Python and NumPy

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Agenda



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Containers

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Python





Python is a high-level, **dynamically** typed multiparadigm programming language. Python code allows you to express very **powerful ideas in very few lines of code** while being very readable.

As of January 1, 2020, Python has officially dropped support for python2. For this class all code will use Python 3.8.

Python



We recommend using the python distribution from **anaconda3**: https://www.anaconda.com/products/individual

Anaconda Individual Edition



For Windows

Python 3.8 • 64-Bit Graphical Installer • 477 MB

Make sure to set "Add Anaconda to my PATH environment variable" to use the conda command from any console.

Python



Setup. Once installed run conda init from any console, then restart it. If using *PowerShell* you might need to run Set-ExecutionPolicy RemoteSigned as Administrator.

Virtual environments.

- conda create -n <venv_name> create a new conda environment.
- conda activate <venv_name> activate (use) the environment.
- conda deactivate deactivate the environment.

Once your environment is active, you can install new packages with the *pip* package installer. **Numpy** can be installed with pip install numpy from your terminal.

Basic data types

x = 3



Like most languages, Python has a number of basic types including integers, floats, booleans, and strings. These data types behave in ways that are familiar from other programming languages.

```
print(type(x)) # Prints "<class 'int'>"
print(x) # Prints "3"

print(x + 1) # Addition; prints "4"
print(x - 1) # Subtraction; prints "2"
print(x * 2) # Multiplication; prints "6"
print(x ** 2) # Exponentiation; prints "9"
```

Basic data types



Note that unlike many languages, Python does not have unary increment (x++) or decrement (x--) operators.

```
x = 3
x += 1
print(x) # Prints "4"
x *= 2
print(x) # Prints "8"
v = 2.5
print(type(y)) # Prints "<class 'float'>"
print(y, y + 1, y * 2, y ** 2) # Prints "2.5 3.5 5.0 6.25"
```



Booleans: Python implements all of the usual operators for Boolean logic, but uses English words rather than symbols (&&, ||, etc.):

```
t = True
f = False

print(type(t)) # Prints "<class 'bool'>"
print(t and f) # Logical AND; prints "False"
print(t or f) # Logical OR; prints "True"
print(not t) # Logical NOT; prints "False"
print(t != f) # Logical XOR; prints "True"
```

Strings



Strings: Python has great support for strings.

```
hello = 'hello'  # String literals can use single quotes
world = "world" # or double quotes: it does not matter.
print(hello) # Prints "hello"
print(len(hello)) # String length; prints "5"
hw = hello + ' ' + world # String concatenation
print(hw) # prints "hello world"
hw12 = '%s %s %d' % (hello, world, 12) # sprintf style string formatting
print(hw12) # prints "hello world 12"
```



String objects have a bunch of useful methods; for example:

```
s = "hello"
print(s.capitalize())
                      # Capitalize a string; prints "Hello"
print(s.upper())
                       # Convert a string to uppercase; prints "HELLO"
print(s.rjust(7))
                       # Right-justify a string, padding with spaces;
                       # prints " hello"
print(s.replace('l', '(ell)')) # Replace all instances of one substring
                                # with another; prints "he(ell)(ell)o"
print('
        world '.strip()) # Strip leading and trailing whitespace;
                           # prints "world"
```

Containers



Python includes several built-in container types: lists, dictionaries, sets, and tuples.



A **list** is the Python equivalent of an array, but is resizeable and can contain elements of different types:

```
xs = [3, 1, 2] # Create a list
print(xs, xs[2]) # Prints "[3, 1, 2] 2"
xs[2] = 'foo'
                 # Lists can contain elements of different types
print(xs)
                 # Prints "[3, 1, 'foo']"
xs.append('bar')
                 # Add a new element to the end of the list
print(xs)
                 # Prints "[3, 1, 'foo', 'bar']"
x = xs.pop()
                 # Remove and return the last element of the list
print(x, xs)  # Prints "bar [3, 1, 'foo']"
```



A **list** is the Python equivalent of an array, but is resizeable and can contain elements of different types:



Slicing: In addition to accessing list elements one at a time, Python provides concise syntax to access sublists; this is known as slicing.

```
L[start:stop:step]
```

Start position End position The increment

```
nums = list(range(5))
                          # that creates a list of integers
                          # Prints "[0, 1, 2, 3, 4]"
print(nums)
print(nums[2:4])
                          # Get a slice from index 2 to 4 (exclusive);
```

range is a built-in function



Slicing: In addition to accessing list elements one at a time, Python provides concise syntax to access sublists: this is known as slicing.

```
L[start:stop:step]
```

Lists



```
nums = list(range(5))
print(nums[:])
                          # Get a slice of the whole list;
                          # prints "[0, 1, 2, 3, 4]"
print(nums[:-1])
                          # Slice indices can be negative:
                          # prints "[0, 1, 2, 37"
nums[2:4] = [8.9]
                          # Assign a new sublist to a slice
print(nums)
                          # Prints "[0, 1, 8, 9, 4]"
```



Loops: You can loop over the elements of a list like this.

```
animals = ['cat', 'dog', 'monkey']

for animal in animals:
    print(animal)

# Prints "cat", "dog", "monkey", each on its own line.
```



If you want access to the **index** of each element within the body of a loop, use the built-in enumerate function:

```
animals = ['cat', 'dog', 'monkey']

for idx, animal in enumerate(animals):
    print('#%d: %s' % (idx + 1, animal))

# Prints "#1: cat", "#2: dog", "#3: monkey", each on its own line
```

List comprehensions



When programming, frequently we want to transform one type of data into another. As a simple example, consider the following code that computes square numbers:

```
nums = [0, 1, 2, 3, 4]
squares = []

for x in nums:
    squares.append(x ** 2)

print(squares) # Prints [0, 1, 4, 9, 16]
```

List comprehensions



You can make this code simpler using a **list comprehension**:

```
nums = [0, 1, 2, 3, 4]
squares = [x ** 2 for x in nums]
print(squares) # Prints [0, 1, 4, 9, 16]
```

List comprehensions



List comprehensions can also contain conditions:

```
nums = [0, 1, 2, 3, 4]
even_squares = [x ** 2 for x in nums if x % 2 == 0]
print(even_squares) # Prints "[0, 4, 16]"
```



A dictionary stores (key, value) pairs, similar to a Map in Java or an object in Javascript. You can use it like this:



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Dictionaries - loops

It is easy to iterate over the keys in a dictionary.



```
d = {'person': 2, 'cat': 4, 'spider': 8}

for animal in d:
    legs = d[animal]
    print('A %s has %d legs' % (animal, legs))
```

Prints "A person has 2 legs", "A cat has 4 legs", "A spider has 8 legs"

Dictionaries - loops



If you want access to keys and their corresponding values, use the items method:

d = {'person': 2, 'cat': 4, 'spider': 8}

```
for animal, legs in d.items():
    print('A %s has %d legs' % (animal, legs))
# Prints "A person has 2 legs", "A cat has 4 legs", "A spider has 8 legs"
```

Dictionary comprehensions



These are similar to list comprehensions, but allow you to easily construct dictionaries. For example:

```
nums = [0, 1, 2, 3, 4]
even_num_to_square = {x: x ** 2 for x in nums if x % 2 == 0}
print(even_num_to_square) # Prints "{0: 0, 2: 4, 4: 16}"
```



A **set** is an unordered collection of distinct elements. As a simple example, consider the following:



A **set** is an unordered collection of distinct elements. As a simple example, consider the following:



Loops: Iterating over a set has the same syntax as iterating over a list; however since sets are unordered, you cannot make assumptions about the order in which you visit the elements of the set:

```
animals = {'cat', 'dog', 'fish'}
for idx, animal in enumerate(animals):
    print('#%d: %s' % (idx + 1, animal))
# Prints "#1: fish", "#2: dog", "#3: cat"
```

Set comprehensions: we can easily construct sets using set comprehensions.

```
from math import sqrt
nums = {int(sqrt(x)) for x in range(30)}
print(nums) # Prints "{0, 1, 2, 3, 4, 5}"
```



A **tuple** is an (immutable) ordered list of values. A tuple is in many ways similar to a list; one of the most important differences is that tuples can be used as keys in dictionaries and as elements of sets, while lists cannot. Here is a trivial example:

You can refer to this page for the differences between lists and tuples.



Python functions are defined using the def keyword. For example:

```
def sign(x):
    if x > 0:
        return 'positive'
    elif x < 0:
        return 'negative'
    else:
        return 'zero'
for x in [-1, 0, 1]: # Prints "negative", "zero", "positive"
    print(sign(x))
```



We will often define functions to take optional keyword arguments, like this:

```
def hello(name, loud=False):
    if loud:
        print('HELLO, %s!' % name.upper())
    else:
        print('Hello, %s' % name)

hello('Bob') # Prints "Hello, Bob"
hello('Fred', loud=True) # Prints "HELLO, FRED!"
```



The syntax for defining classes in Python is straightforward:

```
class AbstractGreeter(object):
    # Constructor
    def __init__(self, name):
        pass
    # Instance method
    def greet(self, loud=False):
        pass
```



```
class Greeter(object):
    # Constructor
    def __init__(self, name):
        self.name = name # Create an instance variable
    # Instance method
    def greet(self, loud=False):
        if loud:
            print('HELLO, %s!' % self.name.upper())
        else:
            print('Hello, %s' % self.name)
```

Classes



```
g = Greeter('Fred') # Construct an instance of the Greeter class
g.greet() # Call an instance method;
# prints "Hello, Fred"

g.greet(loud=True) # Call an instance method;
# prints "HELLO, FRED!"
```

NumPy

NumPy



NumPy is a Python C extension library for array-oriented computing:

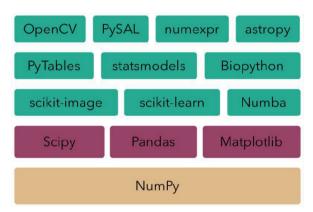
- Efficient
- In-memory
- Contiguous (or Strided)
- Homogeneous (but types can be algebraic)



NumPy



NumPy is the foundation of the Python scientific stack:



Quick Start



```
In [1]: import numpy as np
In [2]: A = np.array([1,2,3,4])
In [3]: A.dtype #type of what is stored in the array - NOT python types!
Out [3]:dtype('int64')
In [4]: A.ndim #number of dimensions (axes in numpy speak)
Out [4]: 1
In [5]: A.shape #size of the dimensions as a tuple
Out [5]: (4,)
In [6]: A.reshape((4,1)).shape #a column vector
Out [6]: (4. 1)
```

Quick Start

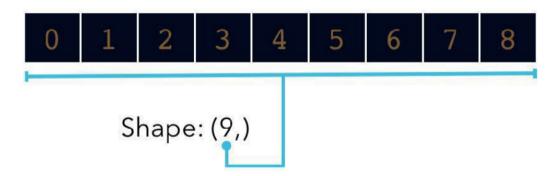


```
In [1]: import numpy as np
In [2]: a = np.array([1,2,3,4,5,6,7,8,9])
In [3]: a
Out[3]: array([1, 2, 3, 4, 5, 6, 7, 8, 9])
In [4]: b = a.reshape((3,3))
                             In [6]: b * 10 + 4
In [5]: b
Out [5]:
                             Out [6]:
array([[1, 2, 3],
                             array([[14, 24, 34],
[4, 5, 6],
                             [44, 54, 64],
[7, 8, 9]])
                             [74, 84, 94]])
```

Array Shape



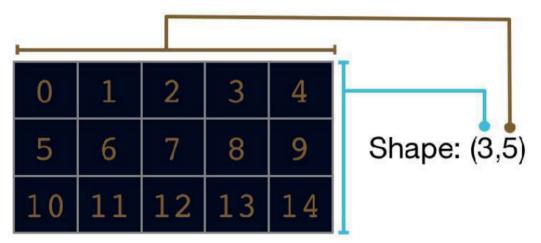
One dimensional arrays have a 1-tuple for their shape:



Array Shape



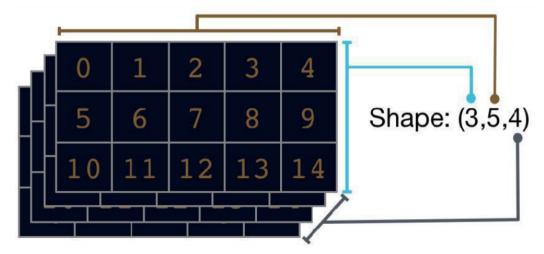
Two dimensional arrays have a 2-tuple:



Array Shape



...and so on:



Array Element Type (dtype)



NumPy arrays comprise elements of a single data type. The type object is accessible through the .dtype attribute.

Here are a few of the most important attributes of dtype objects

- dtype.byteorder big or little endian
- dtype.itemsize element size of this dtype
- dtype.name a name for this dtype object
- dtype.type type object used to create scalars

There are many others...

Array Element Type (dtype)



Array dtypes are usually inferred automatically:

```
In [16]: a = np.array([1,2,3])
In [17]: a.dtype
Out[17]: dtype('int64')
In [18]: b = np.array([1,2,3,4.567])
In [19]: b.dtype
Out[19]: dtype('float64')
In [20]: a = np.array([1,2,3], dtype=np.float32)
In [22]: a
Out[22]: array([ 1., 2., 3.], dtype=float32)
```

Array Creation



Explicitly from a list of values:

```
In [2]: np.array([1,2,3,4])
Out[2]: array([1, 2, 3, 4])
```

As a range of values:

```
In [3]: np.arange(10)
Out[3]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

By specifying the number of elements:

```
In [4]: np.linspace(0, 1, 5)
Out[4]: array([ 0. , 0.25, 0.5 , 0.75, 1. ])
```

Array Creation

7ero-initialized:

In [4]: np.zeros((2,2))



```
Out [4]:
array([[ 0., 0.],
[0.,0.]
One-initialized:
In [5]: np.ones((1,5))
Out[5]: array([[ 1., 1., 1., 1., 1.]])
Uninitialized:
In [4]: np.empty((1,3))
Out[4]: array([[ 2.12716633e-314, 2.12716633e-314, 2.15203762e-314]])
```

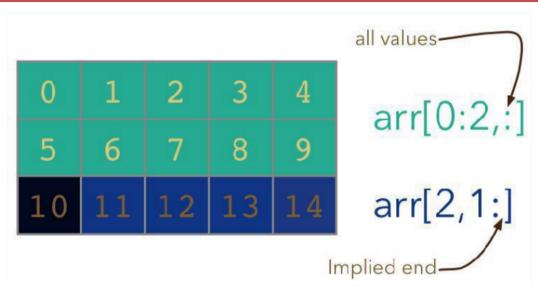
Array Creation



```
Constant diagonal value:
In [6]: np.eye(3)
Out [6]:
array([[ 1., 0., 0.],
[ 0., 1., 0.].
[0., 0., 1.]
Multiple diagonal values:
In [7]: np.diag([1,2,3,4])
Out [7]:
array([[1, 0, 0, 0],
[0, 2, 0, 0],
[0, 0, 3, 0],
\Gamma \cap \cap \cap \Lambda
```

Indexing and Slicing

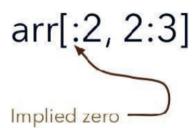




Indexing and Slicing



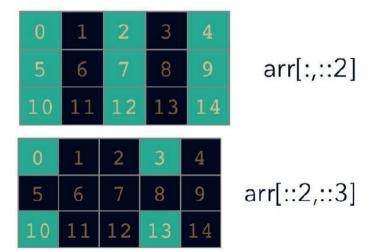
0	1	2	3	4
5	6	7	8	9
10	11	12	13	14



Indexing and Slicing



NumPy array indices can also take an optional stride:



Indexing - Views



Simple assignments do not make copies of arrays (same semantics as Python). Slicing operations do not make copies either; they return views on the original array:

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

In [7]: b.flags.owndata

Out[7]: False

Array views contain a pointer to the original data, but may have different shape or stride values. Views always have flags.owndata equal to False.

Numpy Operations



NumPy ufuncs are functions that operate element-wise on one or more arrays:



ufuncs dispatch to optimized C inner-loops based on array dtype.

Array Element Type (dtype)



NumPy has many built-in ufuncs:

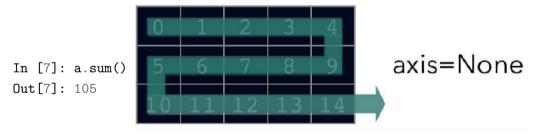
- comparison: <, <=, ==, !=, >=, >
- arithmetic: +, -, *, /, reciprocal, square
- exponential: exp, expm1, exp2, log, log10, log1p, log2, power, sqrt
- trigonometric: sin, cos, tan, acsin, arccos, atctan
- hyperbolic: sinh, cosh, tanh, acsinh, arccosh, atctanh
- bitwise operations: &, |, ~, ^, left_shift, right_shift
- logical operations: and, logical_xor, not, or
- predicates: isfinite, isinf, isnan, signbit
- other: abs, ceil, floor, mod, modf, round, sinc, sign, trunc

There are many others...

Reducing an axis



Array method reductions take an optional axis parameter that specifies over which axes to reduce (axis=None reduces into a single scalar):



axis=None is the default

Reducing an axis

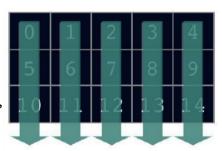


axis=0 reduces into the zeroth dimension:

In [8]: a.sum(axis=0)

Out[8]: array([15, 18, 21,

24, 27])



$$axis=0$$

Reducing an axis



axis=1 reduces into the first dimension:

In [9]: a.sum(axis=1)

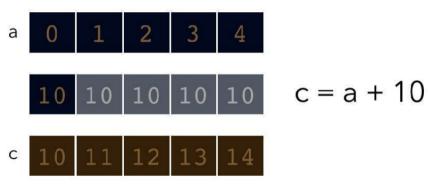
Out[9]: array([10,35,60])



Broadcasting



A key feature of NumPy is broadcasting, where arrays with different, but compatible shapes can be used as arguments to ufuncs:



In this case an array scalar is broadcast to an array with shape (5,)

Broadcasting



A slightly more involved broadcasting example in two dimensions:

Here an array of shape (3, 1) is broadcast to an array with shape (3, 2)

Broadcasting



If the dimensions do not match up, np.newaxis may be useful:

```
In [16]: a = np.arange(6).reshape((2, 3)) # shape((2, 3))
In [17]: b = np.array([10, 100]) # shape (2,)
In [18]: a * b
ValueError
                                        Traceback (most recent call last)
in ()
----> 1 a * b
ValueError: operands could not be broadcast together with shapes (2,3) (2)
In [20]: a * b[:,np.newaxis] # (2, 3) * (2, 1)
Out[20]:
array([[ 0, 10, 20],
[300, 400, 500]])
```

Array Methods



- Predicates: a.any(), a.all()
- Reductions: a.mean(), a.argmin(), a.argmax(),a.trace(), a.cumsum(), a.cumprod()
- Manipulation: a.argsort(), a.transpose(), a.reshape(...),
 a.ravel(), a.fill(...), a.clip(...)
- Complex Numbers: a.real, a.imag, a.conj()

Fancy Indexing



Boolean arrays can also be used as indices into other arrays:

```
In [3]: a
Out[3]:
array([[ 0, 1, 2, 3, 4],
[5, 6, 7, 8, 9],
[10, 11, 12, 13, 14]])
In [4]: b = (a % 3 == 0)
In [5]: b
Out[5]:
array([[ True, False, False, True, False],
[False, True, False, False, True],
[False, False, True, False, False]], dtype=bool)
In [6]: a[b]
Out[6]: arrav([0, 3, 6, 9, 12])
```

NumPy Functions



- Data I/O: fromfile, genfromtxt, load, loadtxt, save, savetxt
- Mesh Creation: mgrid, meshgrid, ogrid
- Manipulation: einsum, hstack, take, vstack

Other Subpackages:

- numpy.fft Fast Fourier transforms
- numpy.polynomial Efficient polynomials
- numpy.linalg Linear algebra cholesky, det, eig, eigvals, inv, lstsq, norm, qr, svd
- numpy.math: C standard library math functions
- numpy.random Random number generation beta, gamma, geometric, hypergeometric, lognormal, normal, poisson, uniform, weibull

Exercise

Shapes and reduction operations



- Write a function that takes a 1d numpy array and computes its reverse vector (last element becomes the first).
- Given the following square array, compute the product of the elements on its diagonal. [[1 3 8] [-1 3 0] [-3 9 2]]
- Create a random vector of size (3, 6) and find its mean value.
- Given two arrays a and b, compute how many time an item of a is higher than the corresponding element of b.

```
a: [[1 5 6 8] [2 -3 13 23] [0 -10 -9 7]] b: [[-3 0 8 1] [-20 -9 -1 32] [7 7 7 7]]
```

• Create and normalize the following matrix (use min-max normalization). [[0.35 -0.27 0.56] [0.15 0.65 0.42] [0.73 -0.78 -0.08]]

Array operations: Python vs Numpy



Let's run a little benchmark! Given a matrix $\mathbf{A} \in \mathbb{R}^{N \times M}$ and a vector $\mathbf{b} \in \mathbb{R}^{M}$, compute the euclidean distance between \mathbf{b} and each row $\mathbf{A}_{i,:}$ of \mathbf{A} :

$$d(\mathbf{a},\mathbf{b}) = \sqrt{(a_1 - b_1)^2 + (a_2 - b_2)^2 + \cdots + (a_M - b_M)^2} = \sqrt{\sum_{j=1}^M (a_j - b_j)^2}.$$

By filling in the blanks in *eucl_distance.py*, implement this simple function **twice**:

- with vanilla Python operators,
- with optimized Numpy operations.

Which one runs faster? Read the provided code carefully and watch out for mistakes;)

Final Disclaimer





If you're one of the lucky ones with access to the GitHub Copilot beta, please **disable it now!**

Resources



- **Reference**: https://numpy.org/doc/stable/reference/
- User guide: https://numpy.org/doc/stable/user/index.html
- Basics tutorial: https://numpy.org/doc/stable/user/quickstart.html
- **Examples**: https://numpy.org/doc/stable/reference/routines.html