Sorting Arrays

Up to this point we have been concerned mainly with **tools to access and operate** on array data with NumPy.

This chapter covers **algorithms related to sorting** values in NumPy arrays.

These algorithms are a **favorite topic in introductory computer science courses**:

Algorithms such as **insertion sorts**, **selection sorts**, **merge sorts**, **quick sorts**, **bubble sorts**, and many, many more.

All are means of accomplishing a similar task: **sorting the values in** a **list or array.**

Python has a couple of built-in functions and methods for sorting lists and other iterable objects.

The **sorted** function accepts a **list** and returns a sorted version of it:

Out[100... [1, 1, 2, 3, 4, 5, 6, 9]

By contrast, the sort method of lists will sort the list in-place:

```
In [102... L.sort() # acts in-place and returns None
print(L)
```

[1, 1, 2, 3, 4, 5, 6, 9]

Python's **sorting methods** are quite **flexible**, and can handle **any iterable** object. **For example**, here we sort a **string**:

```
In [104... sorted('python')
Out[104... ['h', 'n', 'o', 'p', 't', 'y']
```

These built-in sorting methods are convenient.

But as previously discussed, the **dynamism of Python** values means they are **less performant than routines designed specifically for uniform arrays of numbers.**

This is where **NumPy's sorting routines** come in.

Fast Sorting in NumPy: np.sort and np.argsort

The **np.sort** function is **analogous** to Python's built-in **sorted** function, and will **efficiently** return **a sorted copy** of an array:

```
In [107...
          import numpy as np
          x = np.array([2, 1, 4, 3, 5])
           np.sort(x)
Out[107... array([1, 2, 3, 4, 5])
           Similarly to the sort method of Python lists, you can also sort an
           array in-place using the array sort method:
          x.sort()
In [109...
           print(x)
```

```
[1 2 3 4 5]
```

[1 0 3 2 4]

A related function is **argsort**, which instead returns the **indices** of the **sorted elements**:

```
In [111... x = np.array([2, 1, 4, 3, 5])
i = np.argsort(x)
print(i)
```

The first element of this result gives the index of the smallest element, the second value gives the index of the second smallest, and so on.

These **indices can then be used** (via fancy indexing) to **construct the sorted array** if desired:

```
In [113... x[i]
```

```
Out[113... array([1, 2, 3, 4, 5])
```

You'll see an application of argsort later in this chapter.

Sorting Along Rows or Columns

A useful feature of NumPy's sorting algorithms is the ability to sort along specific rows or columns of a multidimensional array using the axis argument. For example:

```
In [116... rng = np.random.default_rng(seed=42)
X = rng.integers(0, 10, (4, 6))
print(X)

[[0 7 6 4 4 8]
     [0 6 2 0 5 9]
     [7 7 7 7 5 1]
     [8 4 5 3 1 9]]
```

```
In [117... # sort each column of X
          np.sort(X, axis=0)
Out[117... array([[0, 4, 2, 0, 1, 1],
                  [0, 6, 5, 3, 4, 8],
                  [7, 7, 6, 4, 5, 9],
                  [8, 7, 7, 7, 5, 9]], dtype=int64)
In [118... # sort each row of X
          np.sort(X, axis=1)
Out [118... array ([0, 4, 4, 6, 7, 8],
                  [0, 0, 2, 5, 6, 9],
                  [1, 5, 7, 7, 7, 7],
                  [1, 3, 4, 5, 8, 9]], dtype=int64)
```

Keep in mind that this treats each row or column as an independent array.

And any relationships between the row or column values will be lost!

Partial Sorts: Partitioning

Sometimes we're not interested in sorting the entire array, but simply want to find the **k** smallest values in the array.

NumPy enables this with the **np.partition** function.

np.partition takes an array and a number *K.*

The result is a new array with the **smallest** *K* **values to the left of the partition** and **the remaining values to the right:**

```
Out[121... array([2, 1, 3, 4, 6, 5, 7])
```

Notice that the **first three values** in the resulting array are **the three smallest in the array**, and the remaining array positions contain the remaining values.

Within the two partitions, the elements have arbitrary order.

Similarly to sorting, we can **partition along an arbitrary axis** of a multidimensional array:

The result is an array where the **first two slots in each row** contain the **smallest values from that row**, with the remaining values filling the remaining slots.

Finally, just as there is an np.argsort function that computes indices of the sort, there is an np.argpartition function that computes indices of the partition.

We'll see both of these in action in the following section.

Example: k-Nearest Neighbors

Let's quickly see how we might use the **argsort** function **along** multiple axes to find the nearest neighbors of each point in a set.

We'll start by creating a random set of 10 points on a twodimensional plane.

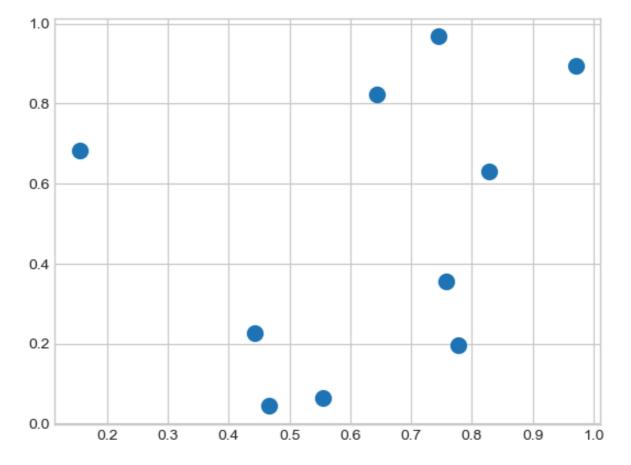
Using the standard convention, we'll arrange these in a 10×2 array:

```
In [127... X = rng.random((10, 2))
In [128... X
```

```
Out[128... array([[0.64386512, 0.82276161], [0.4434142 , 0.22723872], [0.55458479, 0.06381726], [0.82763117, 0.6316644 ], [0.75808774, 0.35452597], [0.97069802, 0.89312112], [0.7783835 , 0.19463871], [0.466721 , 0.04380377], [0.15428949, 0.68304895], [0.74476216, 0.96750973]])
```

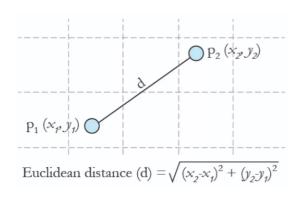
To **get an idea of how these points look,** let's generate a quick **scatter plot:**

```
In [130... %matplotlib inline
   import matplotlib.pyplot as plt
   plt.style.use("seaborn-v0_8-whitegrid")
   plt.scatter(X[:, 0], X[:, 1], s=100);
```



Now we'll compute the distance between each pair of points.

Recall: squared distance between two points is the sum of the squared differences in each dimension:



Using the efficient broadcasting and aggregation routines provided by NumPy we can compute the **matrix of square distances** in a single line of code:

```
In [132... dist_sq = np.sum((X[:, np.newaxis] - X[np.newaxis, :]) ** 2, a
In [133... dist_sq.shape
Out[133... (10, 10)
In [134... dist_sq
```

```
Out[134... array([[0. , 0.39482809, 0.58396752, 0.07028811, 0.232
          29143,
                  0.11177021, 0.41263358, 0.63815537, 0.25920392, 0.031
          13223],
                 [0.39482809, 0. , 0.03906548, 0.31118281, 0.115
          22148,
                  0.7214276 , 0.11326719 , 0.03419159 , 0.29135606 , 0.638
          81176],
                 [0.58396752, 0.03906548, 0. , 0.39700471, 0.125
          92501,
                  0.86089513, 0.06720011, 0.00812058, 0.54368422, 0.852
          82752],
                 [0.07028811, 0.31118281, 0.39700471, 0. , 0.081
          642,
                  0.08882774, 0.19341679, 0.47583627, 0.45602939, 0.119
          65936],
                 [0.23229143, 0.11522148, 0.12592501, 0.081642 , 0.
          ,
                  0.33528787, 0.02597585, 0.18144286, 0.47249968, 0.375
          926671,
                 [0.11177021, 0.7214276 , 0.86089513, 0.08882774, 0.335
```

```
28787,
                 , 0.52486256, 0.97533281, 0.71065321, 0.056
       0.
58068],
       [0.41263358, 0.11326719, 0.06720011, 0.19341679, 0.025
97585,
       0.52486256, 0.
                             , 0.11988469, 0.62803789, 0.598
46002],
       [0.63815537, 0.03419159, 0.00812058, 0.47583627, 0.181
44286,
       0.97533281, 0.11988469, 0. , 0.50624786, 0.930
5396 ],
       [0.25920392, 0.29135606, 0.54368422, 0.45602939, 0.472
49968.
       0.71065321, 0.62803789, 0.50624786, 0. , 0.429
5759 1,
       [0.03113223, 0.63881176, 0.85282752, 0.11965936, 0.375
92667,
       0.05658068, 0.59846002, 0.9305396, 0.4295759, 0.
]])
```

This **operation has a lot packed into it,** and it might be a bit confusing if you're unfamiliar with NumPy's broadcasting rules.

When you come across code like this, it can be useful to **break it** down into its component steps:

```
In [136... # for each pair of points, compute differences in their coordi
    differences = X[:, np.newaxis] - X[np.newaxis, :]
    differences.shape
Out[136... (10, 10, 2)
In [137... differences
```

```
Out[137... array([[[ 0. , 0. ],
                  [ 0.20045092, 0.59552289],
                  [ 0.08928033, 0.75894436],
                  [-0.18376605, 0.19109721],
                 [-0.11422262, 0.46823565],
                 [-0.3268329, -0.07035951],
                 [-0.13451838, 0.62812291],
                 [0.17714412, 0.77895785],
                 [ 0.48957563, 0.13971266],
                 [-0.10089704, -0.14474812]],
                [[-0.20045092, -0.59552289],
                 [0., 0.],
                 [-0.11117059, 0.16342147],
                 [-0.38421697, -0.40442568],
                 [-0.31467354, -0.12728725],
                 [-0.52728383, -0.6658824],
                 [-0.3349693, 0.03260001],
                 [-0.0233068, 0.18343496],
                 [0.28912471, -0.45581023],
                  [-0.30134796, -0.74027101]],
```

```
[[-0.08928033, -0.75894436],
 [0.11117059, -0.16342147],
[0., 0.],
[-0.27304638, -0.56784714],
[-0.20350295, -0.29070871],
[-0.41611324, -0.82930387],
[-0.22379871, -0.13082145],
[0.08786378, 0.02001349],
 [ 0.40029529, -0.6192317 ],
 [-0.19017737, -0.90369248]],
[[0.18376605, -0.19109721],
[0.38421697, 0.40442568],
[ 0.27304638, 0.56784714],
[ 0. , 0.
[ 0.06954343, 0.27713843],
 [-0.14306685, -0.26145672],
[ 0.04924767, 0.43702569],
 [0.36091017, 0.58786063],
```

[0.67334168, -0.05138455],

```
[0.08286902, -0.33584533]],
[[0.11422262, -0.46823565],
[0.31467354, 0.12728725],
[0.20350295, 0.29070871],
[-0.06954343, -0.27713843],
[0. , 0. ],
[-0.21261028, -0.53859515],
[-0.02029576, 0.15988726],
[ 0.29136674, 0.3107222 ],
[ 0.60379825, -0.32852299],
[0.01332558, -0.61298376]],
[[0.3268329, 0.07035951],
[ 0.52728383, 0.6658824 ],
[0.41611324, 0.82930387],
[0.14306685, 0.26145672],
[0.21261028, 0.53859515],
[0., 0.],
[0.19231453, 0.69848241],
[0.50397702, 0.84931736],
```

```
[ 0.81640853, 0.21007217],
 [0.22593587, -0.07438861]],
[[0.13451838, -0.62812291],
[ 0.3349693 , -0.03260001],
[0.22379871, 0.13082145],
[-0.04924767, -0.43702569],
[ 0.02029576, -0.15988726],
[-0.19231453, -0.69848241],
[0., 0.],
[ 0.31166249, 0.15083494],
 [0.62409401, -0.48841025],
 [0.03362134, -0.77287102]],
[[-0.17714412, -0.77895785],
[0.0233068, -0.18343496],
[-0.08786378, -0.02001349],
[-0.36091017, -0.58786063],
[-0.29136674, -0.3107222],
[-0.50397702, -0.84931736],
 [-0.31166249, -0.15083494],
```

```
[0., 0.
[0.31243151, -0.63924519],
 [-0.27804115, -0.92370597]],
[-0.48957563, -0.13971266],
[-0.28912471, 0.45581023],
[-0.40029529, 0.6192317],
[-0.67334168, 0.05138455],
[-0.60379825, 0.32852299],
[-0.81640853, -0.21007217],
[-0.62409401, 0.48841025],
[-0.31243151, 0.63924519],
[0., 0.]
 [-0.59047266, -0.28446078]],
[[0.10089704, 0.14474812],
[0.30134796, 0.74027101],
[ 0.19017737, 0.90369248],
[-0.08286902, 0.33584533],
[-0.01332558, 0.61298376],
[-0.22593587, 0.07438861],
```

[-0.03362134, 0.77287102],

```
Out[139... array([[[0.00000000e+00, 0.00000000e+00],
                   [4.01805718e-02, 3.54647514e-01],
                   [7.97097787e-03, 5.75996537e-01],
                   [3.37699618e-02, 3.65181453e-02],
                   [1.30468069e-02, 2.19244619e-01],
                   [1.06819747e-01, 4.95046037e-03],
                   [1.80951937e-02, 3.94538384e-01],
                   [3.13800380e-02, 6.06775328e-01],
                   [2.39684296e-01, 1.95196274e-02],
                   [1.01802118e-02, 2.09520180e-02]],
                  [4.01805718e-02, 3.54647514e-01],
                   [0.00000000e+00, 0.00000000e+00],
                   [1.23588997e-02, 2.67065754e-02],
                   [1.47622682e-01, 1.63560128e-01],
                   [9.90194376e-02, 1.62020431e-02],
                   [2.78028233e-01, 4.43399370e-01],
                   [1.12204431e-01, 1.06276091e-03],
                   [5.43207155e-04, 3.36483831e-02],
                   [8.35930961e-02, 2.07762967e-01],
                   [9.08105912e-02, 5.48001169e-01]],
```

```
[[7.97097787e-03, 5.75996537e-01],
[1.23588997e-02, 2.67065754e-02],
[0.00000000e+00, 0.00000000e+00],
[7.45543283e-02, 3.22450378e-01],
[4.14134519e-02, 8.45115552e-02],
[1.73150226e-01, 6.87744901e-01],
[5.00858626e-02, 1.71142522e-02],
[7.72004441e-03, 4.00539795e-04],
[1.60236323e-01, 3.83447895e-01],
[3.61674316e-02, 8.16660092e-01]],
[[3.37699618e-02, 3.65181453e-02],
[1.47622682e-01, 1.63560128e-01],
[7.45543283e-02, 3.22450378e-01],
[0.00000000e+00, 0.00000000e+00],
[4.83628892e-03, 7.68057099e-02],
[2.04681243e-02, 6.83596176e-02],
```

[2.42533348e-03, 1.90991455e-01], [1.30256150e-01, 3.45580124e-01], [4.53389018e-01, 2.64037240e-03],

```
[6.86727383e-03, 1.12792088e-01]],
[[1.30468069e-02, 2.19244619e-01],
[9.90194376e-02, 1.62020431e-02],
[4.14134519e-02, 8.45115552e-02],
[4.83628892e-03, 7.68057099e-02],
[0.00000000e+00, 0.00000000e+00],
[4.52031330e-02, 2.90084739e-01],
[4.11917752e-04, 2.55639360e-02],
[8.48945751e-02, 9.65482870e-02],
[3.64572324e-01, 1.07927352e-01],
[1.77571194e-04, 3.75749095e-01]],
[[1.06819747e-01, 4.95046037e-03],
[2.78028233e-01, 4.43399370e-01],
[1.73150226e-01, 6.87744901e-01],
[2.04681243e-02, 6.83596176e-02],
[4.52031330e-02, 2.90084739e-01],
[0.00000000e+00, 0.0000000e+00],
[3.69848774e-02, 4.87877682e-01],
```

[2.53992837e-01, 7.21339970e-01],

```
[6.66522892e-01, 4.41303158e-02],
[5.10470167e-02, 5.53366546e-03]],
[[1.80951937e-02, 3.94538384e-01],
[1.12204431e-01, 1.06276091e-03],
[5.00858626e-02, 1.71142522e-02],
[2.42533348e-03, 1.90991455e-01],
[4.11917752e-04, 2.55639360e-02],
[3.69848774e-02, 4.87877682e-01],
[0.00000000e+00, 0.00000000e+00],
[9.71335098e-02, 2.27511797e-02],
[3.89493327e-01, 2.38544568e-01],
[1.13039458e-03, 5.97329621e-01]],
[[3.13800380e-02, 6.06775328e-01],
[5.43207155e-04, 3.36483831e-02],
[7.72004441e-03, 4.00539795e-04],
[1.30256150e-01, 3.45580124e-01],
[8.48945751e-02, 9.65482870e-02],
```

[2.53992837e-01, 7.21339970e-01], [9.71335098e-02, 2.27511797e-02],

```
[0.00000000e+00, 0.00000000e+00],
[9.76134495e-02, 4.08634410e-01],
[7.73068823e-02, 8.53232713e-01]],
[[2.39684296e-01, 1.95196274e-02],
[8.35930961e-02, 2.07762967e-01],
[1.60236323e-01, 3.83447895e-01],
[4.53389018e-01, 2.64037240e-03],
[3.64572324e-01, 1.07927352e-01],
[6.66522892e-01, 4.41303158e-02],
[3.89493327e-01, 2.38544568e-01],
[9.76134495e-02, 4.08634410e-01],
[0.00000000e+00, 0.00000000e+00],
[3.48657967e-01, 8.09179349e-02]],
[[1.01802118e-02, 2.09520180e-02],
[9.08105912e-02, 5.48001169e-01],
[3.61674316e-02, 8.16660092e-01],
[6.86727383e-03, 1.12792088e-01],
[1.77571194e-04, 3.75749095e-01],
```

[5.10470167e-02, 5.53366546e-03],

```
[7.73068823e-02, 8.53232713e-01],
[3.48657967e-01, 8.09179349e-02],
[0.00000000e+00, 0.00000000e+00]]])

In [140... # sum the coordinate differences to get the squared distance dist_sq = sq_differences.sum(-1) dist_sq.shape

Out[140... (10, 10)

In [141... dist_sq
```

[1.13039458e-03, 5.97329621e-01],

```
Out[141... array([[0. , 0.39482809, 0.58396752, 0.07028811, 0.232
          29143.
                  0.11177021, 0.41263358, 0.63815537, 0.25920392, 0.031
          13223],
                 [0.39482809, 0. , 0.03906548, 0.31118281, 0.115
          22148,
                  0.7214276 , 0.11326719 , 0.03419159 , 0.29135606 , 0.638
          81176],
                 [0.58396752, 0.03906548, 0. , 0.39700471, 0.125
          92501,
                  0.86089513, 0.06720011, 0.00812058, 0.54368422, 0.852
          82752],
                 [0.07028811, 0.31118281, 0.39700471, 0. , 0.081
          642,
                  0.08882774, 0.19341679, 0.47583627, 0.45602939, 0.119
          65936],
                 [0.23229143, 0.11522148, 0.12592501, 0.081642 , 0.
          ,
                  0.33528787, 0.02597585, 0.18144286, 0.47249968, 0.375
          926671,
                 [0.11177021, 0.7214276 , 0.86089513, 0.08882774, 0.335
```

```
28787,
                 , 0.52486256, 0.97533281, 0.71065321, 0.056
       0.
58068],
       [0.41263358, 0.11326719, 0.06720011, 0.19341679, 0.025
97585,
       0.52486256, 0.
                             , 0.11988469, 0.62803789, 0.598
46002],
       [0.63815537, 0.03419159, 0.00812058, 0.47583627, 0.181
44286,
       0.97533281, 0.11988469, 0. , 0.50624786, 0.930
5396 ],
       [0.25920392, 0.29135606, 0.54368422, 0.45602939, 0.472
49968.
       0.71065321, 0.62803789, 0.50624786, 0. , 0.429
5759 1,
       [0.03113223, 0.63881176, 0.85282752, 0.11965936, 0.375
92667,
       0.05658068, 0.59846002, 0.9305396, 0.4295759, 0.
]])
```

As a quick check of our logic, we should see that the diagonal of this matrix (i.e., the set of distances between each point and itself) is all zeros:

```
In [143... dist_sq.diagonal()
Out[143... array([0., 0., 0., 0., 0., 0., 0., 0., 0.])
```

With the **pairwise square distances** converted, we can now use **np.argsort** to sort **along each row.**

The **leftmost columns** will then give the **indices of the nearest neighbors**:

```
In [145... nearest = np.argsort(dist_sq, axis=1)
    print(nearest)
```

```
[[0 9 3 5 4 8 1 6 2 7]
[1 7 2 6 4 8 3 0 9 5]
[2 7 1 6 4 3 8 0 9 5]
[3 0 4 5 9 6 1 2 8 7]
[4 6 3 1 2 7 0 5 9 8]
[5 9 3 0 4 6 8 1 2 7]
[6 4 2 1 7 3 0 5 9 8]
[7 2 1 6 4 3 8 0 9 5]
[8 0 1 9 3 4 7 2 6 5]
[9 0 5 3 4 8 6 1 2 7]
```

Notice that the **first column** gives the **numbers 0 through 9 in order:**

This is due to the fact that each point's closest neighbor is itself.

By using a **full sort** here, we've actually done **more work than we need to in this case.**

If we're simply interested in the **nearest \$k\$ neighbors:**

All we need to do is **partition each row** so that the **smallest** *K*+**1 squared distances come first,** with larger distances filling the remaining positions of the array.

We can do this with the **np.argpartition** function:

```
In [147... K = 2
    nearest_partition = np.argpartition(dist_sq, K + 1, axis=1)

In [148... nearest_partition.shape

Out[148... (10, 10)

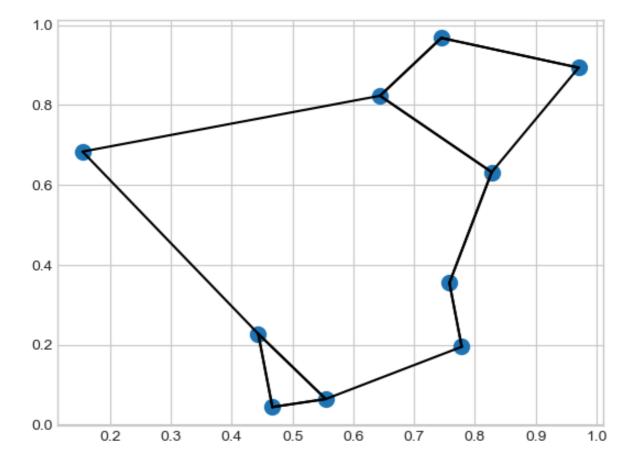
In [149... nearest_partition
```

In order to visualize this network of neighbors:

Let's quickly **plot the points** along with **lines** representing the **connections from each point to its two nearest neighbors:**

```
In [206... plt.scatter(X[:, 0], X[:, 1], s=100)
# draw lines from each point to its two nearest neighbors
K = 2
```

```
for i in range(X.shape[0]):
    for j in nearest_partition[i, :K+1]:
        # plot a line from X[i] to X[j]
        # use some zip magic to make it happen:
        plt.plot(*zip(X[j], X[i]), color='black')
```



Each **point** in the plot has **lines drawn to its two nearest neighbors.**

At first glance, it might seem strange that **some of the points have more than two lines** coming out of them:

This is due to the fact that if point A is one of the two nearest neighbors of point B.

This does not necessarily imply that point B is one of the two nearest neighbors of point A.

Although the **broadcasting and row-wise sorting** of this approach might seem **less straightforward** than **writing a loop**, it turns out to be a very **efficient** way of operating on this data in Python.

You might be tempted to do the same type of operation by manually looping through the data and sorting each set of

neighbors individually.

But this would almost certainly **lead to a slower algorithm** than the **vectorized version** we used.

The **beauty of this approach** is that it's written in a way that's **agnostic to the size of the input data:**

We could as easily compute the neighbors among **100 or 1,000,000 points** in any number of dimensions, and the **code would look the same.**

Finally, when doing **very large nearest neighbor searches**, there are tree-based and/or approximate algorithms that can scale better.