NumPy Tutorial

CS-328 Numerical Methods for Visual Computing and Machine Learning

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Introduction

About NumPy - Motivation

NumPy is the core library for scientific computing in Python.

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Why NumPy?

- High-performance multidimensional array - **matrix operations**.
- Access to a wide ecosystem of efficient numerical libraries that take NumPy arrays as input.
- NumPy arrays are more compact than Python lists - **efficient storage**.

Working with NumPy

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Instead of importing the library into the namespace of our program (which would lead to clutter), we import it into a sub-namespace ("np" is a popular choice).

```
>>> import numpy as np
>>> np.pi
3.141592653589793
```

NumPy Basics

Arrays

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- Indexed by a tuple of nonnegative integers.
- The rank of the array is the number of dimensions.

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>>> print(a.shape)
(3,)
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```
>>> print(a[0], a[1], a[2])
(1, 2, 3)
```

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>>> print(type(a))
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```
>>> print(a.shape)
(3,)
```

```
>>> print(a[0], a[1], a[2])
(1, 2, 3)
```

```
>>> a[0] = 5                  # Change an element of the array
>>> print(a)
[5 2 3]
```

2D Arrays

We can initialize rank 2 arrays (i.e. matrices) from *nested* Python lists.

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```
>>> b = np.array([[1,2,3], [4,5,6]])  # Create a matrix
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(2, 3)
```

2D Arrays

We can initialize rank 2 arrays (i.e. matrices) from *nested* Python lists.

```
>>> b = np.array([[1,2,3], [4,5,6]])  # Create a matrix
>>> print(b.shape)
(2, 3)
```

```
>>> print(b[0, 0], b[0, 1], b[1, 0])
(1, 2, 4)
```

Array creation

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```
>>> a = np.zeros((2,2))   # Create an array of all zeros
>>> print(a)
[[ 0.  0.]
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```

Note that writing $np.zeros(2, 2)$ won't work because it expects a tuple argument.

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```

Note that writing *np.zeros*$(2, 2)$ won't work because it expects a tuple argument.

```
>>> b = np.ones((1,2))    # Create an array of all ones
>>> print(b)
[[ 1.  1.]]
```

Array creation

```
>>> d = np.eye(2)          # Create a 2x2 identity matrix
>>> print(d)
[[ 1.  0.]
 [ 0.  1.]]
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>>> d = np.eye(2)          # Create a 2x2 identity matrix
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```

```
>>> e = np.random.random((2,2))  # Create a random matrix
>>> print(e)
[[ 0.42554464  0.98280237]
 [ 0.86149523  0.22512398]]
```

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[[ 0.42554464  0.98280237]
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```

```
>>> f = np.linspace(1., 4., 6)
>>> print(f)
[ 1.   1.6  2.2  2.8  3.4  4. ]
```

Array indexing, slicing

Different types of indexing are possible. First option **slicing**, which is similar to Python slices.

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```
>>> a = np.array([[0,1,2,3], [4,5,6,7], [8,9,10,11]])
>>> print(a)
[[ 0  1  2  3]
 [ 4  5  6  7]
 [ 8  9 10 11]]
>>> b = a[:2, 1:3]
>>> print(b)
[[1 2]
 [5 6]]
```

Array indexing, slicing

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```
>>> a = np.array([[0,1,2,3], [4,5,6,7], [8,9,10,11]])
>>> b = a[:2, 1:3]
>>> print(a[0, 1])
1
>>> b[0, 0] = 19     # b[0, 0] is the same as a[0, 1]
>>> print(a[0, 1])
19
```

Array indexing, slicing

Danger: A slice of an array references to the same data. Changing it will modify original array.

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>>> a = np.array([[0,1,2,3], [4,5,6,7], [8,9,10,11]])
>>> b = a[:2, 1:3]
>>> print(a[0, 1])
1
>>> b[0, 0] = 19     # b[0, 0] is the same as a[0, 1]
>>> print(a[0, 1])
19
```

```
>>> x = np.array([1, 2, 3])
>>> y = x
>>> z = np.copy(x)
>>> x[0] = 10
>>> x == y
True
>>> x == z
False
```

Array indexing, slicing

```
>>> r1 = a[1, :]   # Rank-1 view of the second row of matrix
>>> r2 = a[1:2, :] # Rank-2 view of the second row of matrix
>>> print(r1)
[4 5 6 7]
>>> print(r2)
[[4 5 6 7]]
```

Array indexing, slicing

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>>> r1 = a[1, :]   # Rank-1 view of the second row of matrix
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>>> print(r1)
[4 5 6 7]
>>> print(r2)
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Remember that the last index in the slice notation is exclusive, so both statements select a single row.

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

Array indexing, indices

A set of indices can be used to modify arbitrary parts of an array:

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```
>>> a = np.array([[1,2,3],[4,5,6]])
>>> a[[0, 1, 1], [0, 0, 1]] -= 20
>>> print(a)
[[-19   2   3]
 [-16 -15   6]]
```

Array indexing, boolean

A part of array can be selected with a given condition:

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```
>>> a = np.array([[1,2,3],[4,5,6]])
>>> print(a>3)
[[False False False]
 [ True  True  True]]
>>> print(a[a>3])
[4 5 6]
```

Datatypes

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```
>>> a = np.array([0, 1, 2])   # No dtype declaration
>>> print(a.dtype)
int64
>>> a = np.array([0, 1, 2.3]) # No dtype declaration
>>> print(a.dtype)
float64
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```

A desired datatype can be specified as well.

```
>>> a = np.array([0, 1, 2], dtype=np.int32)
>>> print(a.dtype)
int32
```

Arithmetic Operations

Universal functions

A universal function is a function that operates on **ndarrays** in an element-by-element fashion.

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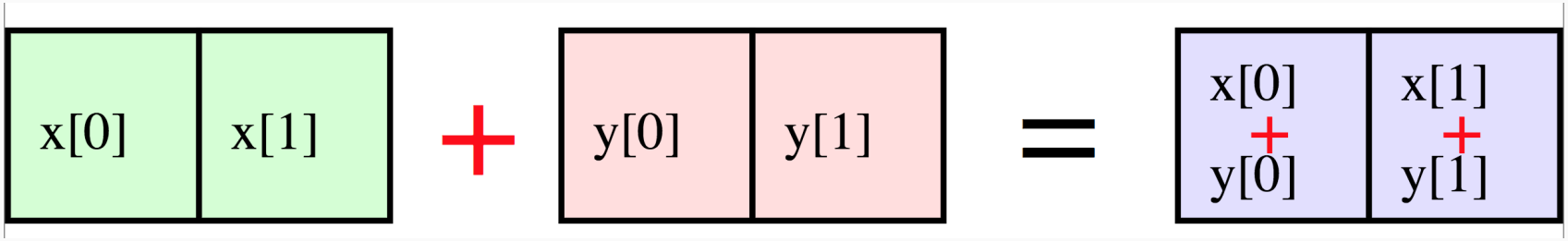

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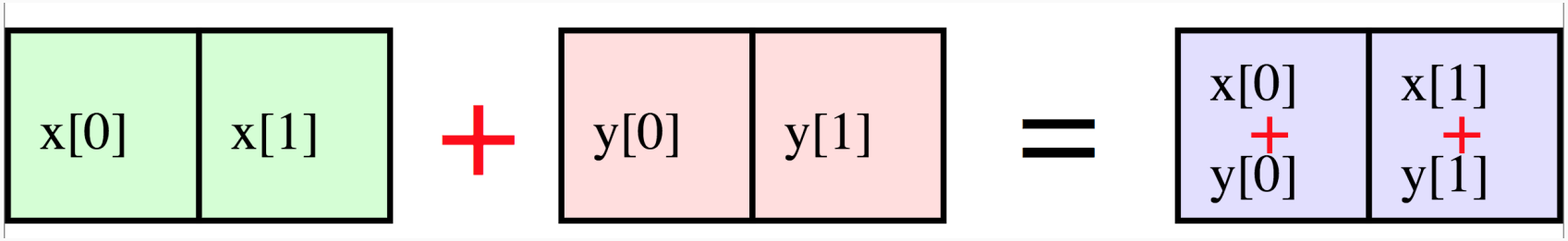

Almost all functions in NumPy are universal.

Universal functions (Elementwise operations)

Basic arithmetic operations work elementwise on arrays.

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```
>>> a = np.array([2, 1], dtype=np.float64)
>>> b = np.array([4, 3], dtype=np.float64)
>>> print(a+b) # add array components element-wise
[ 6.  4.]
>>> print(a*b) # multiply array components element-wise
[ 8.  3.]
>>> print(np.sqrt(b))
[ 2.          1.73205081]
```

Other operations

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It automatically determines which of the three cases is needed based on the shape of the input arguments.

Note that the operator $*$ performs an element-wise array multiplication.

```
>>> a = np.array([[2, 1, 3], [3, 4, 5]], dtype=np.float64)
>>> b = np.array([[8, 2], [5, 5]], dtype=np.float64)
>>> print(b @ a) # matrix multiplication
[[ 22.  16.  34.]
 [ 25.  25.  40.]]
```

Other operations

Many other operations like `sum`, `transpose`, and `max` are available.

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>>> a = np.array([[2, 1, 3], [3, 4, 5]])
>>> print(np.sum(a, axis=0))  # Compute sum of each column
[5 5 8]
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>>> print(np.sum(a, axis=0))  # Compute sum of each column
[5 5 8]
```

```
>>> print(a.T)
[[2 3]
 [1 4]
 [3 5]]
```

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```
>>> a = np.array([[0,1,2,3],[4,5,6,7],[8,9,10,11]]);
>>> b = np.array([-2,-3,0,-1])
>>> c = a + b  # Add b to each row of a
>>> print(a)
[[ 0  1  2  3]
 [ 4  5  6  7]
 [ 8  9 10 11]]
>>> print(c)
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>>> b = np.array([-2,-3,0,-1])
>>> c = a + b  # Add b to each row of a
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[[ 0  1  2  3]
 [ 4  5  6  7]
 [ 8  9 10 11]]
>>> print(c)
[[-2 -2  2  2]
 [ 2  2  6  6]
 [ 6  6 10 10]]
```

Although vector b has a different shape, NumPy assumes that b has also size $4x3$, where each row is a copy of b.

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A two dimensional array multiplied by a one dimensional array results in broadcasting if the number of 1D array elements matches the number of 2D array columns.

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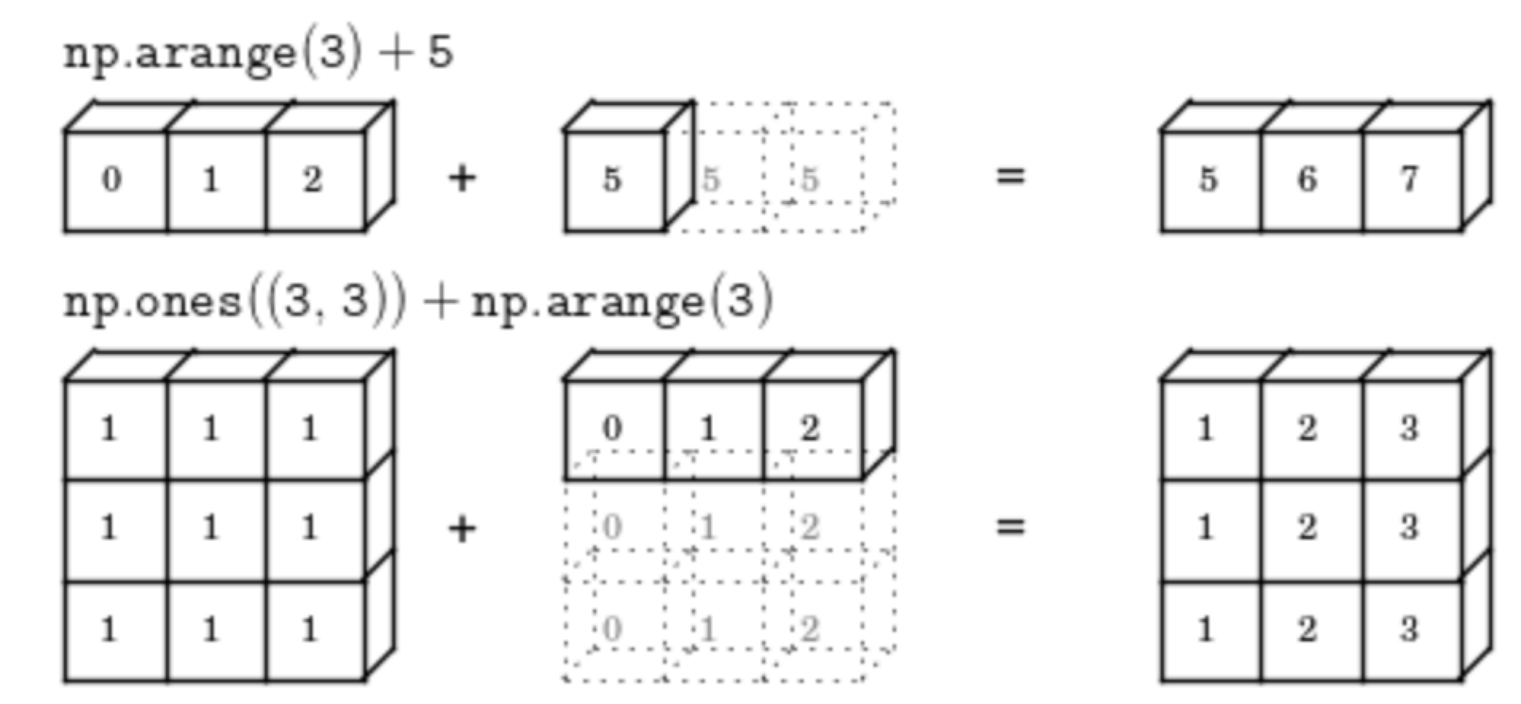

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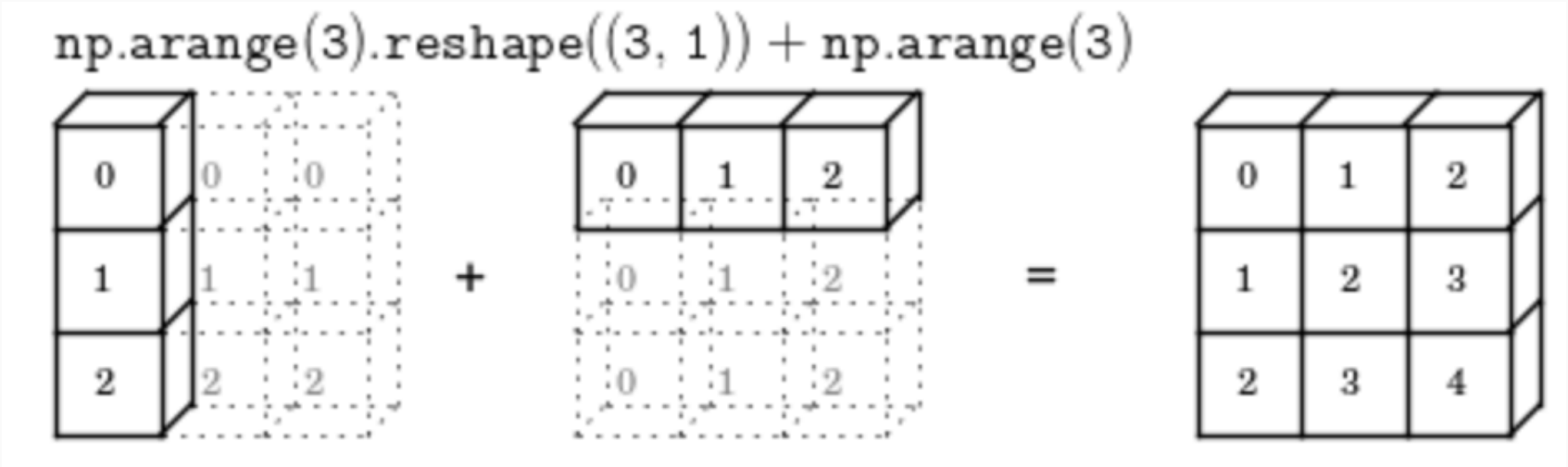

Broadcasting

When operating on two arrays, NumPy compares their shapes element-wise. It starts with the trailing dimensions, and works its way forward. Two dimensions are compatible when

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```
A      (4d array):  8 x 1 x 6 x 1
B      (3d array):      7 x 1 x 5
Result (4d array):  8 x 7 x 6 x 5
```

Broadcasting

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B      (3d array):      7 x 1 x 5
Result (4d array):  8 x 7 x 6 x 5
```

```
A      (2d array):  5 x 4
B      (1d array):      1
Result (2d array):  5 x 4
```

Broadcasting

When operating on two arrays, NumPy compares their shapes element-wise. It starts with the trailing dimensions, and works its way forward. Two dimensions are compatible when

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B      (3d array):      7 x 1 x 5
Result (4d array):  8 x 7 x 6 x 5
```

```
A      (2d array):  5 x 4
B      (1d array):      1
Result (2d array):  5 x 4
```

```
A      (2d array):  5 x 4
B      (1d array):      4
Result (2d array):  5 x 4
```

Broadcasting

When operating on two arrays, NumPy compares their shapes element-wise. It starts with the trailing dimensions, and works its way forward. Two dimensions are compatible when

- they are equal, or
- one of them is 1.

```
A      (1d array):  3
B      (1d array):  4 # trailing dimensions do not match

A      (2d array):      2 x 1
B      (3d array):  8 x 4 x 3 # second from last dimensions mismatched
```

References

- Documentation
  https://numpy.org/doc/stable/
- Official NumPy tutorial:
  https://numpy.org/doc/stable/user/quickstart.html
- NumPy tutorial for MATLAB users:
  https://docs.scipy.org/doc/numpy/user/numpy-for-matlab-users.html
- Jupyter Notebook documentation:
  https://jupyter.readthedocs.io/en/latest/
- Others:
  http://cs231n.github.io/python-numpy-tutorial/#numpy
  http://scipy.github.io/old-wiki/pages/EricsBroadcastingDoc