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Introduction to Numerical Computing with Numpy

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Introduction to Numerical Computing with NumPy

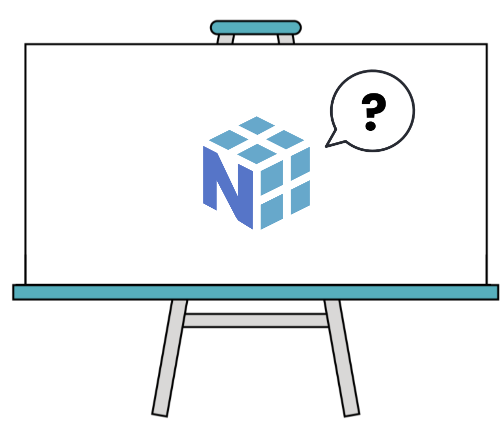
SciPy Conference Tutorial
2023

NumPy

The Standard Numerical Library for Python

NumPy: The Standard Numerical Library for Python

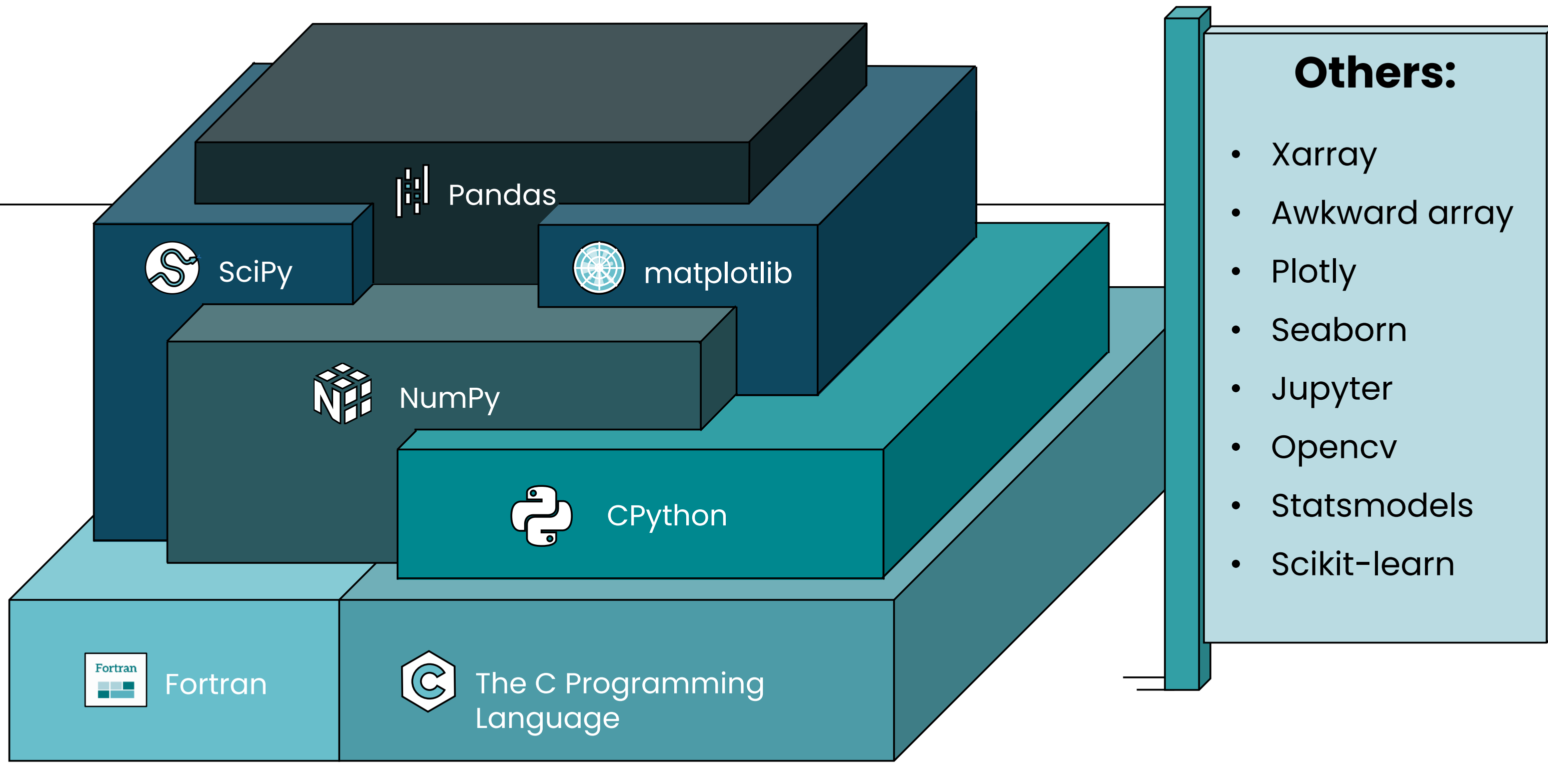
Syllabus



NumPy

Why NumPy?

NumPy : Foundation of Scientific Python



Python Lists and Math

ARITHMETIC

- Python lists are not made for arithmetic.
- For example, list addition is concatenation.

```
>>> a = [1, 2, 3]
>>> b = [4, 5, 6]
>>> a + b
[1, 2, 3, 4, 5, 6]
```

- To mathematically add two lists by position (like we would do with two vectors), we have to use loops.

```
>>> r = []
>>> for v_a, v_b in zip(a, b):
...     r.append(v_a + v_b)
>>> print(r)
[5, 7, 9]
```

- For large lists, Python loops are slow.

MATHMATICAL FUNCTIONS

- Python mathematical functions handle numeric types, not lists.

```
>>> import math
>>> c = [1.1, 2.2, 3.3]
>>> math.trunc(c)
TypeError: type list doesn't define
__trunc__ method
```

- To apply a mathematical function, we have to use loops.

```
>>> r = []
>>> for v_c in c:
...     r.append(math.trunc(v_c))
>>> print(r)
[1, 2, 3]
```

NumPy Arrays and Math

ARITHMETICAL OPERATIONS

- Array addition applies to the entire array and is **addition by position**.
- NumPy arrays are **vectorized**; no loops needed.

```
>>> import numpy as np
>>> a = np.array([1, 2, 3])
>>> b = np.array([4, 5, 6])
>>> a + b
array([5, 7, 9])
```

- No loops needed
  (and really fast even for large arrays).

```
# Other Operations
>>> a * b
array([4, 10, 18])

>>> a / b
array([0.25, 0.4 , 0.5 ])
```

SCALAR AND IN-PLACE OPERATIONS

```
>>> a * 3
array([3, 6, 9])

>>> a += 7
>>> a
array([ 8,  9, 10])
```

MATHMATICAL FUNCTIONS

- NumPy mathematical functions handle arrays.

```
>>> c = np.array([1.1, 2.2, 3.3])
>>> np.trunc(c)
array([1., 2., 3.])

# Other Functions
>>> np.mean(a)
9.0

>>> np.exp(a / b)
array([7.3890561 , 6.04964746, 5.29449005])
```

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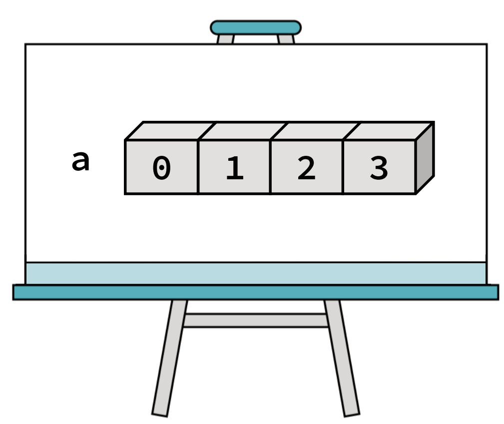

NumPy

Introducing Arrays

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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.itemize
4
```

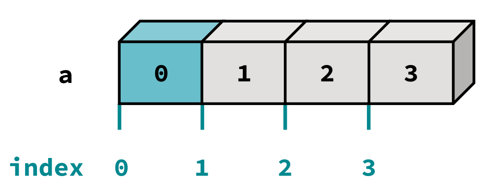
BYTES OF MEMORY USED

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

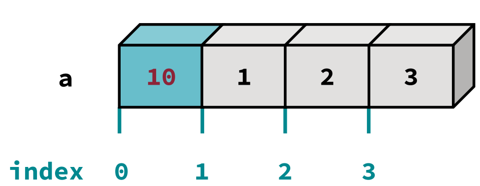

Array Indexing

ARRAY INDEXING

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




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



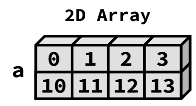
BEWARE OF TYPE COERCION

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

# assigning a float into an int32
# array truncates the decimal part
>>> a[0] = 11.6
>>> a
array([11, 1, 2, 3])

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

Multi-Dimensional Arrays

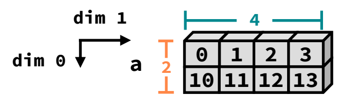
MULTI-DIMENSIONAL ARRAYS

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



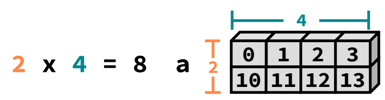
SHAPE = (ROWS, COLUMNS)

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



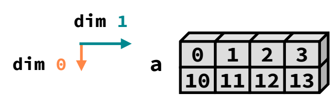
ELEMENT COUNT

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



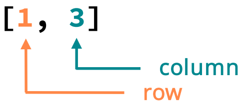
NUMBER OF DIMENSIONS

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

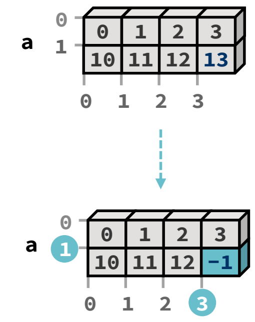


GET / SET ELEMENTS

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

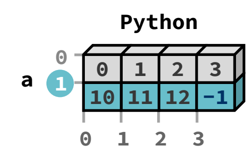



```
>>> a[1, 3] = -1
>>> a
array([[ 0, 1, 2, 3],
       [10,11,12,-1]])
```



ADDRESS 2ND (ONETH) ROW USING SINGLE INDEX

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



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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.])
```

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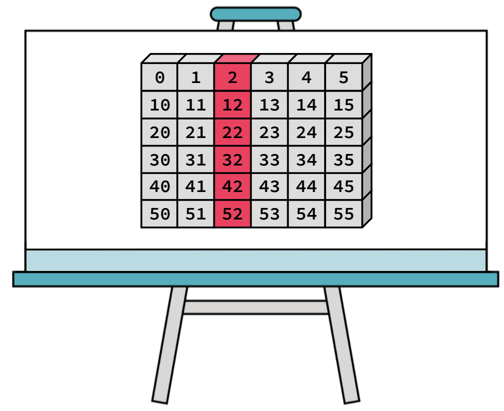


NumPy

Indexing and Slicing

Array 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])
```

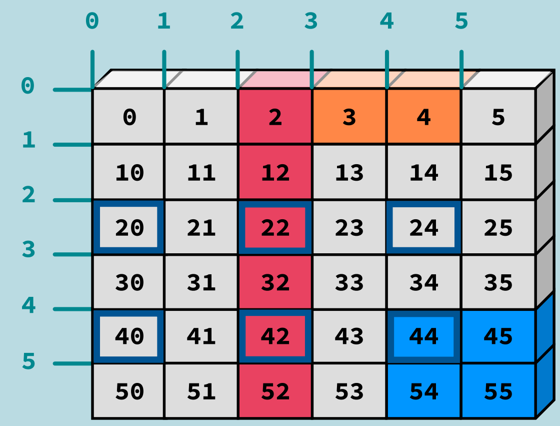
OMITTNG INDICES

```
# 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])
```

Array Slicing in 2-D

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])

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

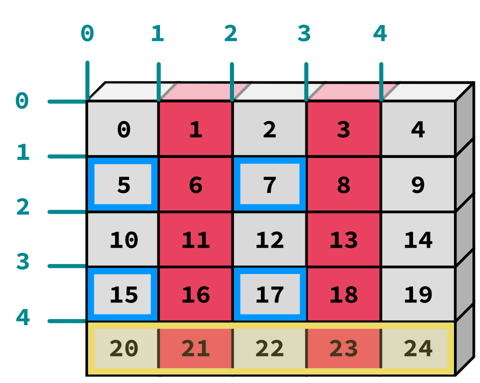


Give it a try! Slicing

1. Create the array below with the command

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

2. Extract the slices as indicated



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])
```


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
```

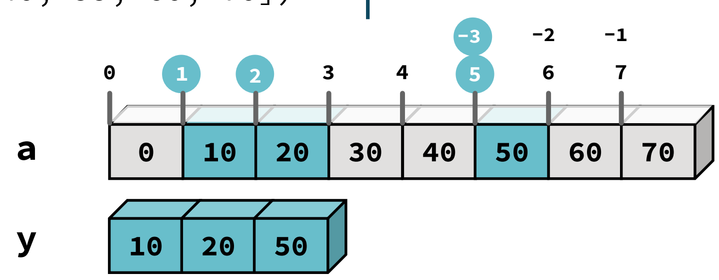
Fancy Indexing

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])
```

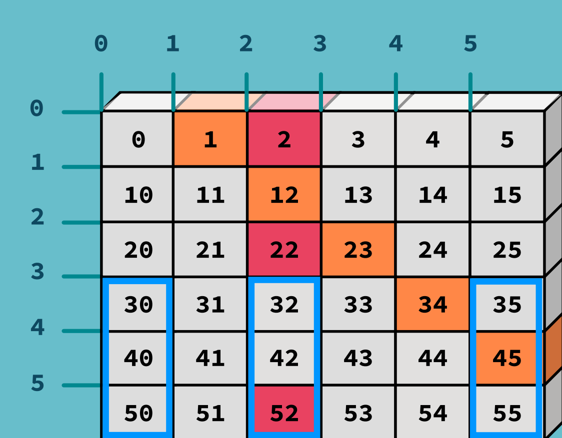
INDEXING WITH BOOLEANS

```
# 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])
```



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.

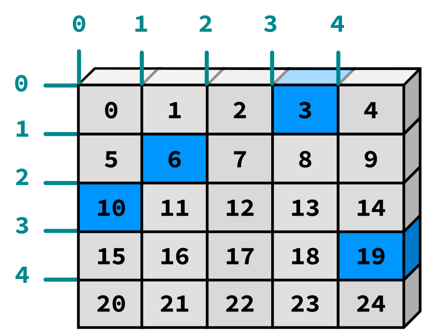
Give it a try! Fancy Indexing

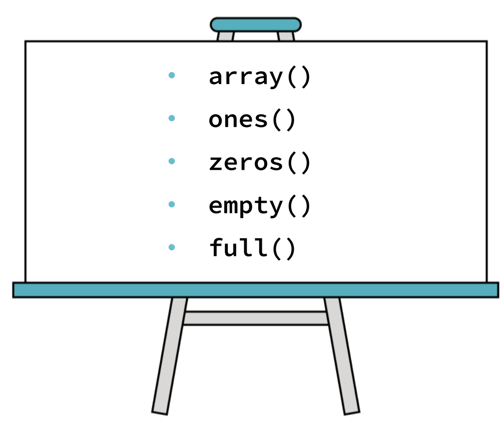
1. Create the array below with

    `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.





NumPy

Creating Arrays

Array Constructor Examples

FLOATING POINT ARRAYS

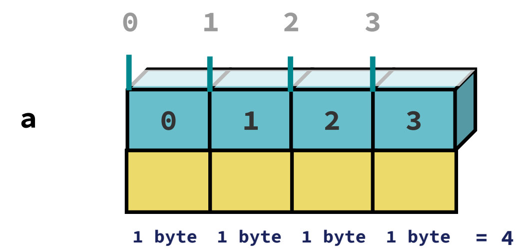
```
# Default to double precision
>>> a = np.array([0, 1.0, 2, 3])
>>> a.dtype
dtype('float64')

>>> 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
```

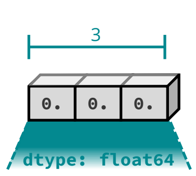

Array Creation Functions

ONES, ZEROS

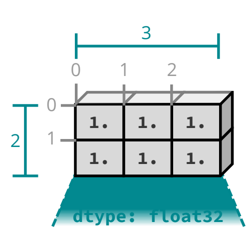
```
ones(shape, dtype='float64')
zeros(shape, dtype='float64')
```

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,))**



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]])
```

Generating Sequences

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])
```

LINSPACE & LOGSPACE

```
# 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])

# 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.])

>>> np.logspace(0, 1, 5, base=np.e)
array([1., 1.28, 1.65, 2.12, 2.72])
```


Generating Random Numbers (Old Style)

INTEGERS (OLD STYLE)

```
# Discrete uniform distribution
# over [0, 5) with N samples
>>> np.random.randint(5, size=3)
array([0, 3, 4])

# Discrete uniform distribution
# over [1, 5) with N samples
>>> np.random.randint(1, 5, 3)
array([2, 2, 3])
```

FLOATS (OLD STYLE)

```
# Uniform distribution over [0.0, 1.0)
# with samples
>>> np.random.rand(3)
array([0.567, 0.183, 0.586])

# Standard normal distribution with
# mean 0 and std 1 with N samples
>>> np.random.standard_normal(3)
array([-0.244, 1.542,  0.596])
```

Generating Random Numbers (New Style)

CREATE RANDOM NUMBER GENERATOR

```
# Create a default random generator
>>> rng = np.random.default_rng(seed=0)
```

INTEGERS (NEW STYLE)

```
# Discrete uniform distribution
# over [0, 5) with N samples
>>> rng.integers(5, size=3)
array([0, 0, 4])

# Discrete uniform distribution
# over [1, 5) with N samples
>>> rng.integers(1, 5, 3)
array([4, 3, 3])
```

FLOATS (NEW STYLE)

```
# Uniform distribution over [0.0, 1.0)
# with N samples
>>> rng.random(3)
array([0.078, 0.588, 0.621])

# Uniform distribution over
# [-1.0, 1.0) with N samples
>>> rng.uniform(-1, 1, 3)
array([-0.595, -0.764, 0.936])

# Standard normal distribution with
# mean 0 and std 1 with N samples
>>> rng.standard_normal(3)
array([-0.244, -0.713,  2.592])
```


Give it a try! Generating Array Data

`import numpy as np`

1. Generate 8 equally spaced points across the interval **`[-10.0, 10.0]`**. Call this **`x`**.
2. Scale this data by **`np.pi / 10`**
   Save this to **x**
3. Calculate **`y = np.cos(x)`**

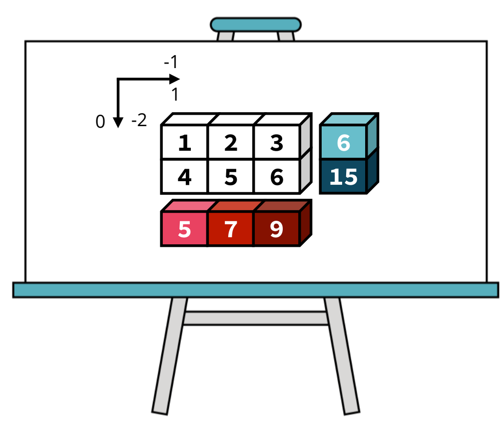
Arrays and Text Files

ARRAYS FROM/TO TXT FILES

```
# 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)
```

```
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



NumPy

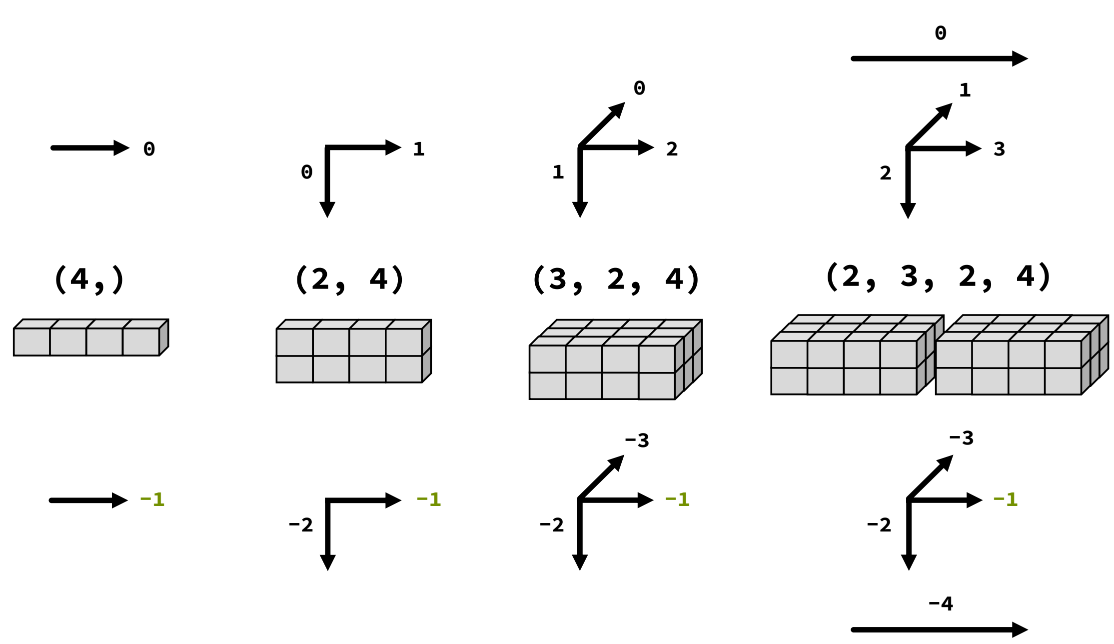
Array Calculation Methods

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

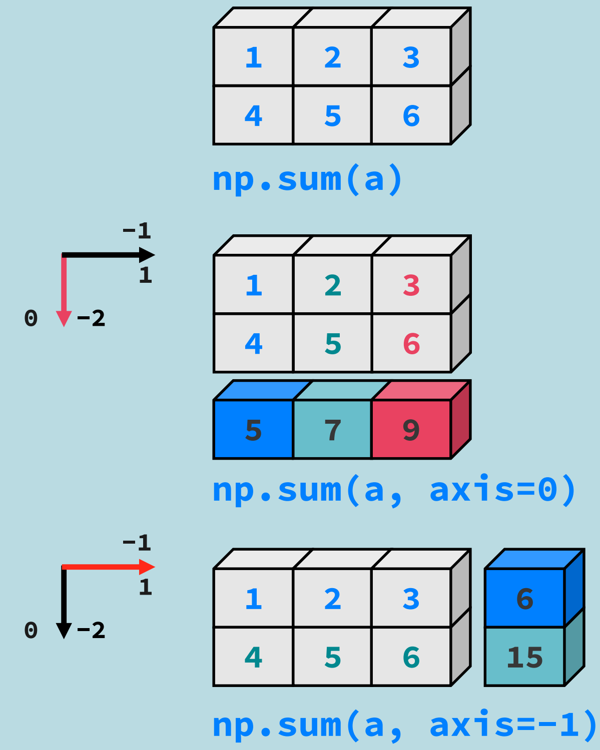
VISUALIZING MULTI-DIMENSIONAL ARRAYS



Array Calculation Methods

SUM METHODS

```
# 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])
```



Other Operations on Arrays

PROD FUNCTION

```
# Functions work on data passed to it
>>> a = np.array([[1, 2, 3],
                  [4, 5, 6]])

# prod() defaults to calculating
# product of all values in an array.
>>> np.prod(a)
720

# supply an axis argument to
# get prod along a specific axis
>>> np.prod(a, axis=0)
array([4, 10, 18])
```

OTHER METHODS AND FUNCTIONS

Mathematical functions

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

Statistics

- `mean, std, var`

Truth value testing

- `any, all`

Min/Max

MIN

```
>>> a = np.array([[5, 4, 1], [2, 3, 6]])
# Prefer NumPy functions to builtins
# when working with arrays
>>> np.min(a)
1
# Most NumPy reducers can be used
# as methods as well as functions
>>> a.min()
1
```

MAX

```
# Use the axis keyword to find max
# values for one dimension
>>> a.max(axis=0)
array([5, 4, 6])
# as a function
>>> np.max(a, axis=1)
array([5, 6])
```

ARGMIN/ARGMAX

```
# Many tasks (like optimization) are
# interested in the location of a
# min/max, not the value
>>> a.argmax()
5

# 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)
(1, 2)
```


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])
```

NumPy 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])
```


Give it a try! Array Calculation Methods

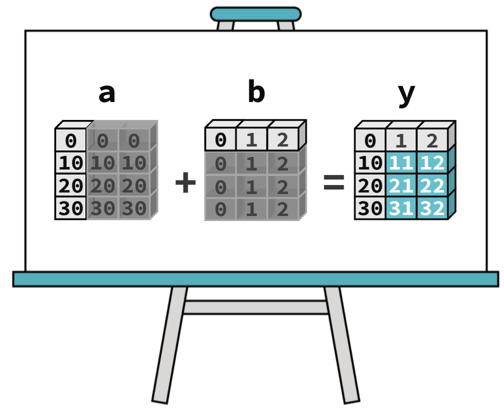
1. Create the array below with

```
a = np.arange(-15, 15).reshape(5, 6) ** 2
```

2. and compute:

- The maximum of each row
- The mean of each column
- 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



NumPy

Array Broadcasting

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**.

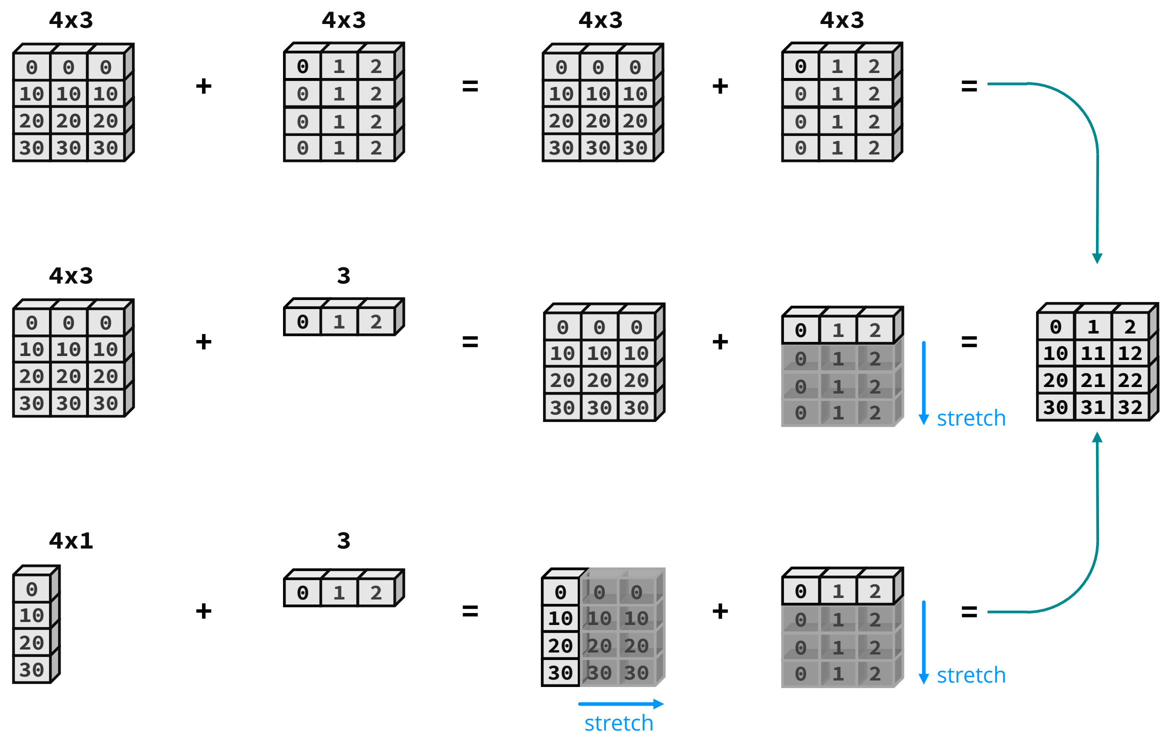
RULE 1: PREPEND ONES TO SMALLER ARRAY'S SHAPE

```
>>> 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!
```

Array Broadcasting



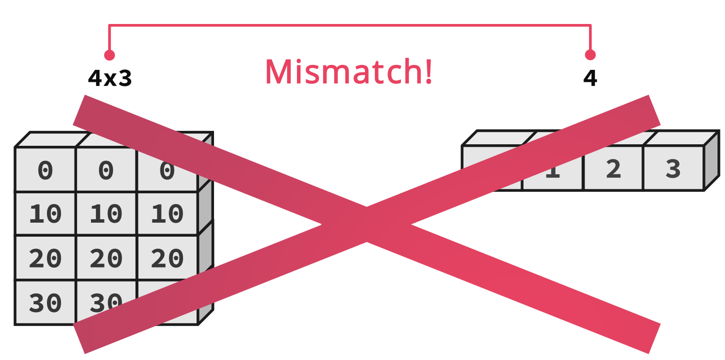
Broadcasting Rules

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

Otherwise, a

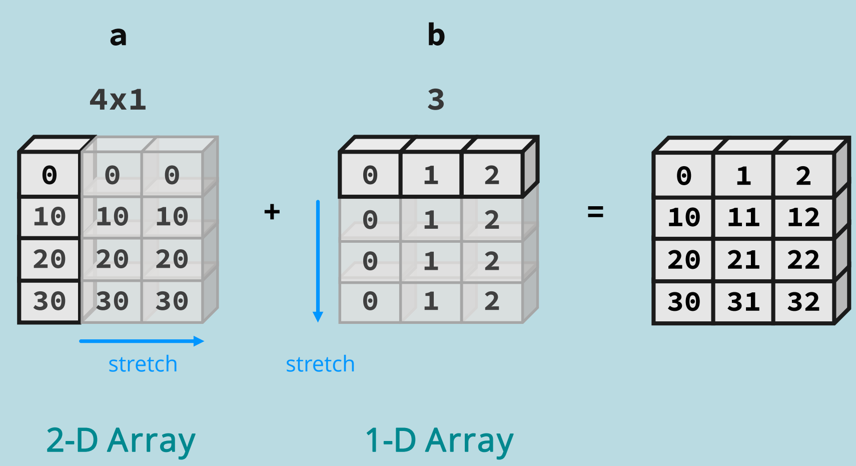
`"ValueError: shape mismatch: objects cannot be broadcast to a single shape"`

exception is thrown.

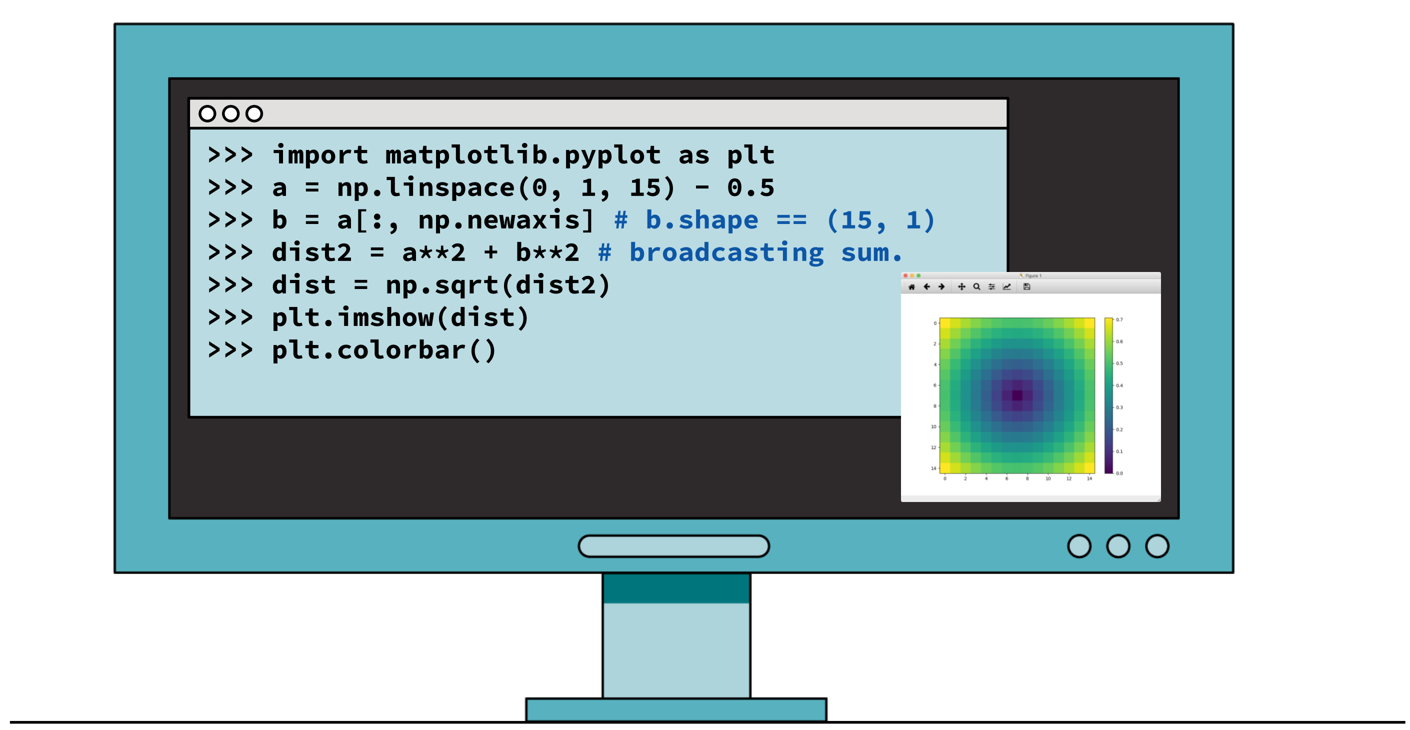


Broadcasting in Action

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



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]
```

Enthought

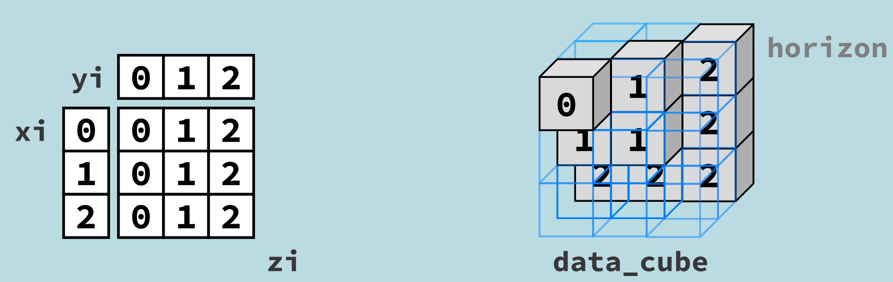
Broadcasting Indices

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



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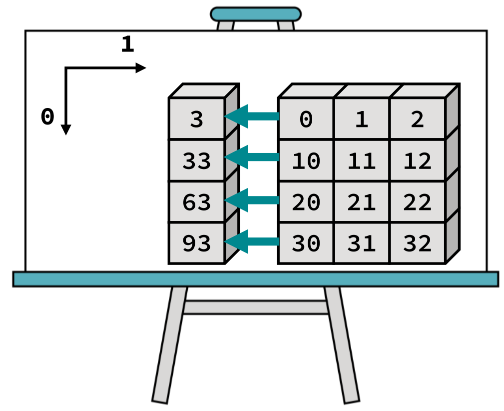


NumPy

Universal Function Methods

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)`

$$= \sum_{n=0}^{N-1} a[n]$$

$$= a[0] + a[1] + ... + a[N-1]$$

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

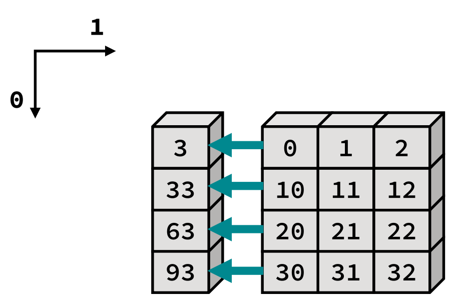
```
>>> a = np.array([1,1,0,1])
>>> np.logical_and.reduce(a)
False
>>> np.logical_or.reduce(a)
True
```


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.

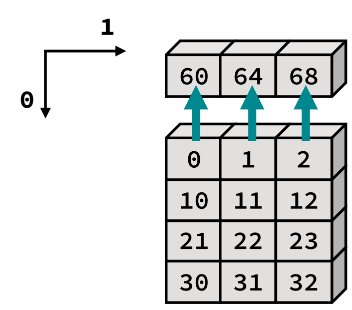
SUMMING UP EACH ROW

```
>>> 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])
```



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)`

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

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])
```


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`.

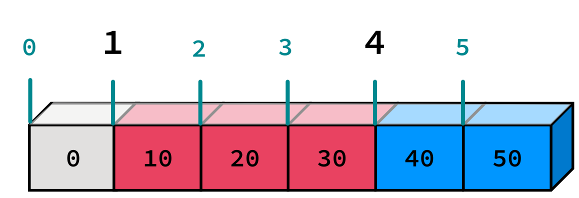
For example:

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

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

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.)

a

a[0]	a[1]	a[2]	a[3]

b

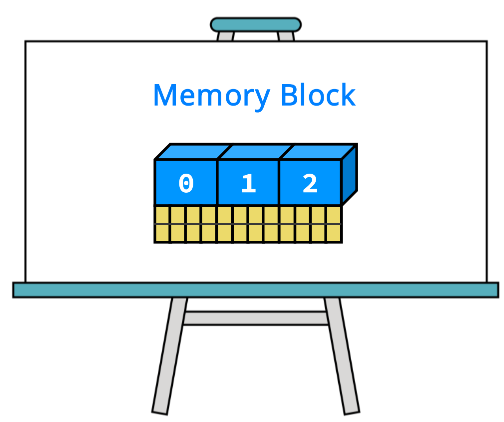
b[0]	b[1]	b[2]

```
>>> 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]
a30]+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]

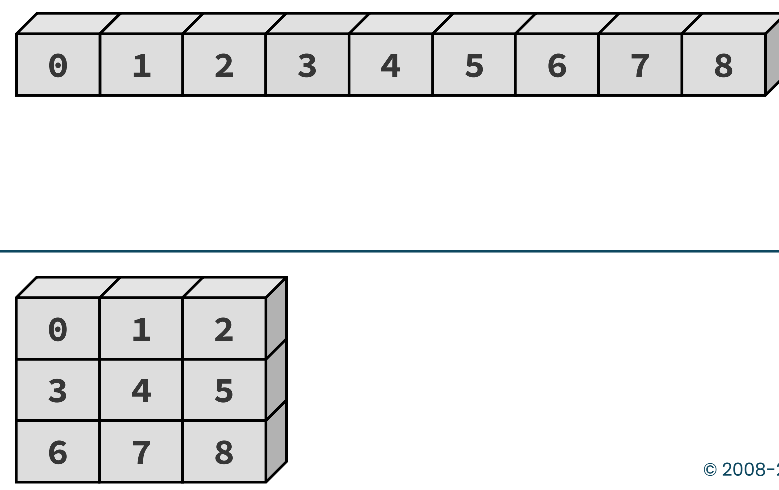


NumPy

The Array Data Structure

Array Data Structure

Memory Block



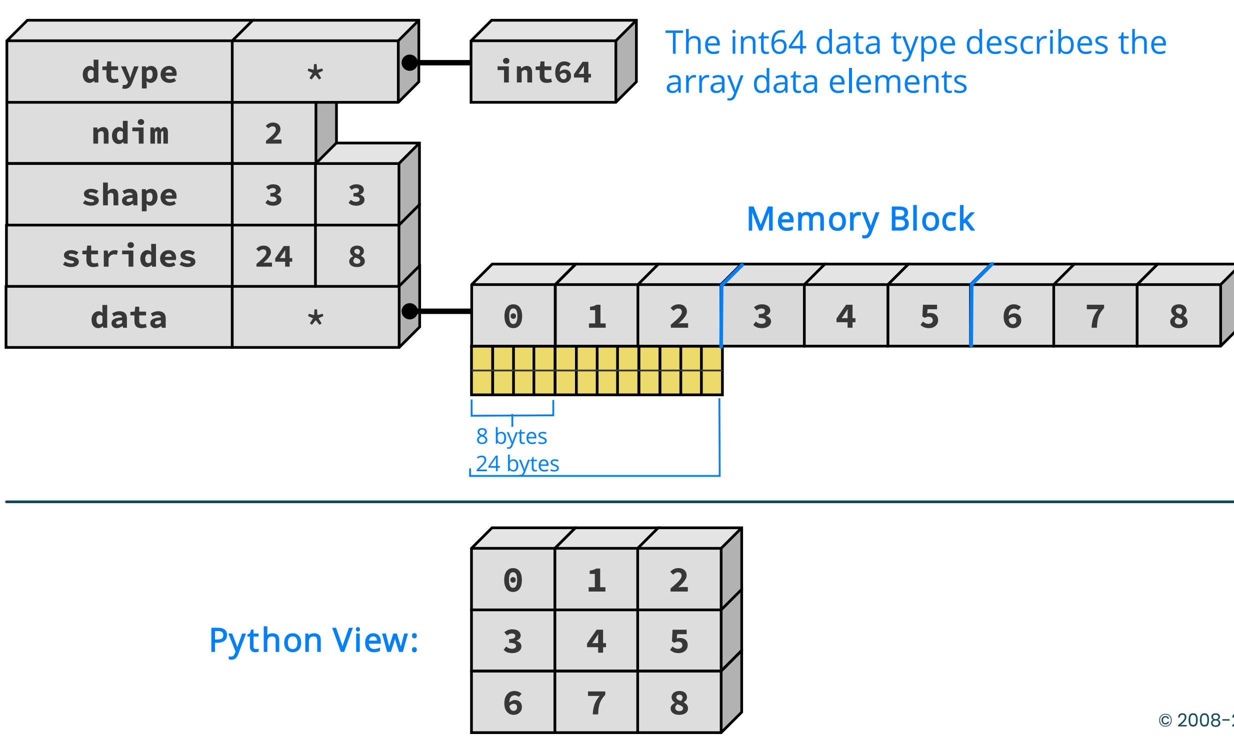
Python View:

Array Data Structure

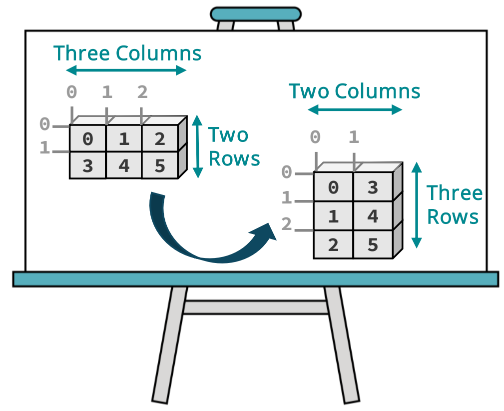
NDArray Data Structure

The int64 data type describes the array data elements

Memory Block



Python View:



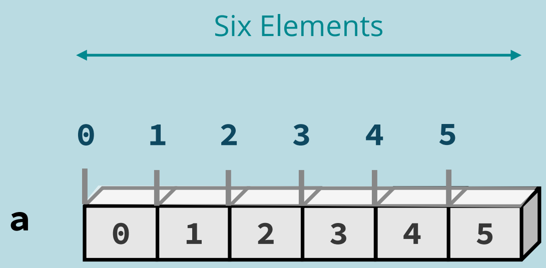
NumPy

Structure Operations

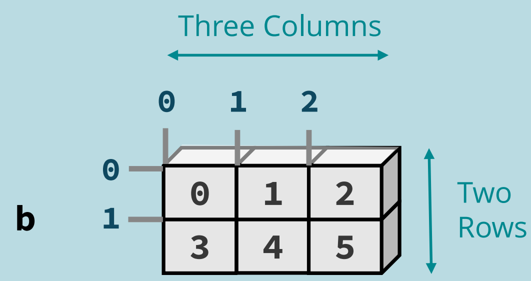
Operations on the Array Structure

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
```

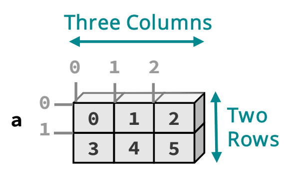


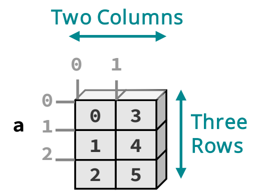
This is not a new copy of the data.
The original data does not get reordered.

Transpose

TRANSPOSE

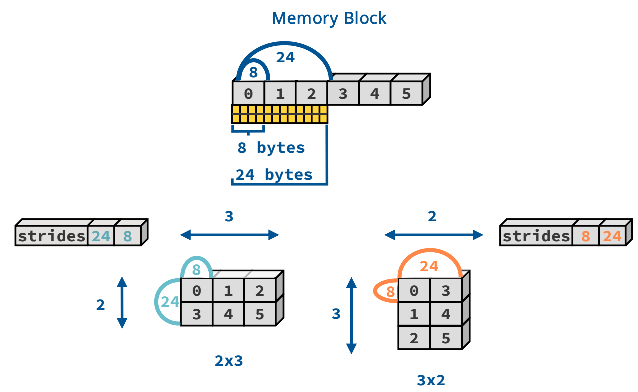
```
>>> a = np.array([[0, 1, 2],
...               [3, 4, 5]])
>>> a.shape
(2,3)

# 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)
```



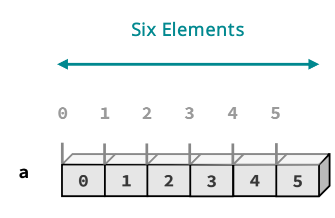
Reshaping Arrays

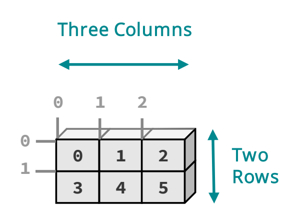
RESHAPE

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



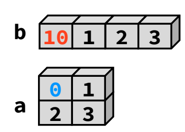


Flattening Arrays

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                no change
array([[0, 1],
       [2, 3]])
```

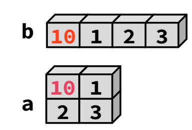


RAVEL (EFFICIENT)

`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                changed!
array([[10, 1],
       [ 2, 3]])
```



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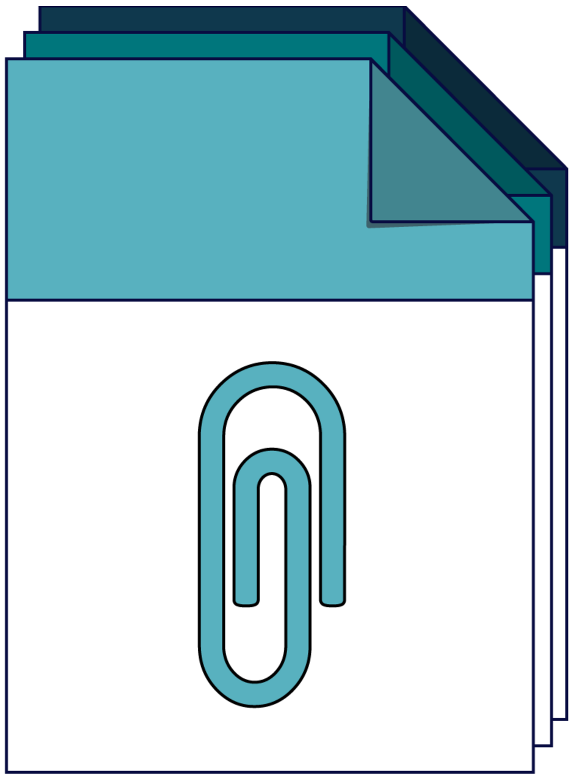

Appendix

Additional Material

Enthought

Enthought

Enthought powers digital transformation for science.

We Partner with Industry Leaders

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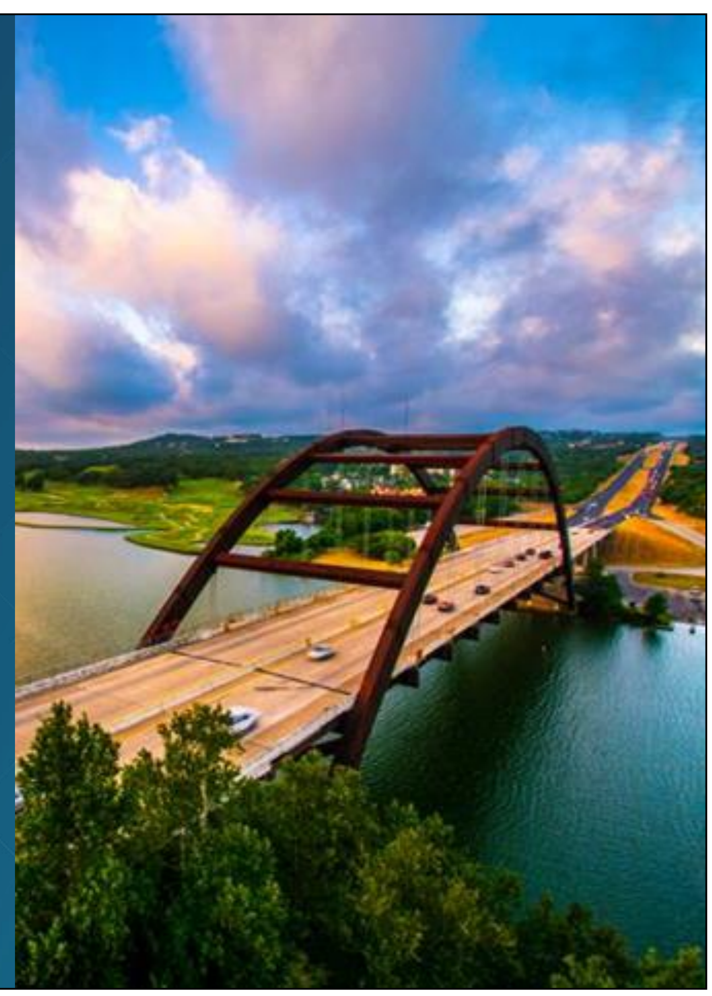
ABOUT ENTHOUGHT

Foundation for Success

- Global, privately-owned company with headquarters in Austin
- Offices in Houston, Texas; Cambridge, United Kingdom; Zürich, Switzerland; and Tokyo, Japan
- Deep roots in the Python community of scientists and engineers
- 80% of employees have graduate degrees or PhDs in science and engineering



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Designed by scientists, for scientists

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Deep scientific expertise and computational knowledge

We empower scientists.
Equipping scientists with digital skills and technology

Enthought