

Ekaterina Tuzova Numpy: Vectorize your brain

K nearest neighbors

https://archive.ics.uci.edu/ml/datasets/Wine



What is NumPy?

Numpy is the fundamental package for scientific computing with Python.



Python and Performance

Python is fast

Python is slow

Euclidian distance

```
import math
def euclidean(xs, ys):
    n = len(xs) # == len(ys)
    acc = 0.
    for i in range(n):
        acc += (xs[i] - ys[i]) ** 2
    return math.sqrt(acc)
```

"Magic" timeit

```
import random
def setup(size):
    xs = [random.random() for _ in range(size)]
    ys = [random.random() for _ in range(size)]
    return xs, ys
```

```
%%timeit xs, ys = setup(8192)
euclidean(xs, ys)
```

100 loops, best of 3: 2.67 ms per loop

Euclidian distance. C

%load_ext biteymagic

```
%%bitey
double euclideanDistance(double x[3], double y[3])
{
    double Sum;
    double distance;
    for(int i=0;i<3;i++)
    {
        Sum = Sum + pow((x[i]-y[i]),2.0);
        distance = sqrt(Sum);
    }
    return distance;
}</pre>
```

Euclidian distance. C

%load_ext biteymagic

```
%%bitey
double euclideanDistance(double x[3], double y[3])
{
    double Sum;
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    for(int i=0;i<3;i++)
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        Sum = Sum + pow((x[i]-y[i]),2.0);
        distance = sqrt(Sum);
    }
    return distance;
}</pre>
```

%%timeit xs, ys = setup(8192)
euclideanDistance(xs, ys)

10000 loops, best of 3: 28 μ s per loop

Euclidian distance

```
import math
def euclidean(xs, ys):
    n = len(xs) # == len(ys)
    acc = 0.
    for i in range(n):
        acc += (xs[i] - ys[i]) ** 2
    return math.sqrt(acc)
```

line_profiler and "magic" lprun

%load_ext line_profiler

%lprun -f euclidean euclidean(*setup(8192))

Euclidian distance

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Timer uni	t: 1e-06 s				
File: <ip< th=""><th>me: 0.015907 Sython-input e euclidean</th><th>-1-51b5d0f5e</th><th>e2ad></th><th></th><th></th></ip<>	me: 0.015907 Sython-input e euclidean	-1-51b5d0f5e	e2ad>		
Line #	Hits	Time H	Per Hit	% Time	Line Contents
2					<pre>def euclidean(xs, ys):</pre>
3	1	3	3.0	0.0	n = len(xs) # == len(ys)
4	1	1	1.0	0.0	acc = 0.
5	8193	6037	0.7	38.0	for i in range(n):
6	8192	9861	1.2	62.0	acc += (xs[i] - ys[i]) ** 2
7	1	5	5.0	0.0	return math.sqrt(acc)

Compiled languages

Interpreted languages

What can be done?



Ufuncs

Universal **func**tions

Special type of function defined within a numpy library and it operate element-wise on arrays.

a = range(4)
b = [value + 1 for value in a]
print(b)

[1, 2, 3, 4]

```
a = range(4)
b = [value + 1 for value in a]
print(b)
```

[1, 2, 3, 4]

import numpy as np

```
a = np.arange(4)
b = a + 1
print(b)
```

[1 2 3 4]

a = np.arange(4)
b = np.full(4, 2)

a*b

array([0., 2., 4., 6.])

%%timeit a = np.arange(100000)
a + 1

10000 loops, best of 3: 108 μ s per loop

%%timeit a = range(100000)
[value + 1 for value in a]

100 loops, best of 3: 8.96 ms per loop

Ufuncs available

- Arithmetic
- Bitwise
- Comparison
- Trigonometric
- Floating

Slicing and indexing

Slicing and indexing

<pre>x = np.arange(4)</pre>
x[:2]
array([0, 1])

y = x[1:] y[0] = 42 print (x)	
[0 42 2	3]

x[:2]	
array([0,	1])

x = np.arange(4)

Slicing and indexing

Multidimensional arrays

```
X = np.arange(6).reshape((2, 3))
X
```

```
array([[0, 1, 2],
[3, 4, 5]])
```

array([[1, 2]])

```
x[0, 1]
1
```

X[:1, 1:]]		

Multidimensional arrays

```
X = np.arange(6).reshape((2, 3))
X
```

array([[0, 1, 2], [3, 4, 5]])

X[:, 1] # X.T[1]

array([1, 4])

X[0, :] # X[0]

array([0, 1, 2])

Index arrays

array([2, 0, 42])

Index arrays

array([2, 0, 42])

$$y[0] = 1$$

Index arrays

array([2, 0, 42])

$$y[0] = 1$$

array([0, 42, 2, 3])



х

array([0, 42, 2, 3])

x[np.array([False, True, True, True])]

array([42, 2, 3])



X
array([0, 42, 2, 3])
<pre>x[np.array([False, True, True, True])]</pre>
x[np.ulluy([lulbe, llue, llue, llue])]
array([42, 2, 3])
x[x >= 2]
array([42, 2, 3])

Test train split

def train_test_split(X, y, ratio):
 mask = np.random.random(len(y)) < ratio
 return X[mask], y[mask], X[~mask], y[~mask]</pre>

Test train split

```
def train test split(X, y, ratio):
    X train = []
    y train = []
    X \text{ test} = []
    y test = []
    numbers = [i for i in range(len(X))]
    shuffle(numbers)
    numbers = numbers[0: int(ratio * len(X))]
    for i in range(len(X)):
        if i in numbers:
            X_train.append(X[i])
            y train.append(y[i])
        else:
            X_test.append(X[i])
            y test.append(y[i])
    return X train, y train, X test, y test
```

Broadcasting

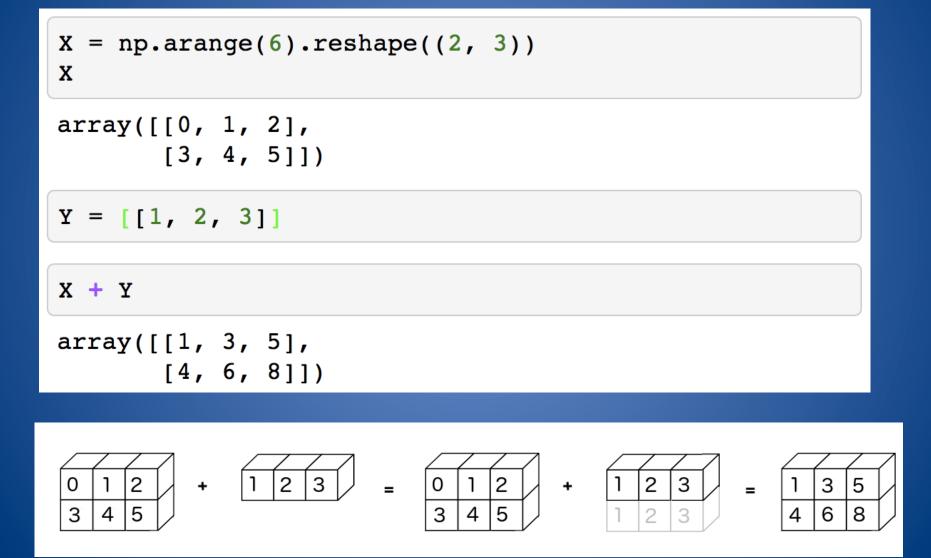
Broadcasting

Broadcasting describes how NumPy treats arrays with different shapes during arithmetic operations.

Broadcasting rules

- 1. If two arrays differ in their number of dimension, the shape of the array with the fewer dimensions is padded with ones on it's leading(left) size.
- 2. If the shape of two arrays doesn't match in any dimension, the array with shape equal to 1 in that dimension is stretched to match the other shape.
- 3. If these conditions are not met, raise a ValueError: operands could not be broadcast together with shapes

Broadcasting. Example



np.newaxis

```
X = np.arange(6).reshape((3, 2))
x
array([[0, 1],
       [2, 3],
       [4, 5]])
```

X + np.array([1, 2, 3])

np.newaxis

```
X = np.arange(6).reshape((3, 2))
X
array([[0, 1],
       [2, 3],
       [4, 5]])
```

```
X + np.array([1, 2, 3])
```

ValueError: operands could not be broadcast together with shapes (3,2) (3,)

np.newaxis

```
X = np.arange(6).reshape((3, 2))
```

Х

array([[0, 1],
 [2, 3],
 [4, 5]])

```
Y = np.array([1, 2, 3])[:, np.newaxis]
Y.shape
```

(3, 1)

Х + Ү

```
array([[1, 2],
      [4, 5],
      [7, 8]])
```

Aggregations

Aggregations

X = np.arange(6).reshape((2, 3))
X.mean()
2.5

Aggregations

X = np.arange(6).reshape((2, 3))
X.mean()
2.5

X.mean(axis=0)
array([1.5, 2.5, 3.5])
X.mean(axis=1)
array([1., 4.])

NumPy resume

Basic ideas to make you code faster:

- Ufuncs
- Slicing and indexing
- Broadcasting
- Aggregations

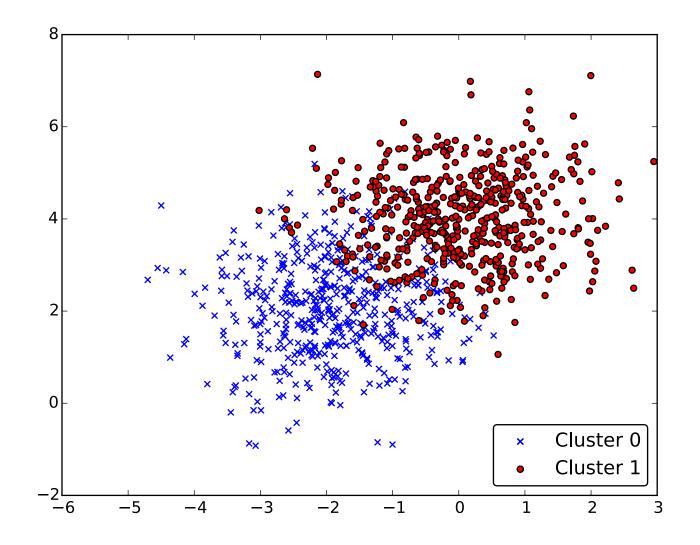
k-means

Algorithm

- 1. Clusters the data into k groups where k is predefined.
- 2. Select k points at random as cluster centers.
- 3. Assign objects to their closest cluster center according to the Euclidean distance function.
- 4. Calculate the centroid or mean of all objects in each cluster.
- 5. Repeat steps 2, 3 and 4 until the same points are assigned to each cluster in consecutive rounds.

Synthetic data

```
import numpy as np
from numpy import random
def sample(size, ratio=.5):
    y = np.random.random(size) <= ratio
    n1 = np.count_nonzero(y)
    n0 = size - n1
    covar = np.diag([1, 1])
    X = np.empty((size, 2))
    X[y == 0, :] = random.multivariate_normal([-2, 2], covar, n0)
    X[y == 1, :] = random.multivariate_normal([0, 4], covar, n1)
    return X, y</pre>
```

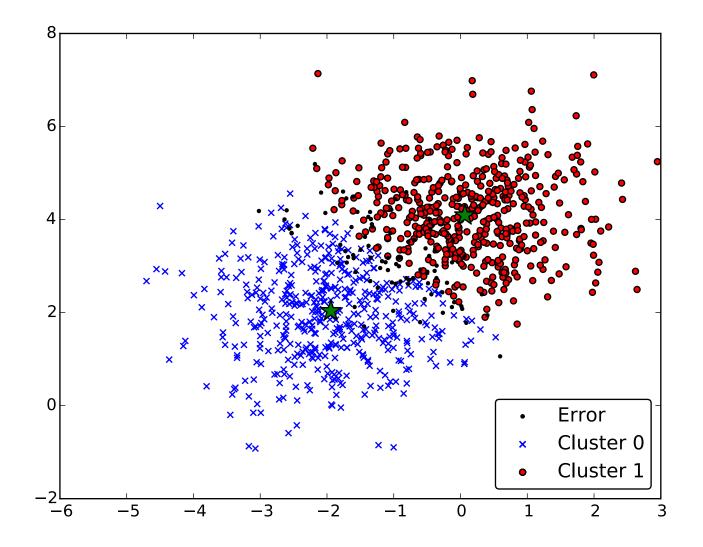


Vectorized euclidian distance

```
def ceuclidean(A, B):
    assert A.ndim == B.ndim == 2
    D = np.empty((len(A), len(B)), dtype=np.float64)
    for i, Ai in enumerate(A):
        D[i, :] = np.sqrt(np.square(Ai - B).sum(axis=1))
    return D
```

k-means

```
def kmeans(X, n_clusters):
    centers = init_centers(X, n_clusters)
    y = None
    while True:
        D = ceuclidean(centers, X)
        new_y = D.argmin(axis=0)
        if np.array_equal(y, new_y):
            break
        y = new_y
        for i in range(n_clusters):
            centers[i] = X[y == i].mean(axis=0)
    return centers, y
```



Thank you.

@ktisha