,)
- A.dtype #object

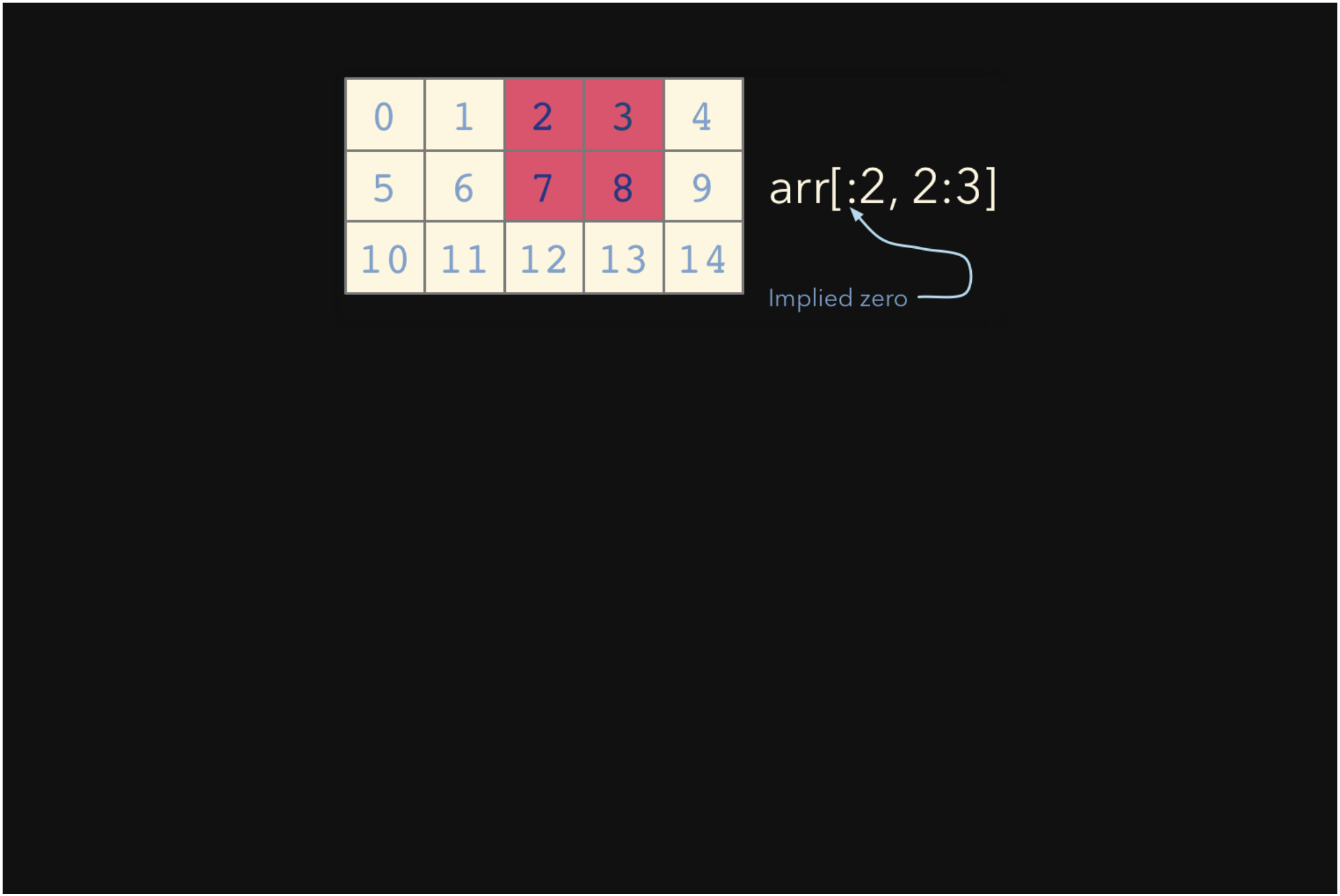
- A = np.array([[1,2,3], [4,5,6], [6,7,8]])
- A.shape #(3,3)
- A.dtype #int32

...And so on

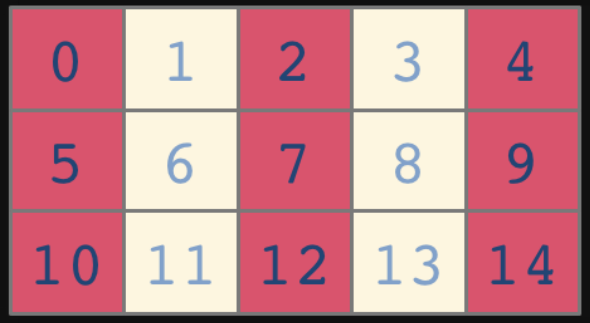


Indexing and Slicing

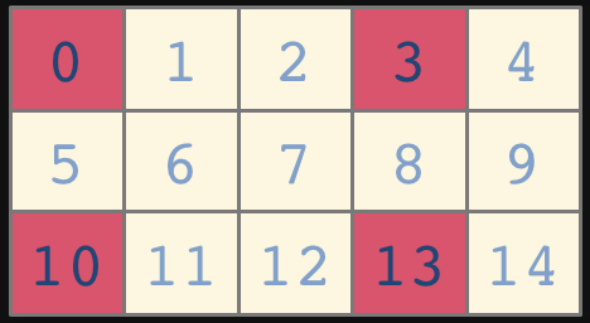



0 1 2 3 4
5 6 7 8 9
10 11 12 13 14
arr[:2, 2:3]
Implied zero

NumPy array indices can also take an optional stride



arr[:,::2]



arr[::2,::3]

Array Views

Simple assigments do not make copies of arrays (same semantics as Python). Slicing operations do not make copies either; they return views on the original array.

```
In [2]: a = np.arange(10)

In [3]: b = a[3:7]

In [4]: b
Out[4]: array([3, 4, 5, 6])

In [5]: b[:] = 0

In [6]: a
Out[6]: array([0, 1, 3, 0, 0, 0, 0, 7, 8, 9])

In [7]: b.flags.owndata
Out[7]: False
```

Array views contain a pointer to the original data, but may have different shape or stride values. Views always have `flags.owndata` equal to `False`,

Numpy – Creating arrays

- Generation functions

```
>>> x = numpy.arange(0, 10, 1) # arguments: start, stop, step
>>> x
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])

>>> numpy.linspace(0, 10, 25)
array([  0.        ,   0.41666667,   0.83333333,   1.25      ,
         1.66666667,   2.08333333,   2.5       ,   2.91666667,
         3.33333333,   3.75      ,   4.16666667,   4.58333333,
         5.        ,   5.41666667,   5.83333333,   6.25      ,
         6.66666667,   7.08333333,   7.5       ,   7.91666667,
         8.33333333,   8.75      ,   9.16666667,   9.58333333,  10.        ])
>>> numpy.logspace(0, 10, 10, base=numpy.e)
array([  1.00000000e+00,   3.03773178e+00,   9.22781435e+00,
         2.80316249e+01,   8.51525577e+01,   2.58670631e+02,
         7.85771994e+02,   2.38696456e+03,   7.25095809e+03,
         2.20264658e+04])
```

Numpy – Creating arrays

```
# a diagonal matrix
>>> numpy.diag([1,2,3])
array([[1, 0, 0],
       [0, 2, 0],
       [0, 0, 3]])

>>> b = numpy.zeros(5)
>>> print(b)
[ 0.  0.  0.  0.  0.]
>>> b.dtype
dtype('float64')
>>> n = 1000
>>> my_int_array = numpy.zeros(n, dtype=numpy.int)
>>> my_int_array.dtype
dtype('int32')

>>> c = numpy.ones((3,3))
>>> c
array([[ 1.,  1.,  1.],
       [ 1.,  1.,  1.],
       [ 1.,  1.,  1.]])
```

Numpy – array creation and use

```
>>> d = numpy.arange(5)  # just like range()
>>> print(d)
[0 1 2 3 4]

>>> d[1] = 9.7
>>> print(d)  # arrays keep their type even if elements changed
[0 9 2 3 4]

>>> print(d*0.4)  # operations create a new array, with new type
[ 0.   3.6  0.8  1.2  1.6]

>>> d = numpy.arange(5, dtype=numpy.float)
>>> print(d)
[ 0.  1.  2.  3.  4.]

>>> numpy.arange(3, 7, 0.5)  # arbitrary start, stop and step
array([ 3. , 3.5, 4. , 4.5, 5. , 5.5, 6. , 6.5])
```

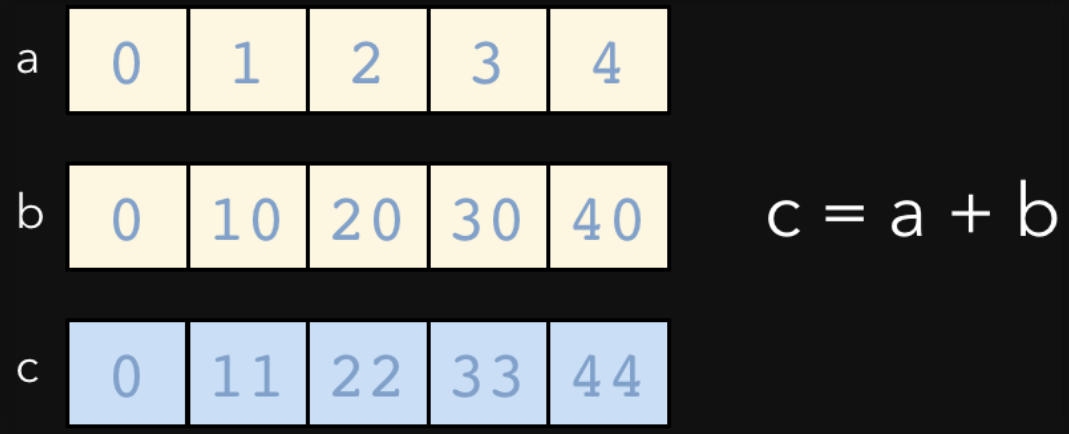
Numpy – array creation and use

```
>>> x, y = numpy.mgrid[0:5, 0:5] # similar to meshgrid in MATLAB
>>> x
array([[0, 0, 0, 0, 0],
       [1, 1, 1, 1, 1],
       [2, 2, 2, 2, 2],
       [3, 3, 3, 3, 3],
       [4, 4, 4, 4, 4]])
# random data
>>> numpy.random.rand(5,5)
array([[ 0.51531133,  0.74085206,  0.99570623,  0.97064334,  0.5819413 ],
       [ 0.2105685 ,  0.86289893,  0.13404438,  0.77967281,  0.78480563],
       [ 0.62687607,  0.51112285,  0.18374991,  0.2582663 ,  0.58475672],
       [ 0.72768256,  0.08885194,  0.69519174,  0.16049876,  0.34557215],
       [ 0.93724333,  0.17407127,  0.1237831 ,  0.96840203,  0.52790012]])
```

https://docs.scipy.org/doc/numpy/user/basics.creation.html
https://docs.scipy.org/doc/numpy/reference/routines.array-creation.html#routines-array-creation

Universal Functions (ufuncs)

NumPy ufuncs are functions that operate element-wise on one or more arrays



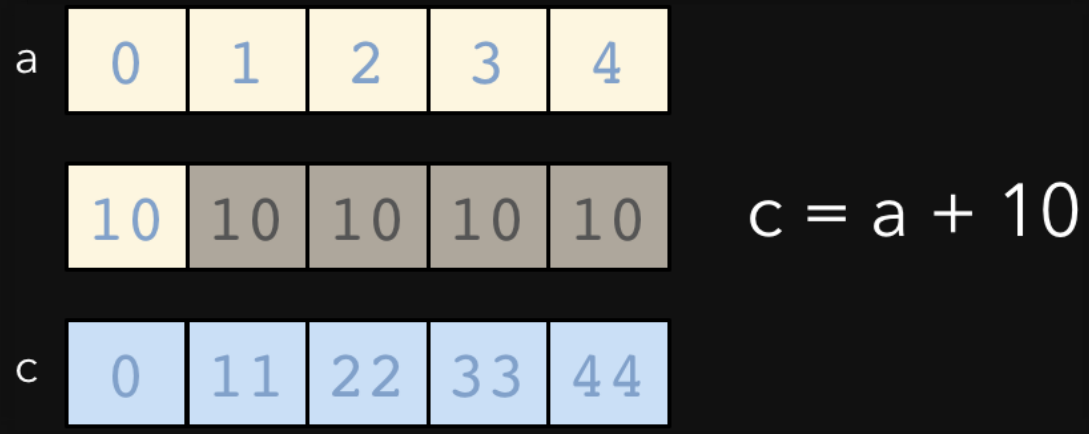
ufuncs dispatch to optimized C inner-loops based on array dtype

NumPy has many built-in ufuncs

- comparison: `<, <=, ==, !=, >=, >`
- arithmetic: `+, -, *, /, reciprocal, square`
- exponential: `exp, expm1, exp2, log, log10, log1p, log2, power, sqrt`
- trigonometric: `sin, cos, tan, acsin, arccos, atctan`
- hyperbolic: `sinh, cosh, tanh, acsinh, arccosh, atctanh`
- bitwise operations: `&, |, ~, ^, left_shift, right_shift`
- logical operations: `and, logical_xor, not, or`
- predicates: `isfinite, isinf, isnan, signbit`
- other: `abs, ceil, floor, mod, modf, round, sinc, sign, trunc`

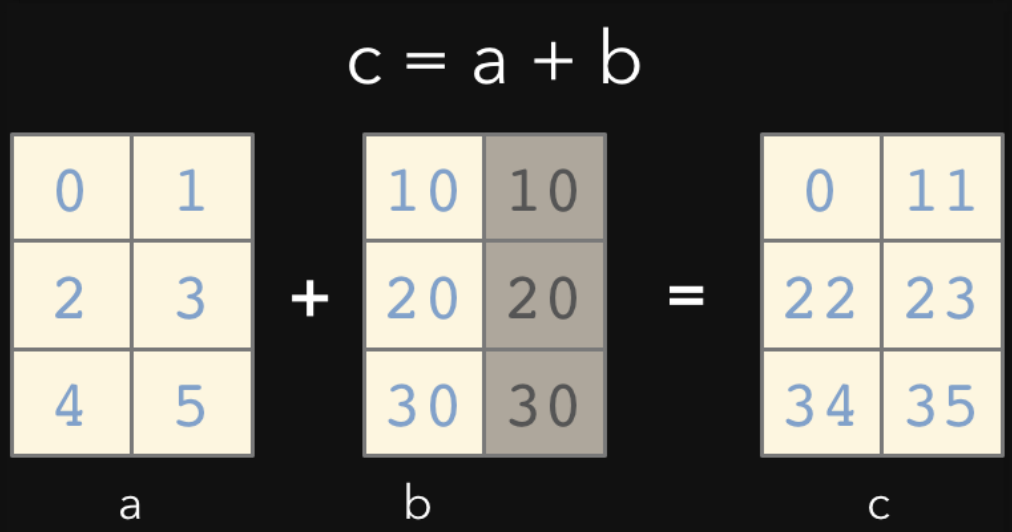
Broadcasting

A key feature of NumPy is broadcasting, where arrays with different, but compatible shapes can be used as arguments to ufuncs



In this case an array scalar is broadcast to an array with shape `(5, )`

A slightly more involved broadcasting example in two dimensions



Here an array of shape `(3, 1)` is broadcast to an array with shape `(3, 2)`

Broadcasting Rules

In order for an operation to broadcast, the size of all the trailing dimensions for both arrays must either:

be **equal** OR be **one**

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

A      (2d array):         6 x 1
B      (3d array):     1 x 6 x 4
Result (3d array):     1 x 6 x 4

A      (4d array):  3 x 1 x 6 x 1
B      (3d array):      2 x 1 x 4
Result (4d array):  3 x 2 x 6 x 4
```

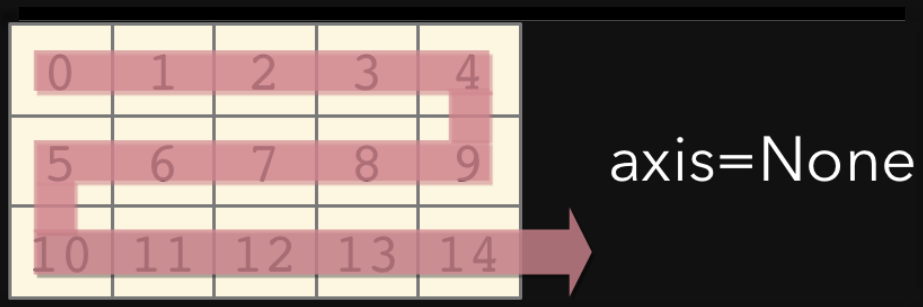
Array Methods

- Predicates
  - `a.any(), a.all()`
- Reductions
  - `a.mean(), a.sum(), a.argmin(), a.argmax(), a.trace(), a.cumsum(), a.cumprod()`
- Manipulation
  - `a.argsort(), a.transpose(), a.reshape(...), a.ravel(), a.fill(...), a.clip(...)`
- Complex Numbers
  - `a.real, a.imag, a.conj()`

Reduction: Axis

Array method reductions take an optional `axis` parameter that specifies over which axes to reduce `axis=None` reduces into a single scalar

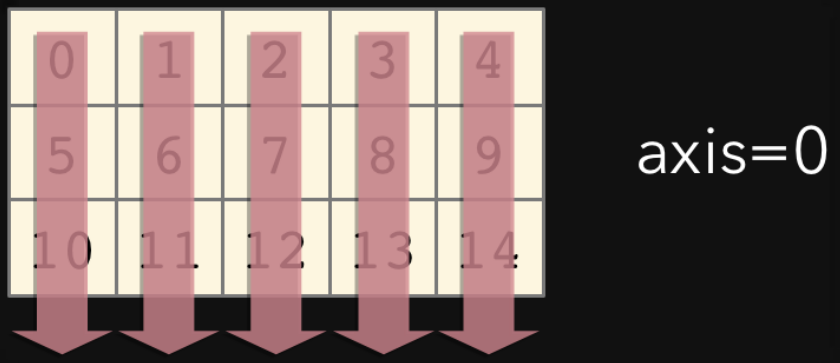
```
In [7]: a.sum()
Out[7]: 105
```



`axis=None` is the default

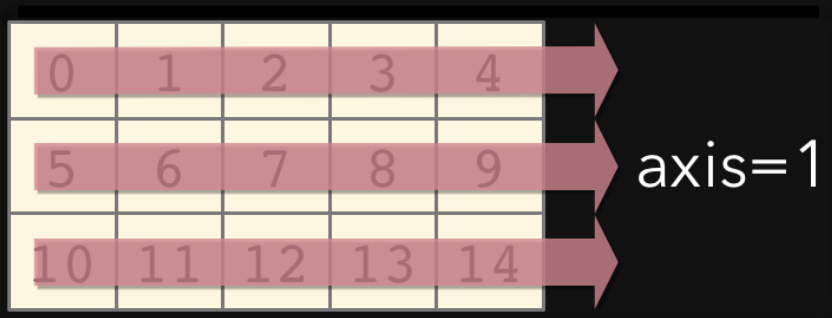
`axis=0` reduces into the zeroth dimension

```
In [8]: a.sum(axis=0)
Out[8]: array([15, 18, 21, 24,
27])
```



`axis=0` reduces into the first dimension

```
In [9]: a.sum(axis=1)
Out[9]: array([10, 35, 60])
```



Numpy – array creation and use

```
>>> arr = numpy.arange(10, 20 )
>>> div_by_3 = arr%3 == 0  # comparison produces boolean array
>>> print(div_by_3)
[ False False  True False False  True False False  True False]
>>> print(arr[div_by_3])  # can use boolean lists as indices
[12 15 18]

>>> arr = numpy.arange(10, 20) . reshape((2,5))
[[10 11 12 13 14]
 [15 16 17 18 19]]
```

Numpy – array methods

```
>>> arr.sum()
145
>>> arr.mean()
14.5
>>> arr.std()
2.8722813232690143
>>> arr.max()
19
>>> arr.min()
10
>>> div_by_3.all()
False
>>> div_by_3.any()
True
>>> div_by_3.sum()
3
>>> div_by_3.nonzero()
(array([2, 5, 8]),)
```

Numpy – array methods - sorting

```
>>> arr = numpy.array([4.5, 2.3, 6.7, 1.2, 1.8, 5.5])
>>> arr.sort()  # acts on array itself
>>> print(arr)
[ 1.2  1.8  2.3  4.5  5.5  6.7]

>>> x = numpy.array([4.5, 2.3, 6.7, 1.2, 1.8, 5.5])
>>> numpy.sort(x)
array([ 1.2,  1.8,  2.3,  4.5,  5.5,  6.7])

>>> print(x)
[ 4.5  2.3  6.7  1.2  1.8  5.5]

>>> s = x.argsort()
>>> s
array([3, 4, 1, 0, 5, 2])
>>> x[s]
array([ 1.2,  1.8,  2.3,  4.5,  5.5,  6.7])
>>> y[s]
array([ 6.2,  7.8,  2.3,  1.5,  8.5,  4.7])
```

Numpy – array operations

```
>>> a = array([[1.0, 2.0], [4.0, 3.0]])
>>> print a
[[ 1. 2.]
 [ 3. 4.]]

>>> a.transpose()
array([[ 1., 3.],
       [ 2., 4.]])

>>> inv(a)
array([[-2. , 1. ],
       [ 1.5, -0.5]])

>>> u = eye(2) # unit 2x2 matrix; "eye" represents "I"

>>> u
array([[ 1., 0.],
       [ 0., 1.]])

>>> j = array([[0.0, -1.0], [1.0, 0.0]])

>>> dot (j, j) # matrix product
array([[-1., 0.],
       [ 0., -1.]])
```

Numpy – statistics

In addition to the mean, var, and std functions, NumPy supplies several other methods for returning statistical features of arrays. The median can be found:

```
>>> a = np.array([1, 4, 3, 8, 9, 2, 3], float)
>>> np.median(a)
3.0
```

The correlation coefficient for multiple variables observed at multiple instances can be found for arrays of the form [[x1, x2, …], [y1, y2, …], [z1, z2, …], …] where x, y, z are different observables and the numbers indicate the observation times:

```
>>> a = np.array([[1, 2, 1, 3], [5, 3, 1, 8]], float)
>>> c = np.corrcoef(a)
>>> c
array([[ 1.        ,  0.72870505],
       [ 0.72870505,  1.        ]])
```

Here the return array c[i,j] gives the correlation coefficient for the ith and jth observables. Similarly, the covariance for data can be found::

```
>>> np.cov(a)
array([[ 0.91666667,  2.08333333],
       [ 2.08333333,  8.91666667]])
```

Numpy – Creating arrays

- File I/O

```
>>> os.system('head DeBilt.txt')
"Stn", "Datum", "Tg", "qTg", "Tn", "qTn", "Tx", "qTx"
001, 19010101,   -49, 00,   -68, 00,   -22, 40
001, 19010102,   -21, 00,   -36, 30,   -13, 30
001, 19010103,   -28, 00,   -79, 30,    -5, 20
001, 19010104,   -64, 00,   -91, 20,   -10, 00
001, 19010105,   -59, 00,   -84, 30,   -18, 00
001, 19010106,   -99, 00,  -115, 30,   -78, 30
001, 19010107,   -91, 00,  -122, 00,   -66, 00
001, 19010108,   -49, 00,   -94, 00,    -6, 00
001, 19010109,    11, 00,   -27, 40,    42, 00

>>> data = numpy.genfromtxt('DeBilt.txt', delimiter=',', skip_header=1)
>>> data.shape
(25568, 8)
```

```
>>> numpy.savetxt('datasaved.txt', data)
>>> os.system('head datasaved.txt')
1.0000000000000000e+00 1.9010101000000000e+07 -4.9000000000000000e+01
0.0000000000000000e+00 -6.8000000000000000e+01 0.0000000000000000e+00 -
2.2000000000000000e+01 4.0000000000000000e+01
```

Numpy – Creating arrays

```
>>> M = numpy.random.rand(3,3)
>>> M
array([[ 0.84188778,  0.70928643,  0.87321035],
       [ 0.81885553,  0.92208501,  0.873464  ],
       [ 0.27111984,  0.82213106,  0.55987325]])
>>>
>>> numpy.save('saved-matrix.npy', M)
>>> numpy.load('saved-matrix.npy')
array([[ 0.84188778,  0.70928643,  0.87321035],
       [ 0.81885553,  0.92208501,  0.873464  ],
       [ 0.27111984,  0.82213106,  0.55987325]])
>>>
>>> os.system('head saved-matrix.npy')
NUMPYF{'descr': '<f8', 'fortran_order': False, 'shape': (3, 3), }
Ï<
£¾ðê?sy²æ?$÷ÒVñë?Ù4ê?%dn¸í?Ã[Äjóë?Ä,ZÑ?Ç
ÎåNê?ó7L{êá?0
>>>
```

https://docs.scipy.org/doc/numpy/user/basics.io.html
https://docs.scipy.org/doc/numpy/reference/routines.io.html

Using arrays wisely

- Array operations are implemented in C or Fortran
- Optimised algorithms - i.e. fast!
- Python loops (i.e. for i in a:…) are much slower
- Prefer array operations over loops, especially when speed important
- Also produces shorter code, often more readable

Numpy – matrices

For **two dimensional** arrays NumPy defined a special matrix class in module matrix. Objects are created either with matrix() or mat() or converted from an array with method asmatrix().

```
>>> import numpy
>>> m = numpy.mat([[1,2],[3,4]])
or
>>> a = numpy.array([[1,2],[3,4]])
>>> m = numpy.mat(a)
or
>>> a = numpy.array([[1,2],[3,4]])
>>> m = numpy.asmatrix(a)
```

Note that the statement m = mat(a) creates a copy of array 'a'.
Changing values in 'a' will not affect 'm'.
On the other hand, method m = asmatrix(a) returns a new reference to the same data.
Changing values in 'a' will affect matrix 'm'.

https://docs.scipy.org/doc/numpy/reference/generated/numpy.matrix.html

Numpy – matrices

For **two dimensional** arrays NumPy defines ... dule matrix.
Objects are created either with matrix() o... rray with method asmatrix().

```
>>> import numpy
>>> m = numpy.mat([[1,2],[3
or
>>> a = numpy.array([[
>>> m = numpy.mat(a)
or
>>> a = numpy
>>> m = num
```

Not... a) creates a copy of array 'a'.
C... affect 'm'.
On t... m = asmatrix(a) returns a new reference to the same data.
Chang... l affect matrix 'm'.

https://docs... org/doc/numpy/reference/generated/numpy.matrix.html

Do not use - confusion guaranteed

Numpy – matrices

Array and matrix operations may be quite different!

```
>>> a = array([[1,2],[3,4]])
>>> m = mat(a) # convert 2-d array to matrix
>>> m = matrix([[1, 2], [3, 4]])
>>> a[0]           # result is 1-dimensional
array([1, 2])
>>> m[0]           # result is 2-dimensional
matrix([[1, 2]])
>>> a*a            # element-by-element multiplication
array([[ 1, 4], [ 9, 16]])
>>> m*m            # (algebraic) matrix multiplication
matrix([[ 7, 10], [15, 22]])
>>> a**3           # element-wise power
array([[ 1, 8], [27, 64]])
>>> m**3           # matrix multiplication m*m*m
matrix([[ 37, 54], [ 81, 118]])
>>> m.T            # transpose of the matrix
matrix([[1, 3], [2, 4]])
>>> m.H            # conjugate transpose (differs from .T for complex matrices)
matrix([[1, 3], [2, 4]])
>>> m.I            # inverse matrix
matrix([[-2. , 1. ], [ 1.5, -0.5]])
```

Numpy – matrices

- Operator *, dot(), and multiply():
  - For array, '*' **means element-wise multiplication**, and the dot() function is used for matrix multiplication.
  - For matrix, '*'**means matrix multiplication**, and the multiply() function is used for element-wise multiplication.
- Handling of vectors (rank-1 arrays)
  - For array, the vector shapes 1xN, Nx1, and N are all different things. Operations like A[:,1] return a rank-1 array of shape N, not a rank-2 of shape Nx1. Transpose on a rank-1 array does nothing.
  - For matrix, rank-1 arrays are always upgraded to 1xN or Nx1 matrices (row or column vectors). A[:,1] returns a rank-2 matrix of shape Nx1.
- Handling of higher-rank arrays (rank > 2)
  - array objects can have rank > 2.
  - matrix objects always have exactly rank 2.
- Convenience attributes
  - array has a .T attribute, which returns the transpose of the data.
  - matrix also has .H, .I, and .A attributes, which return the conjugate transpose, inverse, and asarray() of the matrix, respectively.
- Convenience constructor
  - The array constructor takes (nested) Python sequences as initializers. As in array([[1,2,3],[4,5,6]]).
  - The matrix constructor additionally takes a convenient string initializer. As in matrix("[1 2 3; 4 5 6]")