

Introduction to Numerical Computing with Numpy

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Introduction to Numerical Computing with Numpy

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Introduction to Numerical Computing with Numpy



Hi there!

NumPy

The Standard Numerical Library
for Python

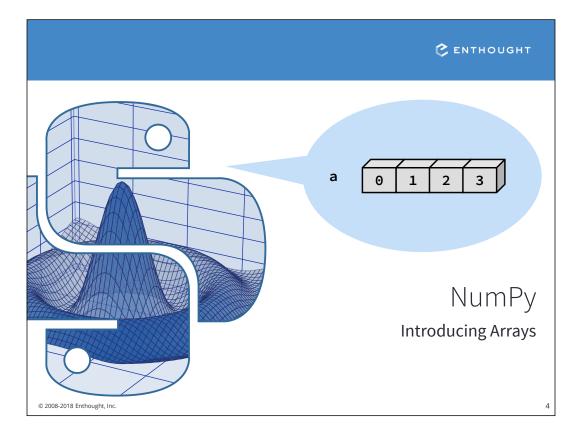
NumPy Arrays

- Introducing Arrays
- Indexing and Slicing
- Creating Arrays
- Array Calculations
- The Array Data Structure
- Structure Operations



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Introducing NumPy Arrays

SIMPLE ARRAY CREATION

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

CHECKING THE TYPE

>>> type(a)

numpy.ndarray

NUMERIC "TYPE" OF ELEMENTS

```
>>> a.dtype
dtype('int32')
```

NUMBER OF DIMENSIONS

```
>>> a.ndim
```

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ARRAY SHAPE

```
# Shape returns a tuple
# listing the length of the
# array along each dimension.
>>> a.shape
(4,)
```

BYTES PER ELEMENT

```
>>> a.itemsize
```

BYTES OF MEMORY USED

```
# Return the number of bytes
# used by the data portion of
# the array.
>>> a.nbytes
16
```



Array Operations

SIMPLE ARRAY MATH

```
>>> a = np.array([1, 2, 3, 4])
>>> b = np.array([2, 3, 4, 5])
>>> a + b
array([3, 5, 7, 9])
>>> a * b
array([ 2, 6, 12, 20])
>>> a ** b
array([ 1, 8, 81, 1024])
```



NumPy defines these constants: pi = 3.14159265359 e = 2.71828182846

MATH FUNCTIONS

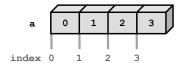
```
# create array from 0.0 to 10.0
>>> x = np.arange(11.0)
# multiply entire array by
# scalar value
>>> c = (2.0 * np.pi) / 10.0
>>> c
0.62831853071795862
>>> c * x
array([0.
            , 0.628, ..., 6.283])
# in-place operations
>>> x *= c
>>> x
array([0. , 0.628, ..., 6.283])
# apply functions to array
>>> y = np.sin(x)
```

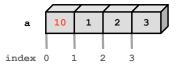
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Setting Array Elements

ARRAY INDEXING

>>> a[0]





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BEWARE OF TYPE COERCION

```
>>> a.dtype
dtype('int32')

# assigning a float into
# an int32 array truncates
# the decimal part
>>> a[0] = 10.6
>>> a
array([10, 1, 2, 3])

# fill has the same behavior
>>> a.fill(-4.8)
>>> a
array([-4, -4, -4, -4])
```

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Multi-Dimensional Arrays

MULTI-DIMENSIONAL ARRAYS

>>> a = np.array([[0, 1, 2, 3], ... [10,11,12,13]])
>>> a

array([[0, 1, 2, 3], [10,11,12,13]])



SHAPE = (ROWS, COLUMNS)

>>> a.shape (2, 4)



ELEMENT COUNT

>>> a.size



NUMBER OF DIMENSIONS

>>> a.ndim 2 © 2008-2018 Enthought, Inc.





GET / SET ELEMENTS

ADDRESS SECOND (ONETH) ROW USING SINGLE INDEX

>>> a[1]
array([10, 11, 12, -1])

Py

a 0 0 1



Formatting Numeric Display

DEFAULT FORMATTING

```
>>> a
array([1. , 1.5, 2. , 2.5])

>>> a * np.pi
array([3.14159265, 4.71238898,
6.28318531, 7.85398163])

>>> a * np.pi * le8
array([3.14159265e+08,
4.71238898e+08, 6.28318531e+08,
7.85398163e+08])

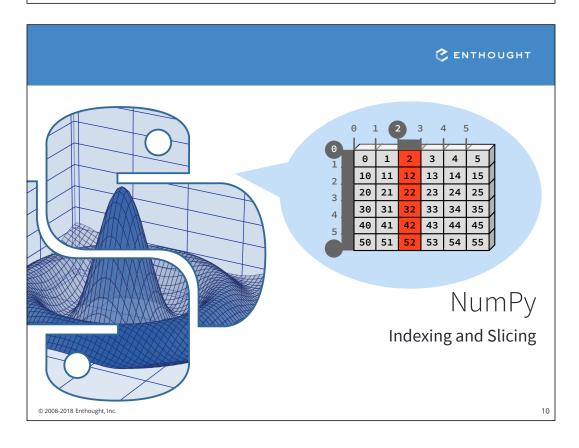
>>> a * np.pi * le-6
array([3.14159265e-06,
4.71238898e-06, 6.28318531e-06,
7.85398163e-06])
```

>>> a = np.arange(1.0, 3.0, 0.5)

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USER FORMATTING

```
# set precision
>>> np.set printoptions(
      precision=2)
array([1. , 1.5, 2. , 2.5])
>>> a * np.pi
array([3.14, 4.71, 6.28, 7.85])
>>> a * np.pi * 1e8
array([3.14e+08, 4.71e+08,
6.28e+08, 7.85e+08])
>>> a * np.pi * 1e-6
array([3.14e-06, 4.71e-06, 6.28e-
06, 7.85e-06])
# suppress scientific notation
>>> np.set printoptions(
     suppress=True)
>>> a * np.pi * 1e-6
array([0., 0., 0., 0.])
                      C ENTHOUGHT 9
```



Slicing

var[lower:upper:step]

Extracts a portion of a sequence by specifying a lower and upper bound. The lower-bound element is included, but the upper-bound element is **not** included. Mathematically: [lower, upper). The step value specifies the stride between elements.

SLICING ARRAYS

```
-5 -4 -3 -2 -1
# indices:
                  0 1 2 3 4
>>> a = np.array([10,11,12,13,14])
# [10, 11, 12, 13, 14]
>>> a[1:3]
array([11, 12])
# negative indices work also
>>> a[1:-2]
array([11, 12])
>>> a[-4:3]
array([11, 12])
```

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OMITTING INDICES

```
# omitted boundaries are
# assumed to be the beginning
# (or end) of the array
# grab first three elements
>>> a[:3]
array([10, 11, 12])
# grab last two elements
>>> a[-2:]
array([13, 14])
# every other element
>>> a[::2]
array([10, 12, 14])
                      C ENTHOUGHT 11
```

Array Slicing

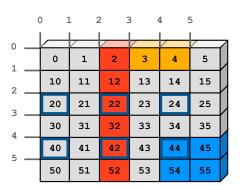
SLICING WORKS MUCH LIKE STANDARD PYTHON SLICING

```
>>> a[0, 3:5]
array([3, 4])
>>> a[4:, 4:]
array([[44, 45],
       [54, 55]])
>>> a[:, 2]
array([2, 12, 22, 32, 42, 52])
```

STRIDED ARE ALSO POSSIBLE

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

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Assigning to a Slice

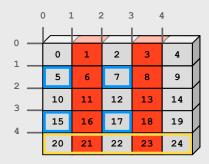
Slices are references to locations in memory. These memory locations can be used in assignment operations.

```
>>> a = np.array([0, 1, 2, 3, 4])
 # slicing the last two elements returns the data there
 >>> a[-2:]
 array([3, 4])
 # we can insert an iterable of length two
 >>> a[-2:] = [-1, -2]
 >>> a
 array([0, 1, 2, -1, -2])
 # or a scalar value
 >>> a[-2:1 = 99]
 >>> a
 array([ 0, 1, 2, 99, 99])
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                                                   ENTHOUGHT 13
```

Give it a try!

Create the array below with the command

and extract the slices as indicated.



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Sliced Arrays Share Data

Arrays created by slicing share data with the originating array. Changing values in a slice also changes the original array.

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

# create a slice containing two elements of a
>>> b = a[2:4]
>>> b
array([2, 3])
>>> b[0] = 10

# changing b changed a!
>>> a
array([ 0,  1, 10, 3, 4])
>>> np.shares_memory(a, b)
True
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```

Fancy Indexing

```
INDEXING BY POSITION
```

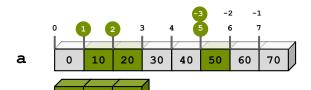
```
>>> a = np.arange(0, 80, 10)
# fancy indexing
>>> indices = [1, 2, -3]
>>> y = a[indices]
>>> y
array([10, 20, 50])
# this also works with setting
>>> a[indices] = 99
>>> a
array([0, 99, 99, 30, 40, 99, 60, 70])
```

У

INDEXING WITH BOOLEANS

```
# manual creation of masks
>>> mask = np.array(
...     [0, 1, 1, 0, 0, 1, 0, 0],
...     dtype=bool)

# fancy indexing
>>> y = a[mask]
>>> y
array([99, 99, 99])
```



20

50

10

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Fancy Indexing in 2-D

```
>>> 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])
```



Unlike slicing, fancy indexing creates copies instead of a view into original array.

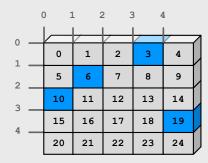
10 20 21 23 24 25 30 32 35 40 41 42 43 50 55

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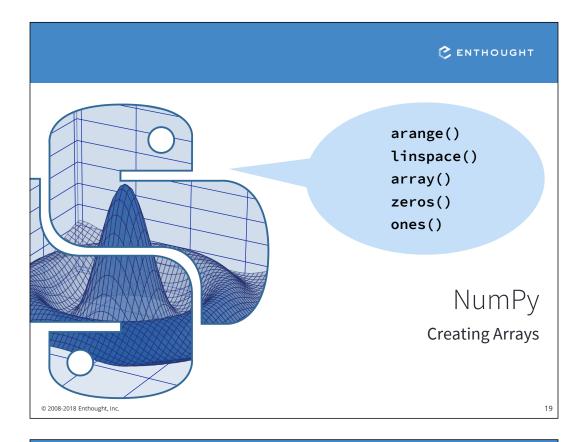
Give it a try!

- 1. Create the array below with
 - a = np.arange(25).reshape(5, 5)
 - and extract the elements indicated in blue.
- 2. Extract all the numbers divisible by 3 using a boolean mask.



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Array Constructor Examples

FLOATING POINT ARRAYS

```
# Default to double precision
>>> a = np.array([0,1.0,2,3])
>>> a.dtype
dtype('float64')
>>> a.nbytes
32
```

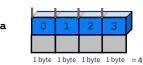
REDUCING PRECISION

```
>>> a = np.array([0,1.,2,3],
              dtype='float32')
>>> a.dtype
dtype('float32')
>>> a.nbytes
16
```

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UNSIGNED INTEGER BYTE

```
>>> a = np.array([0,1,2,3],
               dtype='uint8')
. . .
>>> a.dtype
dtype('uint8')
>>> a.nbytes
          1 2 3
```



```
Base 2
                                   Base 10
                 -> 0 = 0*2**0 + 0*2**1 + ... + 0*2**7

-> 1 = 1*2**0 + 0*2**1 + ... + 0*2**7

-> 2 = 0*2**0 + 1*2**1 + ... + 0*2**7
00000001
00000010
11111111
                -> 255 = 1*2**0 + 1*2**1 + ... + 1*2**7
```

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Array Creation Functions

ARANGE

```
arange([start,] stop[, step],
                 dtype=None)
```

Nearly identical to Python's range (). Creates an array of values in the range [start,stop) with the specified step value. Allows non-integer values for start, stop, and step. Default **dtype** is derived from the start, stop, and step values.

```
>>> np.arange(4)
array([0, 1, 2, 3])
>>> np.arange(0, 2*pi, pi/4)
array([ 0.000, 0.785, 1.571,
2.356, 3.142, 3.927, 4.712,
5.497])
# Be careful...
>>> np.arange(1.5, 2.1, 0.3)
array([ 1.5, 1.8, 2.1])
```

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ONES, ZEROS

```
ones(shape, dtype='float64')
zeros(shape, dtype='float64')
```

shape is a number or sequence specifying the dimensions of the array. If **dtype** is not specified, it defaults to **float64**.

```
>>> np.ones((2, 3),
                dtype='float32')
  array([[ 1., 1., 1.],
          [ 1., 1., 1.]],
          dtype=float32)
  >>> np.zeros(3)
  array([ 0., 0., 0.])
zeros (3) is equivalent to zeros ((3, ))
                          C ENTHOUGHT
```

Array Creation Functions (cont'd)

IDENTITY

```
# Generate an n by n identity
# array. The default dtype is
# float64.
>>> a = np.identity(4)
>>> a
              0.,
                    0.,
array([[ 1.,
                         0.1,
       [ 0., 1., 0.,
                         0.],
       [ 0., 0., 1.,
                        0.],
       [ 0.,
              0.,
                   0.,
                        1.]])
>>> a.dtype
dtype('float64')
>>> np.identity(4, dtype=int)
array([[ 1, 0, 0, 0],
       [ 0, 1, 0, 0],
       [ 0, 0, 1, 0],
```

[0, 0, 0, 1]])

EMPTY AND FULL

```
# empty(shape, dtype=float64,
        order='C')
>>> np.empty(2)
array([1.78021120e-306,
 6.95357225e-308])
# array filled with 5.0
>>> a = np.full(2, 5.0)
array([5., 5.])
# alternative approaches
# (slower)
>>> a = np.empty(2)
>>> a.fill(4.0)
>>> a
array([4., 4.])
>>> a[:] = 3.0
>>> a
array([3., 3.])
```

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Array Creation Functions (cont'd)

LINSPACE

Generate N evenly spaced
elements between (and including)
start and stop values.
>>> np.linspace(0, 1, 5)
array([0., 0.25, 0.5, 0.75, 1.0])

LOGSPACE

Generate N evenly spaced
elements on a log scale
between base**start and
base**stop (default base=10)
>>> np.logspace(0, 1, 5)
array([1., 1.78, 3.16, 5.62, 10.])

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ARRAYS FROM/TO TXT FILES

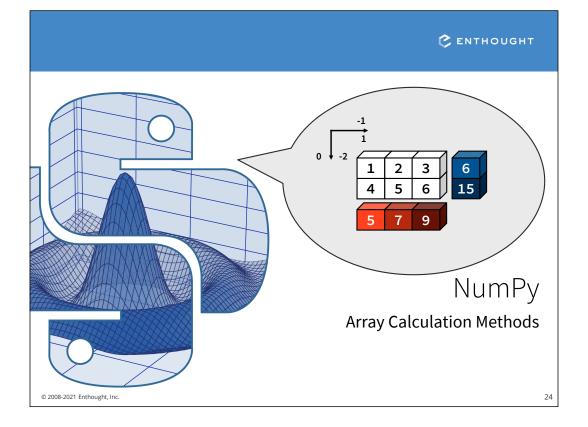
```
BEGINNING OF THE FILE

% Day, Month, Year, Skip, Avg Power
01, 01, 2000, x876, 13 % crazy day!
% we don't have Jan 03rd
04, 01, 2000, xfed, 55

Data.txt
```

```
# loadtxt() automatically
# generates an array from the
# txt file
arr = np.loadtxt('Data.txt',
... skiprows=1,
... dtype=int, delimiter=",",
... usecols = (0,1,2,4),
... comments = "%")
# Save an array into a txt file
np.savetxt('filename.txt', arr)
```

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Computations with Arrays

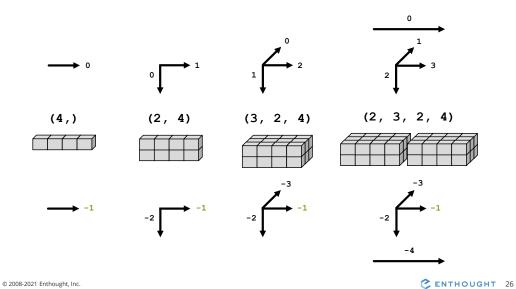
- Operations between multiple array objects are Rule 1: first checked for proper shape match.
- Rule 2: Mathematical operators (+ - * / exp, log, ...) apply element by element, on the values.
- Reduction operations (mean, std, skew, kurt, sum, Rule 3: prod, ...) apply to the whole array, unless an axis is specified.
- Missing values propagate unless explicitly ignored Rule 4: (nanmean, nansum, ...).

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Multi-Dimensional Arrays

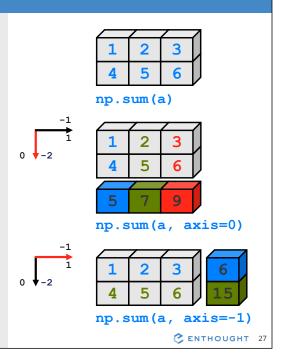
VISUALIZING MULTI-DIMENSIONAL ARRAYS



Array Calculation Methods

SUM METHOD

```
# Methods act on data stored
# in the array
>>> a = np.array([[1,2,3],
                   [4,5,6]])
# .sum() defaults to adding up
all the values in an array.
>>> a.sum()
# supply the keyword axis to
# sum along the 0th axis
>>> a.sum(axis=0)
array([5, 7, 9])
# supply the keyword axis to
# sum along the last axis
>>> a.sum(axis=-1)
array([ 6, 15])
```



Other Operations on Arrays

SUM FUNCTION

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```
# Functions work on data
# passed to it
>>> a = np.array([[1,2,3],
                  [4,5,6]])
# sum() defaults to adding
# up all values in an array.
>>> np.sum(a)
# supply an axis argument to
# sum along a specific axis
>>> np.sum(a, axis=0)
array([5, 7, 9])
```

OTHER METHODS AND FUNCTIONS

Mathematical functions

- sum, prod
- min, max, argmin, argmax
- ptp (max min)

Statistics

• mean, std, var

Truth value testing

· any, all

See the NumPy appendix for more.

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Min/Max

MIN

```
>>> a = np.array([[2, 3], [0, 1]])
# Prefer NumPy functions to
# builtins when working with
# arrays
>>> np.min(a)
# Most NumPy reducers can be used
# as methods as well as functions
>>> a.min()
```

MAX

```
# Use the axis keyword to find
# max values for one dimension
>>> a.max(axis=0)
array([2, 3])
# as a function
>>> np.max(a, axis=1)
array([3, 1])
```

ARGMIN/MAX

```
# Many tasks (like optimization)
# are interested in the location
# of a min/max, not the value
>>> a.argmax()
# arg methods return the
# location in a 1D, flattened
# version of the original array
>>> np.argmin(a)
```

UNRAVELING

```
# NumPy includes a function
# to un-flatten 1D locations
>>> np.unravel index(
        a.argmax(), a.shape)
(0, 1)
```

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Where

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COORDINATE LOCATIONS

```
# NumPy's where function has two
# distinct uses. One is to
# provide coordinates from masks.
>>> a = np.arange(-2, 2) ** 2
>>> a
array([4, 1, 0, 1])
>>> mask = a % 2 == 0
>>> mask
array([ True, False, True, False])
# Coordinates are returned as
# a tuple of arrays, one for
# each axis.
>>> np.where(mask)
(array([0, 2]),)
```

CONDITIONAL ARRAY CREATION

```
# Where can also be used to
# construct a new array by
# choosing values from other
# arrays of the same shape.
>>> positives = np.arange(1, 5)
>>> negatives = -positives
>>> np.where(mask, positives,
             negatives)
array([1, -2, 3, -4])
# Or from scalar values.
# This can be useful for
# recoding arrays.
>>> np.where(mask, 1, 0)
array([1, 0, 1, 0])
# Or from both.
>>> np.where(mask, positives, 0)
array([1, 0, 3, 0])
```

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Statistics Array Methods

MEAN

```
>>> a = np.array([[1,2,3],
                  [4,5,6]])
# mean value of each column
>>> a.mean(axis=0)
array([ 2.5, 3.5, 4.5])
>>> np.mean(a, axis=0)
array([ 2.5, 3.5, 4.5])
```

STANDARD DEV./VARIANCE

```
# Standard Deviation
>>> a.std(axis=0)
array([ 1.5, 1.5, 1.5])
# For sample, set ddof=1
>>> a.std(axis=0, ddof=1)
array([ 2.12, 2.12, 2.12])
```

variance >>> a.var(axis=0) array([2.25, 2.25, 2.25])

>>> np.var(a, axis=0) array([2.25, 2.25, 2.25])

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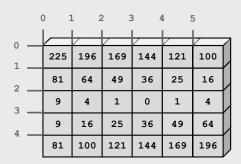
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Give it a try!

Create the array below with

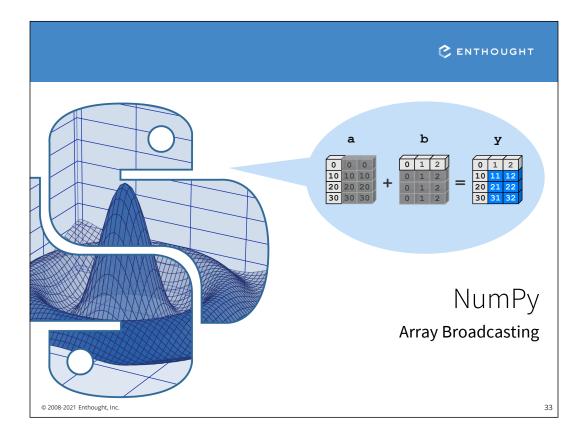
a = np.arange(-15, 15).reshape(5, 6) ** 2and compute:

- The maximum of each row
- The mean of each column
- 3. The position of the overall minimum



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Array Broadcasting

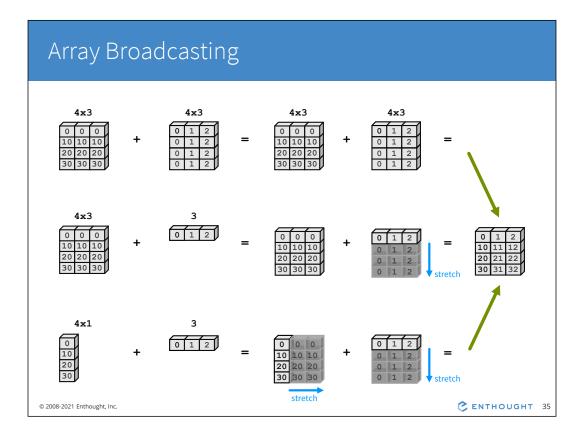
NumPy arrays of different dimensionality can be combined in the same expression. Arrays with smaller dimension are broadcasted to match the larger arrays, without copying data. Broadcasting has **two rules**.

RULE 1: PREPEND ONES TO SMALLER ARRAY'S SHAPE

```
>>> import numpy as np
>>> a = np.ones((3, 5)) \# a.shape == (3, 5)
>>> b = np.ones((5,)) # b.shape == (5,)
>>> b.reshape(1, 5) # result is a (1,5)-shaped array.
>>> b[np.newaxis, :] # equivalent, more concise.
```

RULE 2: DIMENSIONS OF SIZE 1 ARE REPEATED WITHOUT COPYING

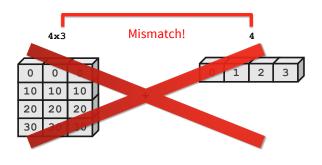
```
>>> c = a + b \# c.shape == (3, 5)
# is logically equivalent to...
>>> tmp b = b.reshape(1, 5)
>>> tmp_b_repeat = tmp_b.repeat(3, axis=0)
>>> c = a + tmp b repeat
# But broadcasting makes no copies of "b"s data!
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```



Broadcasting Rules

The trailing axes of either arrays must be 1 or both must have the same size for broadcasting to occur. Otherwise, a

"ValueError: shape mismatch: objects cannot be broadcast to a single shape" exception is thrown.

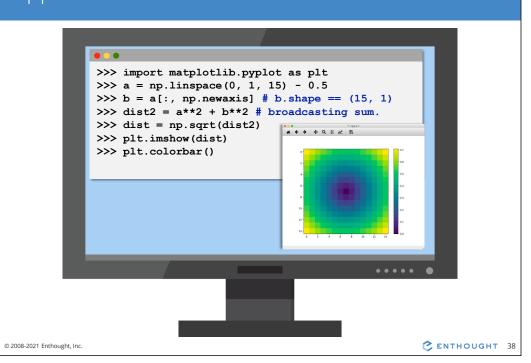


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Broadcasting in Action

```
>>> a = array([0, 10, 20, 30])
>>> b = array([0, 1, 2])
>>> y = a[:, newaxis] + b
                                         b
                    a
                                         3
                   4x1
                  10 10
                                                          10
                                                              11
                                                                  12
                   20 20
                                                                  22
                   30 30
                    stretch
                                stretch
                2-D Array
                                      1-D Array
                                                                      ENTHOUGHT 37
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```

Application: Distance from Center



Broadcasting's Usefulness

Broadcasting can often be used to replace needless data replication inside a NumPy array expression.

np.meshgrid() - use newaxis appropriately in broadcasting expressions.

np.repeat() - broadcasting makes repeating an array along a dimension of size 1 unnecessary.

MESHGRID: COPIES DATA

```
>>> x, y = \
    np.meshgrid([1,2],
                  [3,4,5])
>>> z = x + y
```

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BROADCASTING: NO COPIES

```
>>> x = np.array([1, 2])
>>> y = np.array([3, 4, 5])
>>> z = x[np.newaxis, :] 
       + y[:, np.newaxis]
```

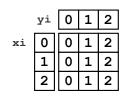
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Broadcasting Indices

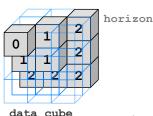
Broadcasting can also be used to slice elements from different "depths" in a 3-D (or any other shape) array. This is a very powerful feature of indexing.

```
>>> data_cube = np.arange(27).reshape(3, 3, 3)
>>> yi, xi = np.meshgrid(np.arange(3), np.arange(3),
                         sparse=True)
>>> zi = np.array([[0, 1, 2],
                   [1, 1, 2],
. . .
                   [2, 2, 2]])
>>> horizon = data cube[xi, yi, zi]
```

Indices



Selected Data



data_cube

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Universal Function Methods

The mathematical, comparative, logical, and bitwise operators op that take two arguments (binary operators) have special methods that operate on arrays:

```
>>> op.reduce(a,axis=0)
>>> op.accumulate(a,axis=0)
>>> op.outer(a,b)
>>> op.reduceat(a,indices)
```

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op.reduce()

op.reduce(a) applies op to all the elements in a 1-D array a reducing it to a single value.

For example:

```
y = add.reduce(a)
 =\sum_{n=0}^{N-1}a[n]
  = a[0] + a[1] + ... + a[N-1]
```

ADD EXAMPLE

```
>>> a = np.array([1,2,3,4])
>>> np.add.reduce(a)
10
```

STRING LIST EXAMPLE

```
>>> a = np.array(
    ['ab','cd','ef'],
    dtype='object')
>>> np.add.reduce(a)
'abcdef'
```

LOGICAL OP EXAMPLES

```
>>> a = np.array([1,1,0,1])
>>> np.logical and.reduce(a)
False
>>> np.logical or.reduce(a)
True
```

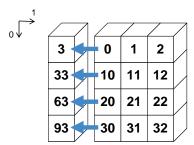
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op.reduce()

For multidimensional arrays, **op.reduce** (**a**, **axis**) applies **op** to the elements of **a** along the specified **axis**. The resulting array has dimensionality one less than **a**. The default value for **axis** is 0.

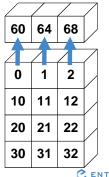
SUMMING UP EACH ROW



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SUM COLUMNS BY DEFAULT





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op.accumulate()

op.accumulate (a) creates a new array containing the intermediate results of the reduce operation at each element in a.

For example:

y = add.accumulate(a)
=
$$\left[\sum_{n=0}^{0} a[n], \sum_{n=0}^{1} a[n], ..., \sum_{n=0}^{N-1} a[n]\right]$$

ADD EXAMPLE

>>> a = np.array([1,2,3,4])
>>> np.add.accumulate(a)
array([1, 3, 6, 10])

STRING LIST EXAMPLE

LOGICAL OP EXAMPLES

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op.reduceat()

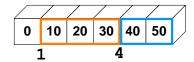
op.reduceat (a, indices) applies op to ranges in the 1-D array a defined by the values in indices. The resulting array has the same length as indices.

For example:

y = add.reduceat(a, indices)

$$y[i] = \sum_{n=indices[i]}^{indices[i]} a[n]$$

EXAMPLE





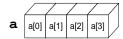
For multidimensional arrays, reduceat() is always applied along the *last* axis (sum of rows for 2-D arrays). This is different from the default for reduce() and accumulate().

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op.outer()

op.outer (a,b) forms all possible combinations of elements between a and b using op. The shape of the resulting array results from concatenating the shapes of a and b. (Order matters.)





>>> np.add.outer(a,b)

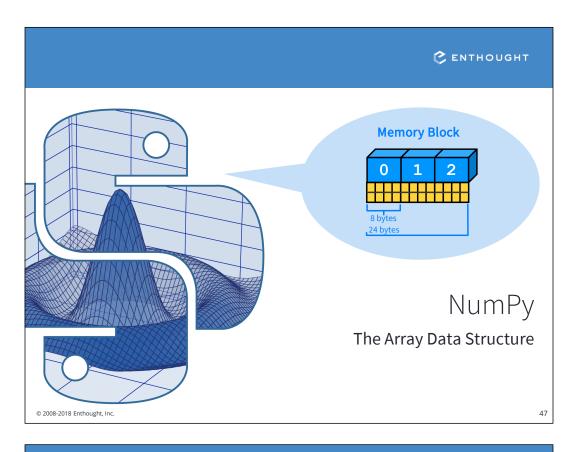
		\angle	
a[0]+b[0]	a[0]+b[1]	a[0]+b[2]	
a[1]+b[0]	a[1]+b[1]	a[1]+b[2]	
a[2]+b[0]	a[2]+b[1]	a[2]+b[2]	
a[3]+b[0]	a[3]+b[1]	a[3]+b[2]	

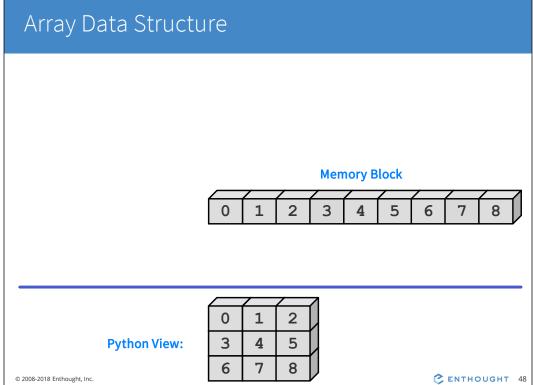
>>> np.add.outer(b,a)

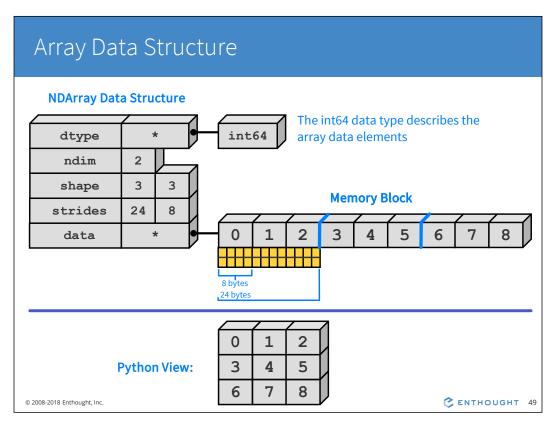


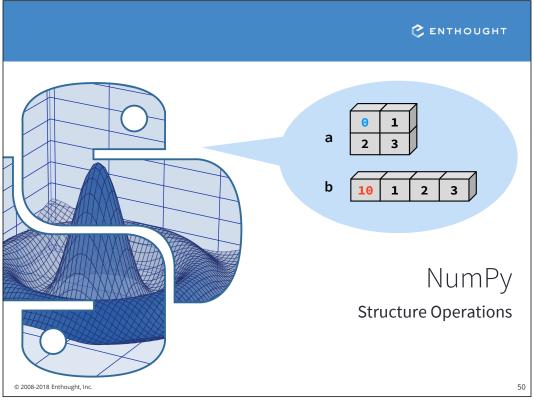
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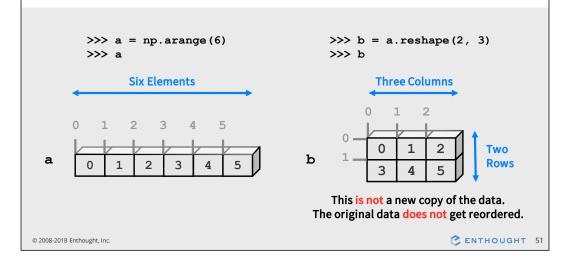






Operations on the Array Structure

Operations that only affect the array structure, not the data, can usually be executed without copying memory.



Transpose

TRANSPOSE >>> a = np.array([[0,1,2], [3,4,5]]) >>> a.shape (2,3)# Transpose swaps the order # of axes. >>> a.T array([[0, 3], [1, 4], [2, 5]]) >>> a.T.shape (3, 2)**Two Columns Three Columns** 0 1 2 © 2008-2018 Enthought, Inc.

Reshaping Arrays

RESHAPE

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SHAPE

Flattening Arrays

FLATTEN (SAFE)

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a.flatten() converts a multi-dimensional array into a 1-D array. The new array is a *copy* of the original data.

```
# Create a 2D array
>>> a = np.array([[0,1],
                   [2,3]])
# Flatten out elements to 1D
>>> b = a.flatten()
>>> b
array([0,1,2,3])
# Changing b does not change a
>>> b[0] = 10
>>> b
array([10,1,2,3])
                 no change
>>> a
array([[0, 1],
                        b 10 1 2 3
       [2, 3]])
```

RAVEL (EFFICIENT)

a.ravel() is the same as a.flatten(), but returns a reference (or view) of the array if possible (i.e., the memory is contiguous). Otherwise the new array copies the data.







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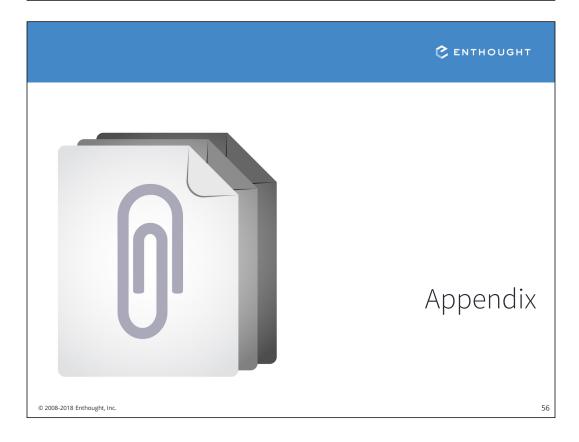




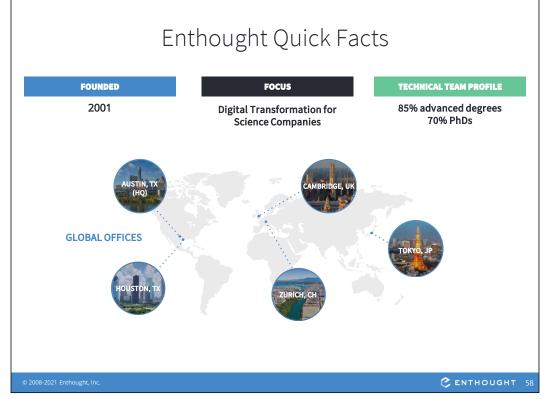
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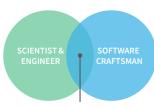
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