

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

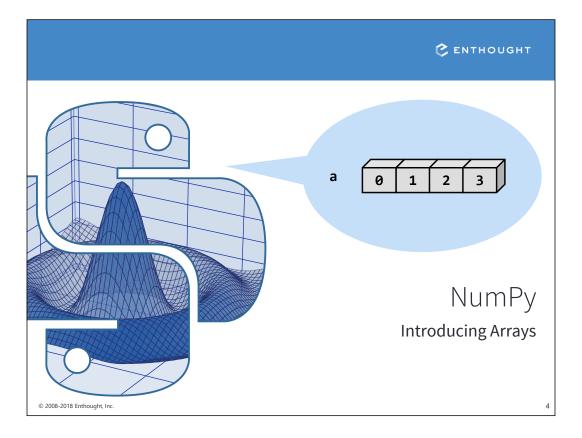
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# NumPy Arrays

- 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
```

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# **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

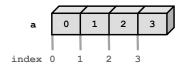
### **MATH FUNCTIONS**

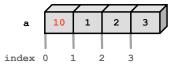
```
# create array from 0.0 to 10.0
>>> x = np.arange(11.0)
# multiply entire array by
# scalar value
>>> c = (2.0 * np.pi) / 10.0
>>> c
0.62831853071795862
>>> c * x
array([0.
            , 0.628, ..., 6.283])
# in-place operations
>>> x *= c
>>> x
array([0. , 0.628, ..., 6.283])
# apply functions to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

# 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], 2D Array
[10,11,12,13]])
a 0 1 2 3
10 11 12 13

### SHAPE = (ROWS, COLUMNS)

>>> a.shape (2, 4)



### **ELEMENT COUNT**

>>> a.size
8 2 x 4 = 8 a 2 10011 1211

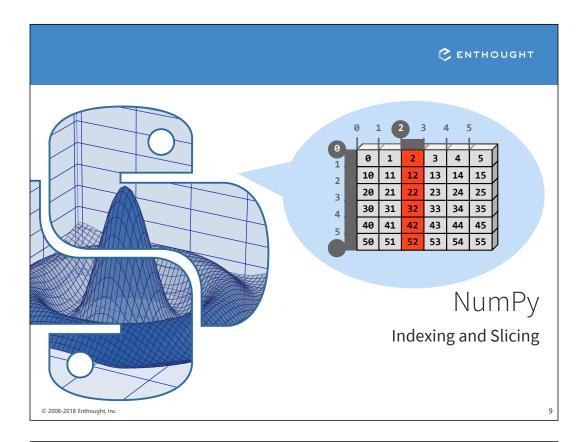
#### **NUMBER OF DIMENSIONS**

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



### **GET / SET ELEMENTS**

# ADDRESS SECOND (ONETH) ROW USING SINGLE INDEX



# 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**

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### **OMITTING INDICES**

```
# omitted boundaries are
# assumed to be the beginning
# (or end) of the list

# grab first three elements
>>> a[:3]
array([10, 11, 12])

# grab last two elements
>>> a[-2:]
array([13, 14])

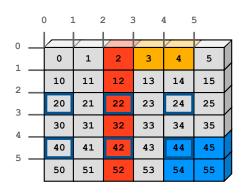
# every other element
>>> a[::2]
array([10, 12, 14])
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```

# Array Slicing

# SLICING WORKS MUCH LIKE STANDARD PYTHON SLICING

#### STRIDED ARE ALSO POSSIBLE

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# Assigning to a Slice

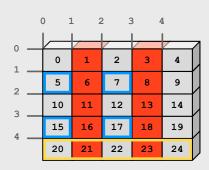
Slices are references to locations in memory. These memory locations can be used in assignment operations.

```
>>> 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:] = 99
>>> a
array([0, 1, 2, 99, 99])
```

# Give it a try!

Create the array below with the command

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

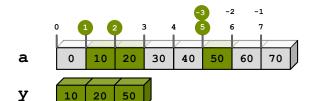
# Fancy Indexing

#### **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
array([ 0, 99, 99, 30, 40, 99,
60, 70])
```

#### **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])
```



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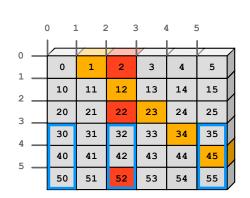
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# Fancy Indexing in 2-D

```
>>> 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])
```

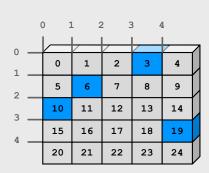


Unlike slicing, fancy indexing creates copies instead of a view into original array.

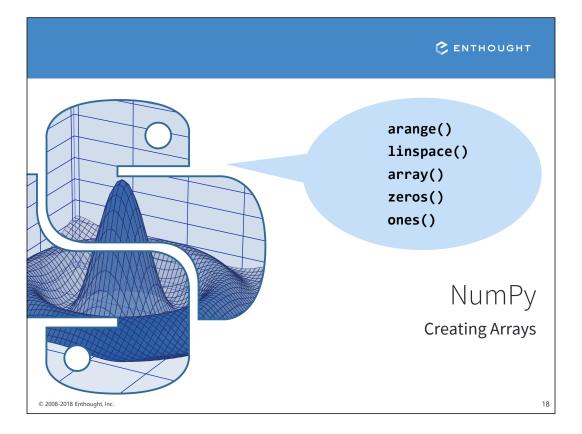


# Give it a try!

- 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**

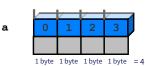
```
# Default to double precision
>>> a = np.array([0,1.0,2,3])
>>> a.dtype
dtype('float64')
>>> a.nbytes
32
```

#### **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**



```
Base 2

00000000 -> 0 = 0*2**0 + 0*2**1 + ... + 0*2**7
00000001 -> 1 = 1*2**0 + 0*2**1 + ... + 0*2**7
00000010 -> 2 = 0*2**0 + 1*2**1 + ... + 0*2**7
...

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

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# **Array Creation Functions**

### **ARANGE**

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)
```

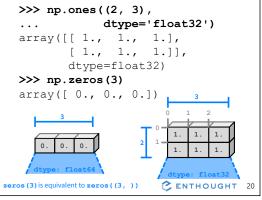
array([ 1.5, 1.8, 2.1])

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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**.



# Array Creation Functions (cont'd)

#### **IDENTITY**

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

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#### **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])
```

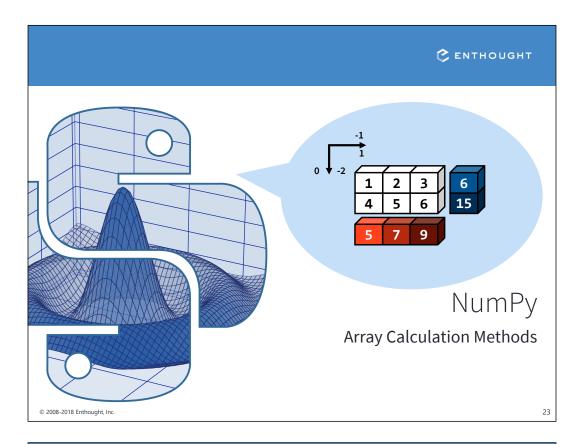
### **LOGSPACE**

```
# 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.])
```

#### 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
```

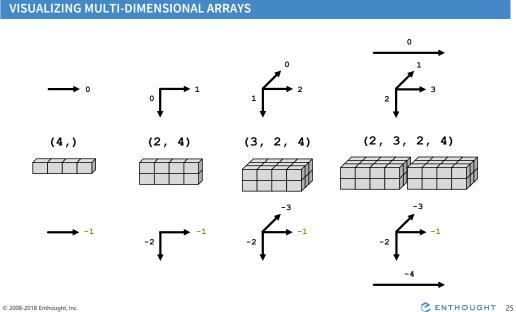
```
# loadtxt() automatically
# generates an array from the
# txt file
arr = np.loadtxt('Data.txt',
        skiprows=1,
        dtype=int, delimiter=",",
. . .
        usecols = (0,1,2,4),
. . .
        comments = "%")
# Save an array into a txt file
np.savetxt('filename.txt', arr)
```



# Computations with Arrays

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

# Multi-Dimensional Arrays

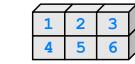


# Array Calculation Methods

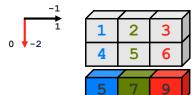
### **SUM METHOD**

- # 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() 21
- # 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])

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sum(a)



sum(a, axis=0)



sum(a, axis=-1)

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# Other Operations on Arrays

#### **SUM FUNCTION**

```
# 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])
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```

### **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)
```

# Where

#### **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]),)
```

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### **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

```
[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])
```

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

### 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])
```

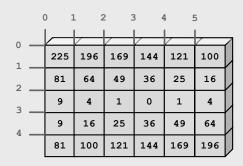
>>> np.var(a, axis=0) array([2.25, 2.25, 2.25])

# Give it a try!

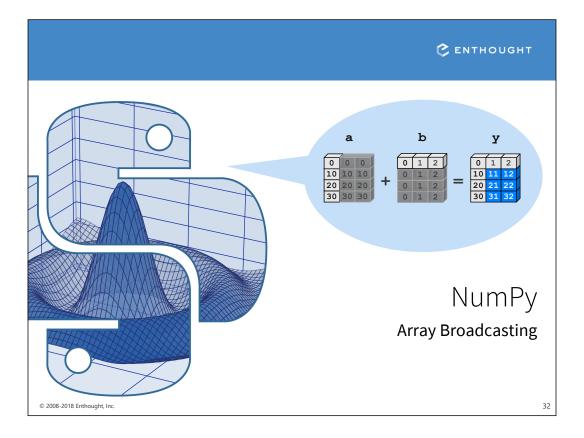
### Create the array below with

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

- 1. The maximum of each row
- 2. 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.
```

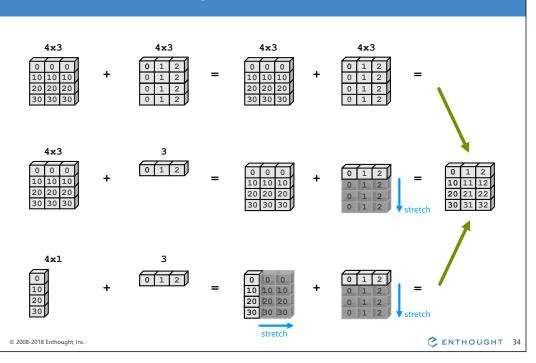
### **RULE 2: DIMENSIONS OF SIZE 1 ARE REPEATED WITHOUT COPYING**

```
>>> 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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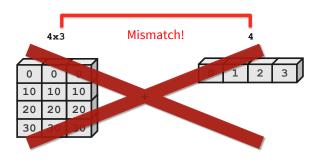
# Array Broadcasting



# **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.

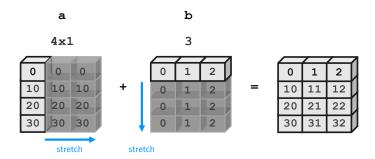


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# Broadcasting in Action

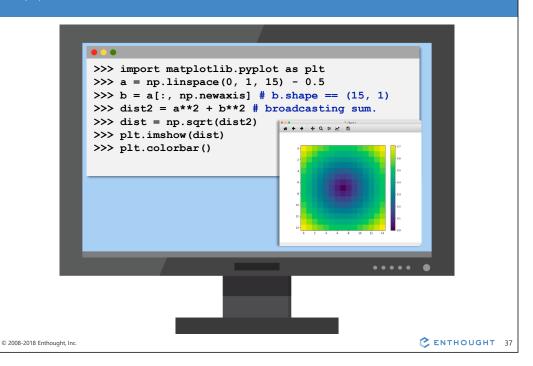
```
>>> a = array([0, 10, 20, 30])
>>> b = array([0, 1, 2])
>>> y = a[:, newaxis] + b
```



2-D Array 1-D Array



# 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
```

### **BROADCASTING: NO COPIES**

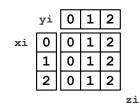
```
>>> x = np.array([1, 2])
>>> y = np.array([3, 4, 5])
>>> z = x[np.newaxis, :] 
        + y[:, np.newaxis]
```

# 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.

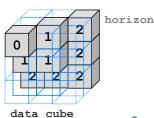
```
>>> data cube = np.arange(27).reshape(3, 3, 3)
>>> yi, xi = np.meshgrid(np.arange(3), np.arange(3),
                         sparse=True)
>>> zi = np.array([[0, 1, 2],
                   [1, 1, 2],
                   [2, 2, 2]])
>>> horizon = data_cube[xi, yi, zi]
```

### **Indices**



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### Selected Data



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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)
```

## 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:

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

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#### **ADD EXAMPLE**

### STRING LIST EXAMPLE

### **LOGICAL OP EXAMPLES**

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

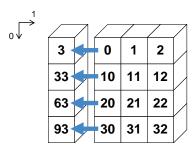
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## op.reduce()

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**

```
>>> a = np.arange(3) + np.arange(0, 40,
                    10).reshape(-1, 1)
>>> np.add.reduce(a,1)
array([ 3, 33, 63, 93])
```

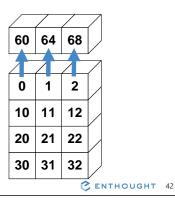


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#### **SUM COLUMNS BY DEFAULT**

>>> np.add.reduce(a) array([60, 64, 68])





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

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### **ADD EXAMPLE**

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

### STRING LIST EXAMPLE

### **LOGICAL OP EXAMPLES**

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

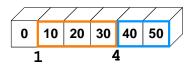
### op.reduceat()

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:

$$y[i] = \sum_{n=indices[i]}^{indices[i+1]} a[n]$$

### **EXAMPLE**

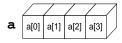




For multidimensional arrays, reduceat () is always applied along the last axis (sum of rows for 2-D arrays). This is different from the default for reduce() and accumulate().

# 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)

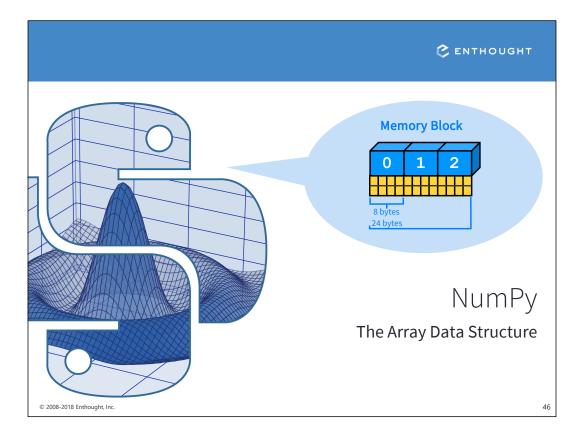
a[0]+b[0]	a[0]+b[1]	a[0]+b[2]	
a[1]+b[0]	a[1]+b[1]	a[1]+b[2]	
a[2]+b[0]	a[2]+b[1]	a[2]+b[2]	
a[3]+b[0]	a[3]+b[1]	a[3]+b[2]	

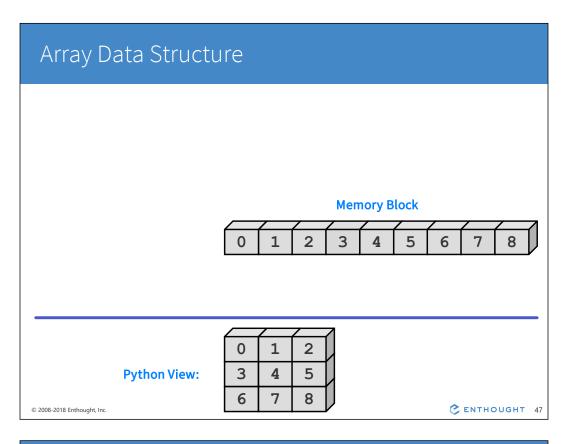
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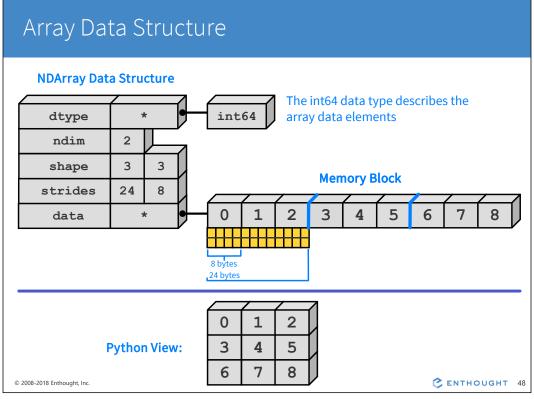
>>> np.add.outer(b,a)

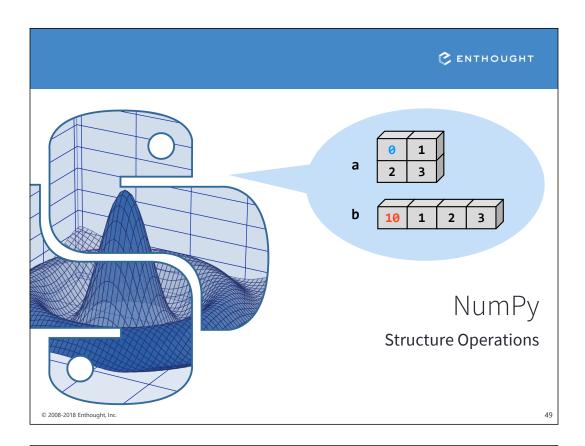
				/
b[0]+a[0]	b[0]+a[1]	b[0]+a[2]	b[0]+a[3]	
b[1]+a[0]	b[1]+a[1]	b[1]+a[2]	b[1]+a[3]	
b[2]+a[0]	b[2]+a[1]	b[2]+a[2]	b[2]+a[3]	

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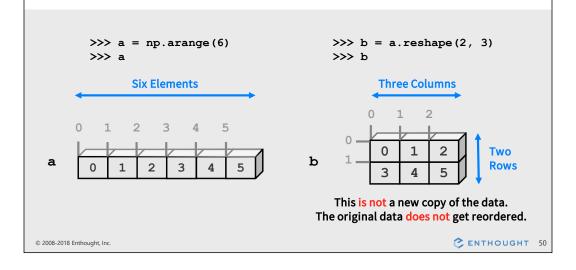






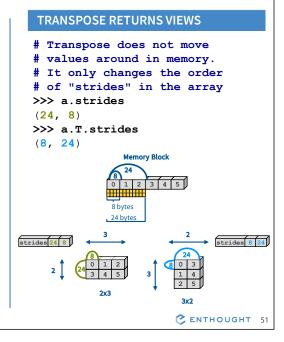
# Operations on the Array Structure

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 0 3 0 1 2 3 4 5 Rows



# Reshaping Arrays

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**RESHAPE** 

# Flattening Arrays

### **FLATTEN (SAFE)**

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])
>>> a
array([10,1,2,3])
>>> a
array([10,1,2,3])
>>> a
array([10,1],
[2,3]])
```

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### **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.