



# Introduction to Numerical Computing with Numpy

## Use Restrictions:

Use only permitted under license or agreement. Copying, sharing, redistributing or other unauthorized use is strictly prohibited. The Enthought Training Materials (ETM) are provided for the individual and sole use of the paid attendee of the class ("Student") for which the Training Services are provided. The virtual training sessions may not be shared, reproduced, transmitted, or retransmitted in any form or by any means, electronic or mechanical, including photocopying, recording, or any information storage and retrieval system. Furthermore, neither Customer nor any Student shall:

Copy, disclose, transfer or distribute ETM to any party in any form. Remove, modify or obscure any copyright, trademark, legal notices or other proprietary notations in ETM. Make derivative works of ETM or combine ETM or any part of ETM with any other works. Use ETM in any manner that could be detrimental to Enthought. © 2001-2022, Enthought, Inc. All Rights Reserved. All trademarks and registered trademarks are the property of their respective owners.

Enthought, Inc. 200 W Cesar Chavez Suite 202 Austin, TX 78701  
[www.enthought.com](http://www.enthought.com)

Q2-2022  
letter  
3.5.5



# Introduction to Numerical Computing with Numpy

Enthought, Inc.  
[www.enthought.com](http://www.enthought.com)

## Introduction 1

## NumPy 2

- Introducing NumPy Arrays 4
- Multi-Dimensional Arrays 8
- Slicing/Indexing Arrays 10
- Fancy Indexing 16
- Creating arrays 19
- Array Creation Functions 21
- Array Calculation Methods 24
- Array Broadcasting 33
- Universal Function Methods 41
- The array data structure 47

## Closing words 55

## Appendix 56

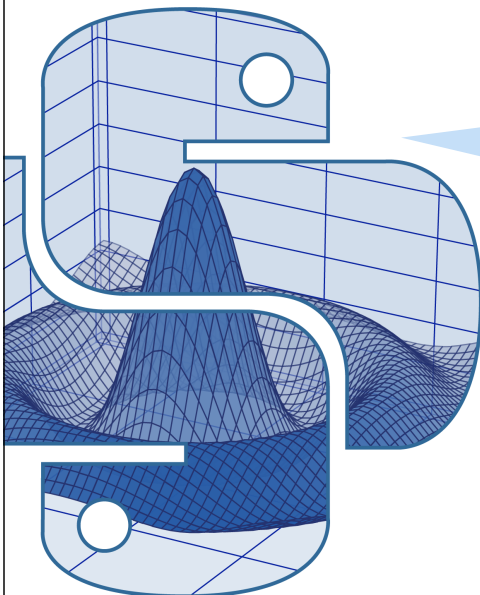
## About Enthought 57



# Introduction to Numerical Computing with Numpy



1

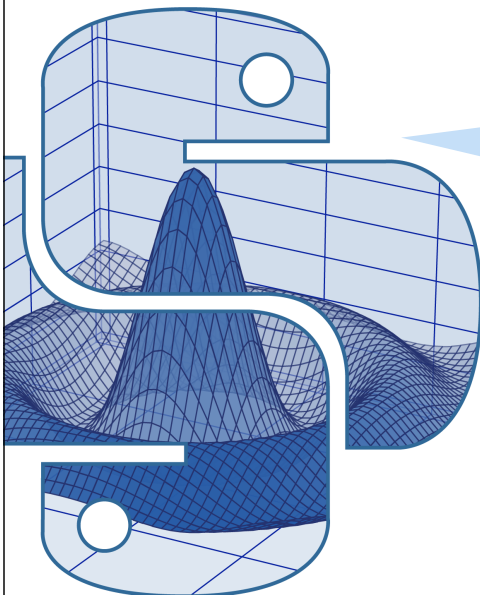
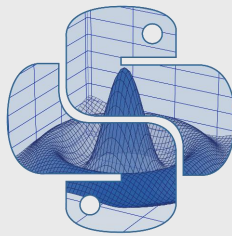


Hi there!

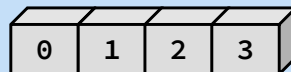
NumPy  
The Standard Numerical Library  
for Python

# NumPy Arrays

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



a



NumPy  
Introducing Arrays

# Introducing NumPy Arrays

## SIMPLE ARRAY CREATION

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

## ARRAY SHAPE

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

## BYTES PER ELEMENT

```
>>> a.itemsize
4
```

## 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])

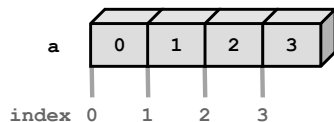
# in-place operations
>>> x *= c
>>> x
array([0.    , 0.628, ..., 6.283])

# apply functions to array
>>> y = np.sin(x)
```

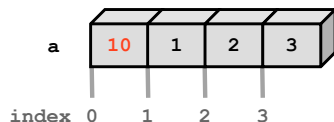
# Setting Array Elements

## ARRAY INDEXING

```
>>> a[0]
0
```



```
>>> a[0] = 10
>>> a
array([10, 1, 2, 3])
```



© 2008-2022 Enthought, Inc.



## 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])
```

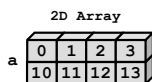
Enthought

7

# Multi-Dimensional Arrays

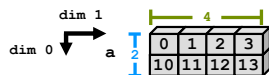
## MULTI-DIMENSIONAL ARRAYS

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



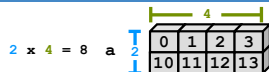
## SHAPE = (ROWS, COLUMNS)

```
>>> a.shape
(2, 4)
```



## ELEMENT COUNT

```
>>> a.size
8
```



## NUMBER OF DIMENSIONS

```
>>> a.ndim
2
```



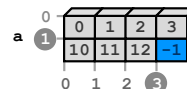
© 2008-2022 Enthought, Inc.

## GET / SET ELEMENTS

```
>>> a[1, 3]
13
```

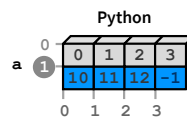


```
>>> a[1, 3] = -1
>>> a
array([[ 0, 1, 2, 3],
       [10,11,12,-1]])
```



## ADDRESS SECOND (ONETH) ROW USING SINGLE INDEX

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



Enthought

8

# Formatting Numeric Display

## DEFAULT FORMATTING

```
>>> a = np.arange(1.0, 3.0, 0.5)
>>> a
array([1. , 1.5, 2. , 2.5])
```

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

```
>>> a * np.pi * 1e8
array([3.14159265e+08,
       4.71238898e+08, 6.28318531e+08,
       7.85398163e+08])
```

```
>>> a * np.pi * 1e-6
array([3.14159265e-06,
       4.71238898e-06, 6.28318531e-06,
       7.85398163e-06])
```

## USER FORMATTING

```
# set precision
```

```
>>> np.set_printoptions(
    precision=2)
```

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

```
>>> a * np.pi
array([3.14, 4.71, 6.28, 7.85])
```

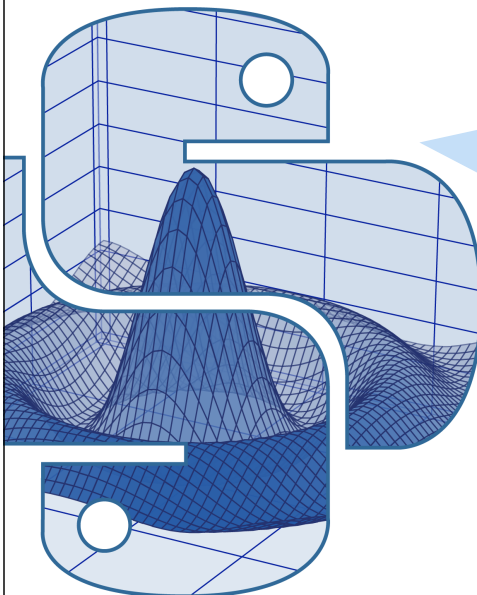
```
>>> a * np.pi * 1e8
array([3.14e+08, 4.71e+08,
       6.28e+08, 7.85e+08])
```

```
>>> 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.])
```



	0	1	2	3	4	5
0	0	1	2	3	4	5
1	10	11	12	13	14	15
2	20	21	22	23	24	25
3	30	31	32	33	34	35
4	40	41	42	43	44	45
5	50	51	52	53	54	55

NumPy  
Indexing and Slicing



# 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])
```

## 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])
```

© 2008-2022 Enthought, Inc.

# 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]])
```

	0	1	2	3	4	5
0	0	1	2	3	4	5
1	10	11	12	13	14	15
2	20	21	22	23	24	25
3	30	31	32	33	34	35
4	40	41	42	43	44	45
5	50	51	52	53	54	55

© 2008-2022 Enthought, Inc.

## 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.

	0	1	2	3	4
0	0	1	2	3	4
1	5	6	7	8	9
2	10	11	12	13	14
3	15	16	17	18	19
4	20	21	22	23	24

## 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
```

© 2008-2022 Enthought, Inc.

Enthought 15

## Fancy Indexing

### INDEXING BY POSITION

```
>>> a = np.arange(0, 80, 10)

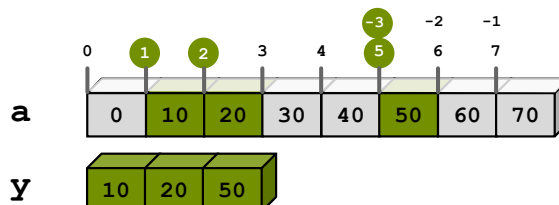
# fancy indexing
>>> indices = [1, 2, -3]
>>> y = a[indices]
>>> y
array([10, 20, 50])

# this also works with setting
>>> a[indices] = 99
>>> a
array([ 0, 99, 99, 30, 40, 99, 60, 70])
```

### 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])
```



© 2008-2022 Enthought, Inc.

Enthought 16

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

	0	1	2	3	4	5
0	0	1	2	3	4	5
1	10	11	12	13	14	15
2	20	21	22	23	24	25
3	30	31	32	33	34	35
4	40	41	42	43	44	45
5	50	51	52	53	54	55

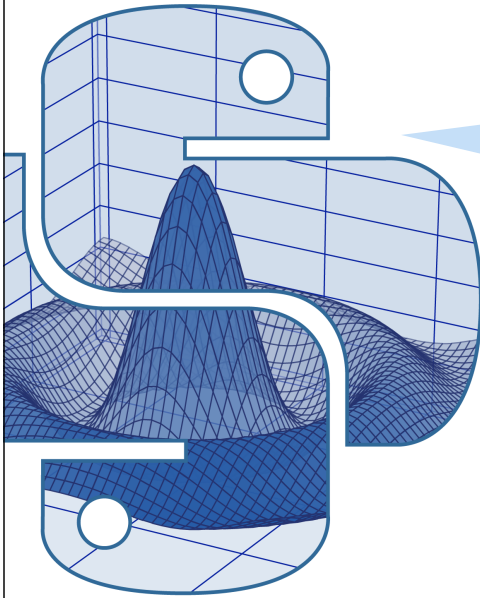


Unlike slicing, fancy indexing creates copies instead of a view into original array.

## 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.

	0	1	2	3	4
0	0	1	2	3	4
1	5	6	7	8	9
2	10	11	12	13	14
3	15	16	17	18	19
4	20	21	22	23	24



`arange()`  
`linspace()`  
`array()`  
`zeros()`  
`ones()`

## NumPy

### Creating Arrays

© 2008-2022 Enthought, Inc.

19

## Array Constructor Examples

### FLOATING POINT ARRAYS

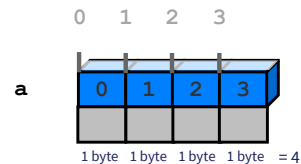
```
# Default to double precision
>>> a = np.array([0,1.0,2,3])
>>> a.dtype
dtype('float64')
>>> a.nbytes
32
```

### REDUCING PRECISION

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

### UNSIGNED INTEGER BYTE

```
>>> a = np.array([0,1,2,3],
...               dtype='uint8')
>>> a.dtype
dtype('uint8')
>>> a.nbytes
4
```



Base 2

Base 10

```
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
```

© 2008-2022 Enthought, Inc.

# 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])
```

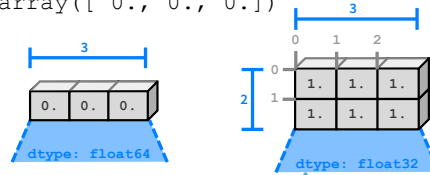
© 2008-2022 Enthought, Inc.

## 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.]])
>>> np.zeros(3)
array([ 0.,  0.,  0.])
```



Enthought

21

# Array Creation Functions (cont'd)

## IDENTITY

```
# Generate an n by n identity
# array. The default dtype is
# float64.
```

```
>>> a = np.identity(4)
>>> a
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]])
```

## 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.])
```

© 2008-2022 Enthought, Inc.

Enthought

22

# 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.])
```

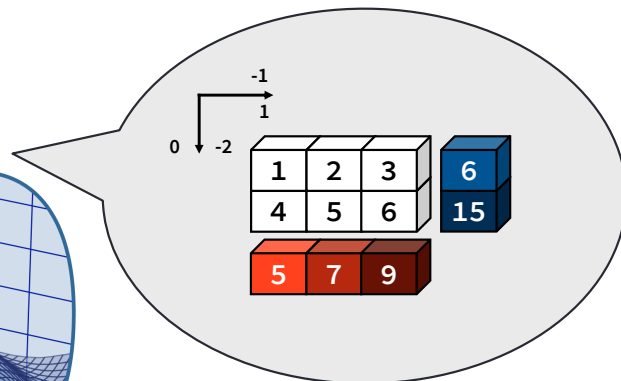
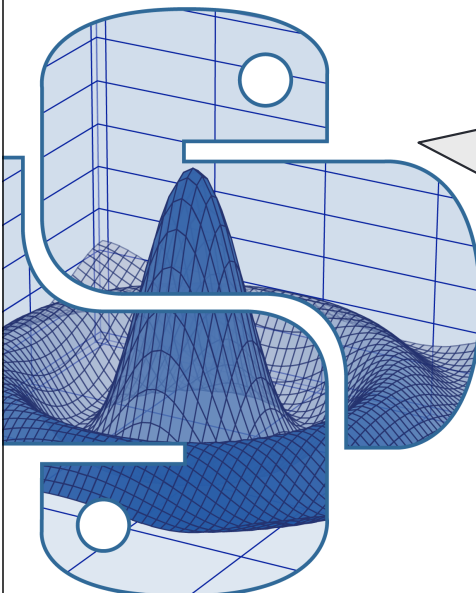
## Arrays from/to txt files

```
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
```

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)
```



NumPy

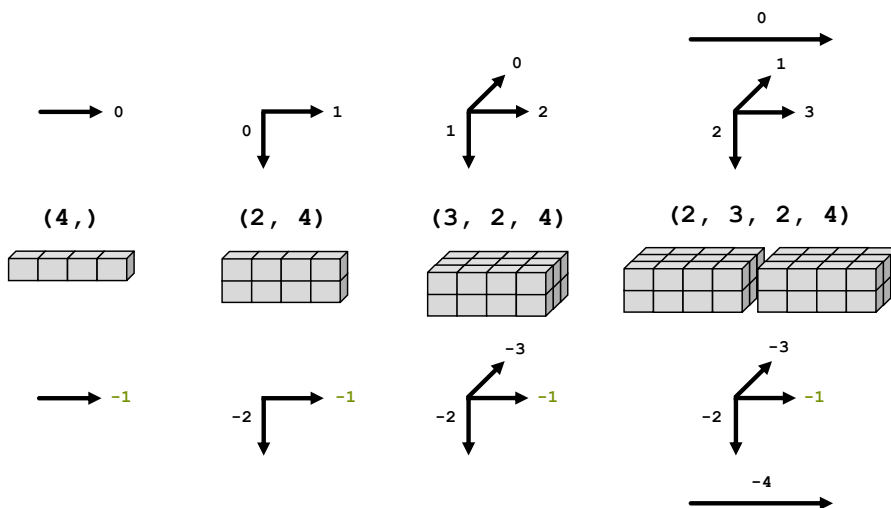
Array Calculation Methods

# Computations with Arrays

- Rule 1:** Operations between multiple array objects are first checked for proper shape match.
- Rule 2:** Mathematical operators (+ - \* / exp, log, ...) apply 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

## VISUALIZING MULTI-DIMENSIONAL ARRAYS





# Array Calculation Methods

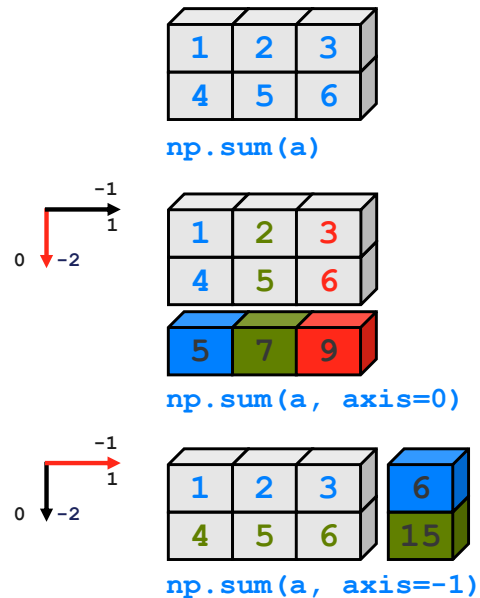
## SUM METHOD

```
# 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()
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])
```



© 2008-2022 Enthought, Inc.

# 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)
21

# 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.

© 2008-2022 Enthought, Inc.

# Min/Max

## MIN

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

## 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()
1
# arg methods return the
# location in a 1D, flattened
# version of the original array
>>> np.argmin(a)
2
```

## 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]),)
```

## 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])
```

# 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])
```

## Give it a try!

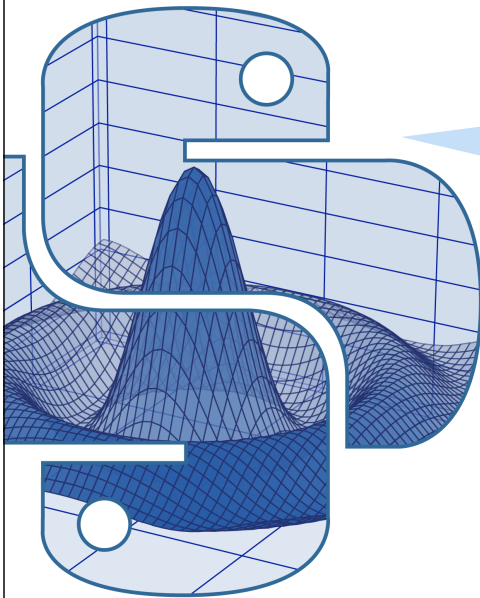
Create the array below with

```
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

	0	1	2	3	4	5
0	225	196	169	144	121	100
1	81	64	49	36	25	16
2	9	4	1	0	1	4
3	9	16	25	36	49	64
4	81	100	121	144	169	196



a	b			=	y		
0	0	0			0	1	2
10	10	10	+		10	11	12
20	20	20			20	21	22
30	30	30			30	31	32

## NumPy Array Broadcasting

© 2008-2022 Enthought, Inc.

33

## 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

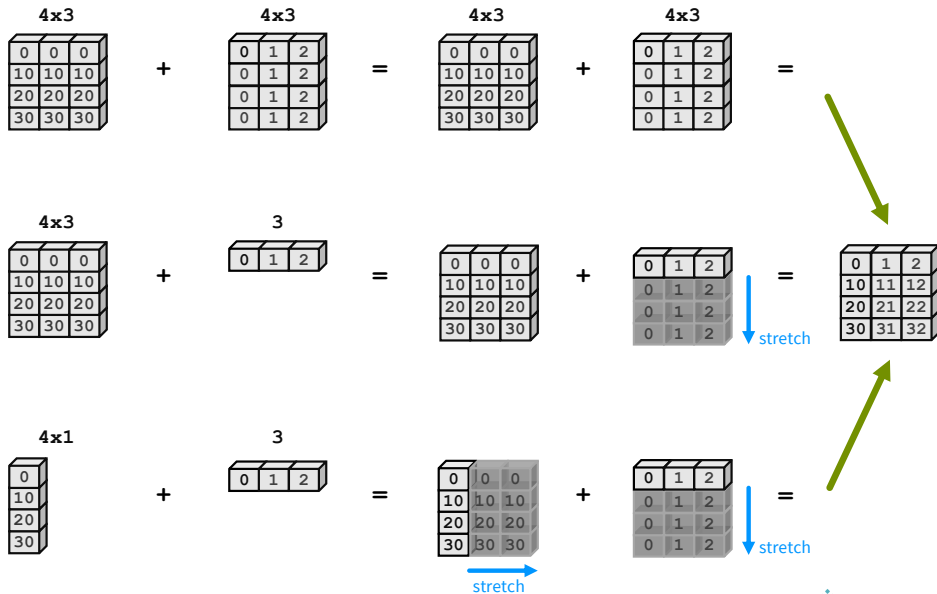
```
>>> import numpy as np
>>> a = np.ones((3, 5)) # a.shape == (3, 5)
>>> b = np.ones((5,)) # b.shape == (5,)
>>> b.reshape(1, 5) # result is a (1,5)-shaped array.
>>> b[np.newaxis, :] # equivalent, more concise.
```

### 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!
```

© 2008-2022 Enthought, Inc.

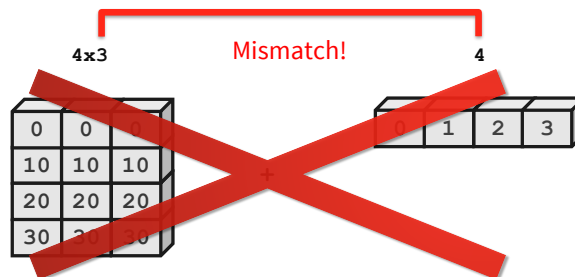
# Array Broadcasting



© 2008-2022 Enthought, Inc.

# Broadcasting Rules

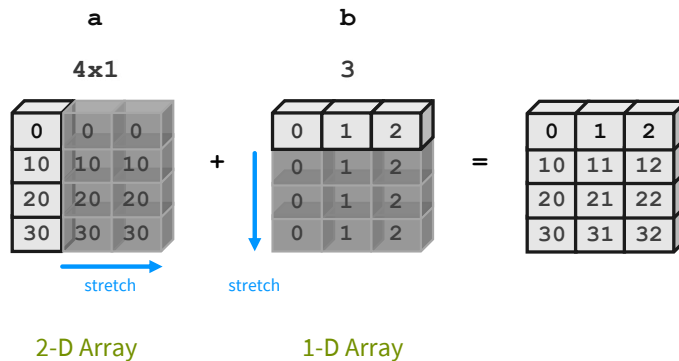
The trailing axes of either arrays must be 1 or both must have the same size for broadcasting to occur. Otherwise, a `"ValueError: shape mismatch: objects cannot be broadcast to a single shape"` exception is thrown.



© 2008-2022 Enthought, Inc.

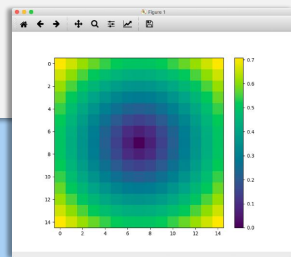
# Broadcasting in Action

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



# Application: Distance from Center

```
>>> import matplotlib.pyplot as plt
>>> a = np.linspace(0, 1, 15) - 0.5
>>> b = a[:, np.newaxis] # b.shape == (15, 1)
>>> dist2 = a**2 + b**2 # broadcasting sum.
>>> dist = np.sqrt(dist2)
>>> plt.imshow(dist)
>>> plt.colorbar()
```



# 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

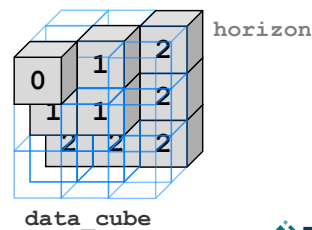
Broadcasting can also be used to slice elements from different “depths” in a 3-D (or any other shape) array. This is a very powerful feature of indexing.

```
>>> 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

		yi		
		0	1	2
xi	0	0	1	2
	1	0	1	2
	2	0	1	2
		zi		

## Selected Data



# 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:

$$\begin{aligned} y &= \text{add.reduce}(a) \\ &= \sum_{n=0}^{N-1} a[n] \\ &= a[0] + a[1] + \dots + a[N-1] \end{aligned}$$

### 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
```

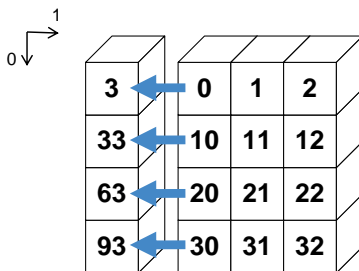


## op.reduce()

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.

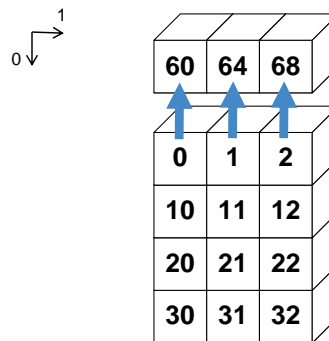
### SUMMING UP EACH ROW

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



### SUM COLUMNS BY DEFAULT

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



© 2008-2022 Enthought, Inc.

## op.accumulate()

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

For example:

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

### ADD EXAMPLE

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

### STRING LIST EXAMPLE

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

### 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])
```

© 2008-2022 Enthought, Inc.

## 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**.

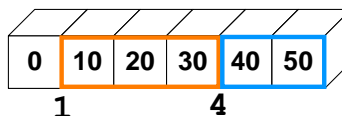
For example:

**y = add.reduceat(a, indices)**

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

### EXAMPLE

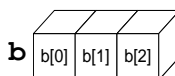
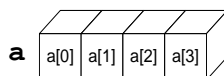
```
>>> a = np.array([0, 10, 20, 30, 40, 50])
>>> indices = np.array([1, 4])
>>> np.add.reduceat(a, indices)
array([ 60,  90])
```



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.)

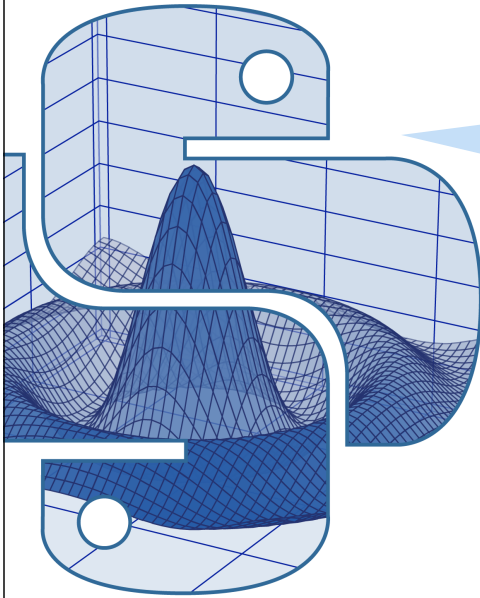


```
>>> np.add.outer(a, b)
```

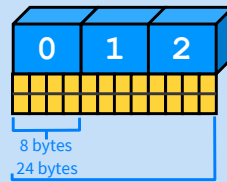
a[0]+b[0]	a[0]+b[1]	a[0]+b[2]
a[1]+b[0]	a[1]+b[1]	a[1]+b[2]
a[2]+b[0]	a[2]+b[1]	a[2]+b[2]
a[3]+b[0]	a[3]+b[1]	a[3]+b[2]

```
>>> 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]



Memory Block



NumPy

The Array Data Structure

## Array Data Structure

Memory Block

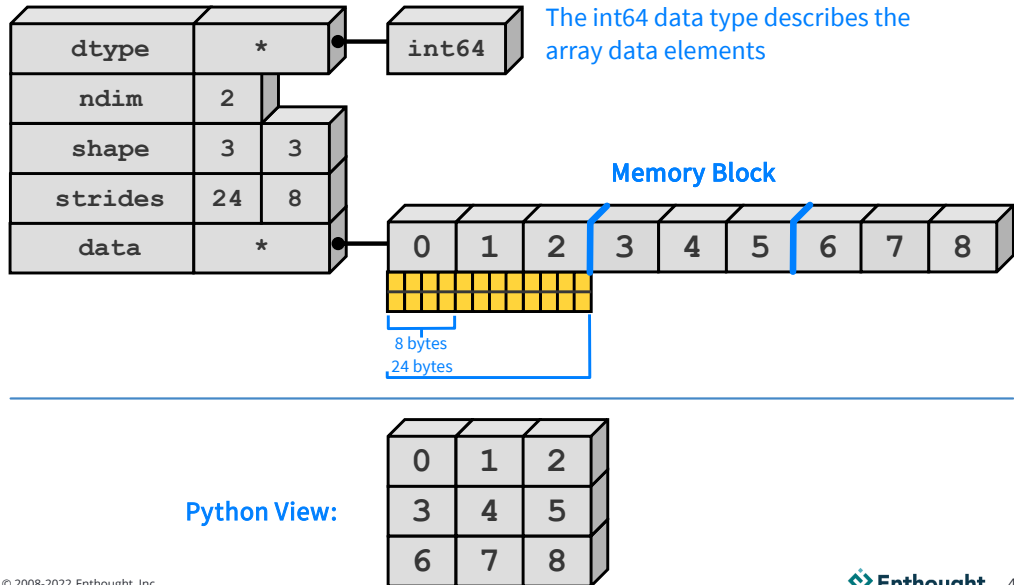


Python View:



# Array Data Structure

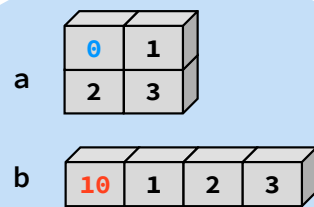
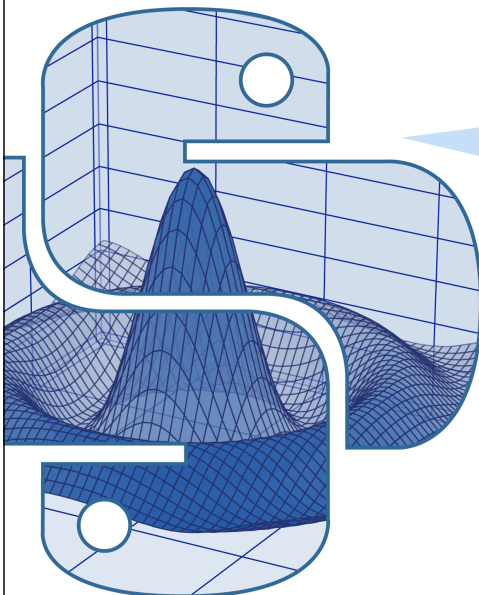
## NDArray Data Structure



© 2008-2022 Enthought, Inc.

Enthought 49

Enthought



NumPy  
Structure Operations

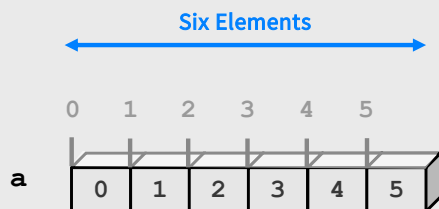
© 2008-2022 Enthought, Inc.

50

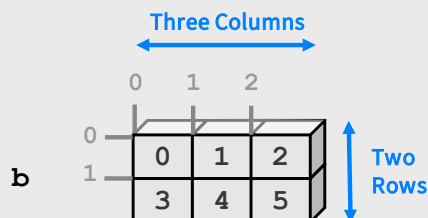
# Operations on the Array Structure

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

```
>>> a = np.arange(6)
>>> a
```



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



This **is not** a new copy of the data.  
The original data **does not** get reordered.

## Transpose

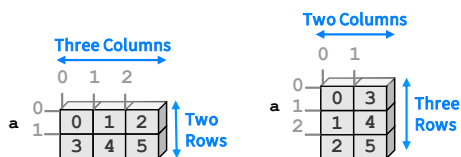
### TRANSPOSE

```
>>> 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]])
```

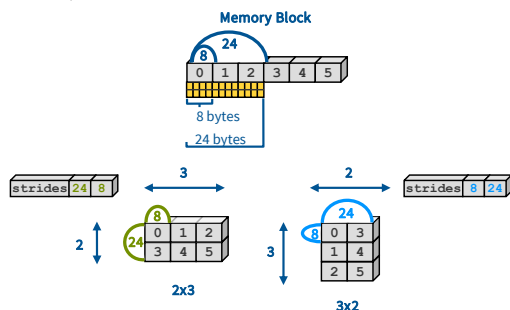
```
>>> a.T.shape
(3,2)
```



### TRANSPOSE RETURNS VIEWS

# Transpose does not move  
# values around in memory.  
# It only changes the order  
# of "strides" in the array

```
>>> a.strides
(24, 8)
>>> a.T.strides
(8, 24)
```



# Reshaping Arrays

## RESHAPE

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

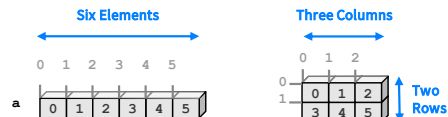
# Return a new array with a
# different shape (a view
# where possible)
>>> a.reshape(3,2)
array([[0, 1],
       [2, 3],
       [4, 5]])

# Reshape cannot change the
# number of elements in an
# array
>>> a.reshape(4,2)
ValueError: total size of new
array must be unchanged
```

## SHAPE

```
>>> a = np.arange(6)
>>> a
array([0, 1, 2, 3, 4, 5])
>>> a.shape
(6,)

# Reshape array in-place to
# 2x3
>>> a.shape = (2,3)
>>> a
array([[0, 1, 2],
       [3, 4, 5]])
```



# Flattening Arrays

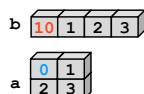
## FLATTEN (SAFE)

**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([[0, 1],
       [2, 3]])
```

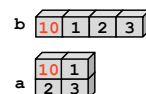


## RAVEL (EFFICIENT)

**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. **np.ravel()** can be applied to non-array objects.

```
# Flatten out elements to 1-D
>>> b = a.ravel()
>>> b
array([0,1,2,3])

# Changing b does change a
>>> b[0] = 10
>>> b
array([10,1,2,3])
>>> a
array([[10, 1],
       [ 2, 3]])
```



Stay in touch!



@enthought



Enthought  
Media



Enthought



Enthought

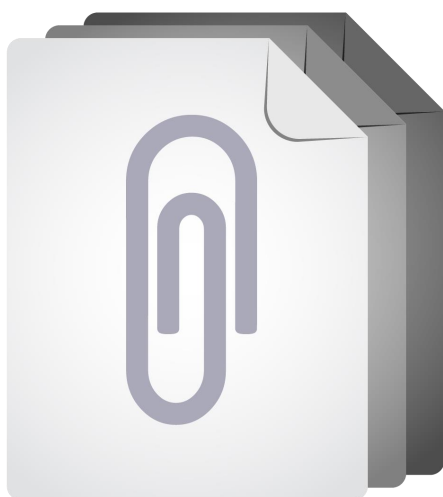


**SciPy**



**EuroSciPy**

Please complete the online survey!  
(link on course web page)



Appendix



## About Enthought

## Enthought Quick Facts

### FOUNDED

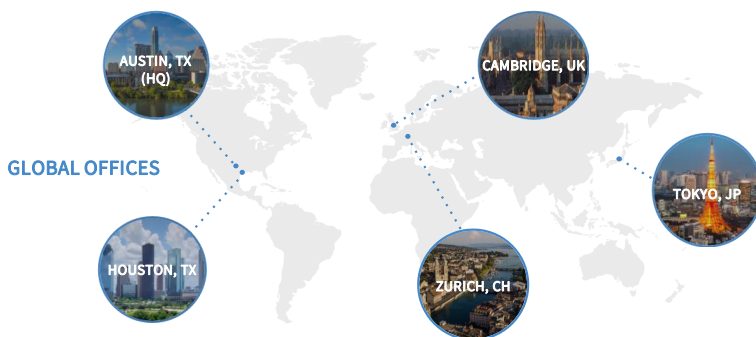
2001

### FOCUS

Digital Transformation for  
Science Companies

### TECHNICAL TEAM PROFILE

85% advanced degrees  
70% PhDs





# Enthought at a Glance

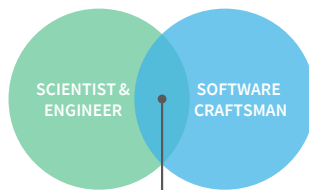
Enthought is a leader in  
Scientific Computing,  
AI, Modeling & Simulation

Industries:  
Bioscience, Oil & Gas,  
Polymers and  
Semiconductors

Enthought is engineering and  
science focused. We build  
solutions that accelerate  
research and engineering  
analysis

## ENGINEER / SCIENTIST SKILLS

- Hard Science Education
- Machine Learning
- Deep Learning
- Statistics
- Image/Signal Processing
- Engineering Intuition
- Modeling and Simulation
- Optimization
- Pragmatic Business Sense



*Enthought team members have the unique  
combined skill set*

## SOFTWARE ENGINEERING SKILLS

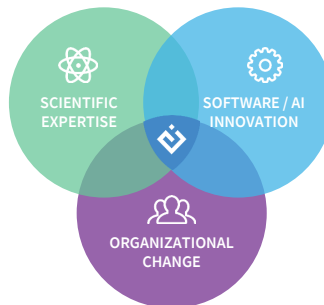
- Application Architecture
- System Architecture
- Object-Oriented Design
- Big Data Architecture
- Database Design
- Visualization
- Cloud Architecture

# Enthought Accelerates Science

## BUSINESS IMPACT THROUGH ACCELERATING SCIENCE

### SCIENTIFIC EXPERTISE

85% of the Enthought technical team have advanced scientific, math, or engineering degrees, 70% with PhDs in mathematics, physics, chemistry, engineering, bioscience, and education.



### SOFTWARE / AI INNOVATION

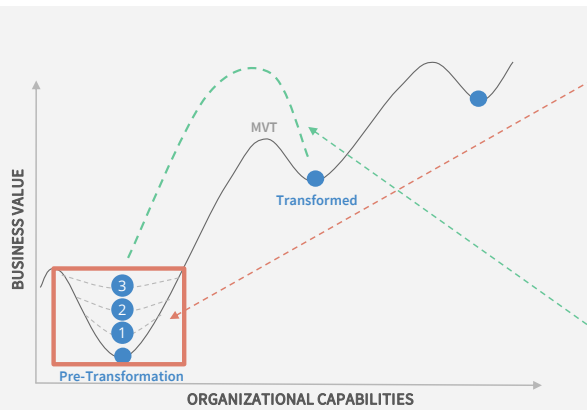
For 17 years, Enthought has been building powerful domain-specific applications powered by our purpose-built Python platform for computational science, data management, and AI.

### ORGANIZATIONAL CHANGE

Enthought has a team dedicated to de-mystifying 'digital transformation'. We work from the C-suite to the scientist to align process and train nearly 1,000 technical experts per year.

# Digital Transformation: More Than a Sum of Projects

Stable state | Restorative forces resist change | Local optimization | Minimum viable transformation | **Strategy**



**Technology Solutions:** What digital technologies are strategic to the business?

**Capability Building:** What new digital skills and capabilities are needed?

**Change Mgmt & Org Design:** How do we evolve the organization to support higher-value business models leveraging new digital affordances?

**Governance:** How do we lead the business through the transition, and prepare leaders for the new digital paradigm?

# Digital Transformation Approach

