The Basics of NumPy Arrays

Data manipulation in Python is nearly synonymous with NumPy array manipulation: even newer tools like Pandas (Chapter 3) are built around the NumPy array. This section will present several examples using NumPy array manipulation to access data and subarrays, and to split, reshape, and join the arrays. While the types of operations shown here may seem a bit dry and pedantic, they comprise the building blocks of many other examples used throughout the book. Get to know them well!

We'll cover a few categories of basic array manipulations here:

Attributes of arrays
: Determining the size, shape, memory consumption, and data types of arrays

Indexing of arrays
: Getting and setting the value of individual array elements

Slicing of arrays
: Getting and setting smaller subarrays within a larger array

Reshaping of arrays
: Changing the shape of a given array

Joining and splitting of arrays
: Combining multiple arrays into one, and splitting one array into many

NumPy Array Attributes

First let's discuss some useful array attributes. We'll start by defining three random arrays: a one-dimensional, two-dimensional, and three-dimensional array. We'll use NumPy's random number generator, which we will *seed* with a set value in order to ensure that the same random arrays are generated each time this code is run:

```
In[1]: import numpy as np
       np.random.seed(0)  # seed for reproducibility

       x1 = np.random.randint(10, size=6)  # One-dimensional array
       x2 = np.random.randint(10, size=(3, 4))  # Two-dimensional array
       x3 = np.random.randint(10, size=(3, 4, 5))  # Three-dimensional array
```

Each array has attributes `ndim` (the number of dimensions), `shape` (the size of each dimension), and `size` (the total size of the array):

```
In[2]: print("x3 ndim: ", x3.ndim)
       print("x3 shape:", x3.shape)
       print("x3 size: ", x3.size)

x3 ndim:  3
x3 shape: (3, 4, 5)
x3 size:  60
```

Another useful attribute is the `dtype`, the data type of the array (which we discussed previously in "Understanding Data Types in Python" on page 34):

```
In[3]: print("dtype:", x3.dtype)
```

```
dtype: int64
```

Other attributes include `itemsize`, which lists the size (in bytes) of each array element, and `nbytes`, which lists the total size (in bytes) of the array:

```
In[4]: print("itemsize:", x3.itemsize, "bytes")
       print("nbytes:", x3.nbytes, "bytes")
```

```
itemsize: 8 bytes
nbytes: 480 bytes
```

In general, we expect that `nbytes` is equal to `itemsize` times `size`.

Array Indexing: Accessing Single Elements

If you are familiar with Python's standard list indexing, indexing in NumPy will feel quite familiar. In a one-dimensional array, you can access the i^{th} value (counting from zero) by specifying the desired index in square brackets, just as with Python lists:

```
In[5]: x1
```

```
Out[5]: array([5, 0, 3, 3, 7, 9])
```

```
In[6]: x1[0]
```

```
Out[6]: 5
```

```
In[7]: x1[4]
```

```
Out[7]: 7
```

To index from the end of the array, you can use negative indices:

```
In[8]: x1[-1]
```

```
Out[8]: 9
```

```
In[9]: x1[-2]
```

```
Out[9]: 7
```

In a multidimensional array, you access items using a comma-separated tuple of indices:

```
In[10]: x2
```

```
Out[10]: array([[3, 5, 2, 4],
                [7, 6, 8, 8],
                [1, 6, 7, 7]])
```

```
In[11]: x2[0, 0]
```

```
Out[11]: 3
```

```
In[12]: x2[2, 0]
```

```
Out[12]: 1
```

```
In[13]: x2[2, -1]
```

```
Out[13]: 7
```

You can also modify values using any of the above index notation:

```
In[14]: x2[0, 0] = 12
        x2
```

```
Out[14]: array([[12,  5,  2,  4],
                [ 7,  6,  8,  8],
                [ 1,  6,  7,  7]])
```

Keep in mind that, unlike Python lists, NumPy arrays have a fixed type. This means, for example, that if you attempt to insert a floating-point value to an integer array, the value will be silently truncated. Don't be caught unaware by this behavior!

```
In[15]: x1[0] = 3.14159  # this will be truncated!
        x1
```

```
Out[15]: array([3, 0, 3, 3, 7, 9])
```

Array Slicing: Accessing Subarrays

Just as we can use square brackets to access individual array elements, we can also use them to access subarrays with the *slice* notation, marked by the colon (`:`) character. The NumPy slicing syntax follows that of the standard Python list; to access a slice of an array `x`, use this:

```
x[start:stop:step]
```

If any of these are unspecified, they default to the values `start=0`, `stop=`*`size of dimension`*, `step=1`. We'll take a look at accessing subarrays in one dimension and in multiple dimensions.

One-dimensional subarrays

```
In[16]: x = np.arange(10)
        x
```

```
Out[16]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

```
In[17]: x[:5]  # first five elements
```

```
Out[17]: array([0, 1, 2, 3, 4])
```

```
In[18]: x[5:]  # elements after index 5
```

```
Out[18]: array([5, 6, 7, 8, 9])
```

```
In[19]: x[4:7]  # middle subarray
```

```
Out[19]: array([4, 5, 6])
```

```
In[20]: x[::2]  # every other element
```

```
Out[20]: array([0, 2, 4, 6, 8])
```

```
In[21]: x[1::2]  # every other element, starting at index 1
```

```
Out[21]: array([1, 3, 5, 7, 9])
```

A potentially confusing case is when the `step` value is negative. In this case, the defaults for `start` and `stop` are swapped. This becomes a convenient way to reverse an array:

```
In[22]: x[::-1]  # all elements, reversed
```

```
Out[22]: array([9, 8, 7, 6, 5, 4, 3, 2, 1, 0])
```

```
In[23]: x[5::-2]  # reversed every other from index 5
```

```
Out[23]: array([5, 3, 1])
```

Multidimensional subarrays

Multidimensional slices work in the same way, with multiple slices separated by commas. For example:

```
In[24]: x2
```

```
Out[24]: array([[12,  5,  2,  4],
                [ 7,  6,  8,  8],
                [ 1,  6,  7,  7]])
```

```
In[25]: x2[:2, :3]  # two rows, three columns
```

```
Out[25]: array([[12,  5,  2],
                [ 7,  6,  8]])
```

```
In[26]: x2[:3, ::2]  # all rows, every other column
```

```
Out[26]: array([[12,  2],
                [ 7,  8],
                [ 1,  7]])
```

Finally, subarray dimensions can even be reversed together:

```
In[27]: x2[::-1, ::-1]
```

```
Out[27]: array([[ 7,  7,  6,  1],
                [ 8,  8,  6,  7],
                [ 4,  2,  5, 12]])
```

Accessing array rows and columns. One commonly needed routine is accessing single rows or columns of an array. You can do this by combining indexing and slicing, using an empty slice marked by a single colon (`:`):

```
In[28]: print(x2[:, 0])  # first column of x2
```

```
[12  7  1]
```

```
In[29]: print(x2[0, :])  # first row of x2
```

```
[12  5  2  4]
```

In the case of row access, the empty slice can be omitted for a more compact syntax:

```
In[30]: print(x2[0])  # equivalent to x2[0, :]
```

```
[12  5  2  4]
```

Subarrays as no-copy views

One important—and extremely useful—thing to know about array slices is that they return *views* rather than *copies* of the array data. This is one area in which NumPy array slicing differs from Python list slicing: in lists, slices will be copies. Consider our two-dimensional array from before:

```
In[31]: print(x2)
```

```
[[12  5  2  4]
 [ 7  6  8  8]
 [ 1  6  7  7]]
```

Let's extract a 2×2 subarray from this:

```
In[32]: x2_sub = x2[:2, :2]
        print(x2_sub)
```

```
[[12  5]
 [ 7  6]]
```

Now if we modify this subarray, we'll see that the original array is changed! Observe:

```
In[33]: x2_sub[0, 0] = 99
        print(x2_sub)
```

```
[[99  5]
 [ 7  6]]
```

```
In[34]: print(x2)
```

```
[[99  5  2  4]
 [ 7  6  8  8]
 [ 1  6  7  7]]
```

This default behavior is actually quite useful: it means that when we work with large datasets, we can access and process pieces of these datasets without the need to copy the underlying data buffer.

Creating copies of arrays

Despite the nice features of array views, it is sometimes useful to instead explicitly copy the data within an array or a subarray. This can be most easily done with the `copy()` method:

```
In[35]: x2_sub_copy = x2[:2, :2].copy()
        print(x2_sub_copy)

[[99  5]
 [ 7  6]]
```

If we now modify this subarray, the original array is not touched:

```
In[36]: x2_sub_copy[0, 0] = 42
        print(x2_sub_copy)

[[42  5]
 [ 7  6]]

In[37]: print(x2)

[[99  5  2  4]
 [ 7  6  8  8]
 [ 1  6  7  7]]
```

Reshaping of Arrays

Another useful type of operation is reshaping of arrays. The most flexible way of doing this is with the `reshape()` method. For example, if you want to put the numbers 1 through 9 in a 3×3 grid, you can do the following:

```
In[38]: grid = np.arange(1, 10).reshape((3, 3))
        print(grid)

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

Note that for this to work, the size of the initial array must match the size of the reshaped array. Where possible, the `reshape` method will use a no-copy view of the initial array, but with noncontiguous memory buffers this is not always the case.

Another common reshaping pattern is the conversion of a one-dimensional array into a two-dimensional row or column matrix. You can do this with the `reshape` method, or more easily by making use of the `newaxis` keyword within a slice operation:

```
In[39]: x = np.array([1, 2, 3])

        # row vector via reshape
        x.reshape((1, 3))

Out[39]: array([[1, 2, 3]])

In[40]: # row vector via newaxis
        x[np.newaxis, :]

Out[40]: array([[1, 2, 3]])
```

```
In[41]: # column vector via reshape
        x.reshape((3, 1))

Out[41]: array([[1],
                [2],
                [3]])

In[42]: # column vector via newaxis
        x[:, np.newaxis]

Out[42]: array([[1],
                [2],
                [3]])
```

We will see this type of transformation often throughout the remainder of the book.

Array Concatenation and Splitting

All of the preceding routines worked on single arrays. It's also possible to combine multiple arrays into one, and to conversely split a single array into multiple arrays. We'll take a look at those operations here.

Concatenation of arrays

Concatenation, or joining of two arrays in NumPy, is primarily accomplished through the routines `np.concatenate`, `np.vstack`, and `np.hstack`. `np.concatenate` takes a tuple or list of arrays as its first argument, as we can see here:

```
In[43]: x = np.array([1, 2, 3])
        y = np.array([3, 2, 1])
        np.concatenate([x, y])

Out[43]: array([1, 2, 3, 3, 2, 1])
```

You can also concatenate more than two arrays at once:

```
In[44]: z = [99, 99, 99]
        print(np.concatenate([x, y, z]))

[ 1  2  3  3  2  1 99 99 99]
```

`np.concatenate` can also be used for two-dimensional arrays:

```
In[45]: grid = np.array([[1, 2, 3],
                         [4, 5, 6]])

In[46]: # concatenate along the first axis
        np.concatenate([grid, grid])

Out[46]: array([[1, 2, 3],
                [4, 5, 6],
                [1, 2, 3],
                [4, 5, 6]])

In[47]: # concatenate along the second axis (zero-indexed)
        np.concatenate([grid, grid], axis=1)
```

```
Out[47]: array([[1, 2, 3, 1, 2, 3],
                [4, 5, 6, 4, 5, 6]])
```

For working with arrays of mixed dimensions, it can be clearer to use the `np.vstack` (vertical stack) and `np.hstack` (horizontal stack) functions:

```
In[48]: x = np.array([1, 2, 3])
        grid = np.array([[9, 8, 7],
                         [6, 5, 4]])

        # vertically stack the arrays
        np.vstack([x, grid])

Out[48]: array([[1, 2, 3],
                [9, 8, 7],
                [6, 5, 4]])

In[49]: # horizontally stack the arrays
        y = np.array([[99],
                      [99]])
        np.hstack([grid, y])

Out[49]: array([[ 9,  8,  7, 99],
                [ 6,  5,  4, 99]])
```

Similarly, `np.dstack` will stack arrays along the third axis.

Splitting of arrays

The opposite of concatenation is splitting, which is implemented by the functions `np.split`, `np.hsplit`, and `np.vsplit`. For each of these, we can pass a list of indices giving the split points:

```
In[50]: x = [1, 2, 3, 99, 99, 3, 2, 1]
        x1, x2, x3 = np.split(x, [3, 5])
        print(x1, x2, x3)

[1 2 3] [99 99] [3 2 1]
```

Notice that *N* split points lead to *N + 1* subarrays. The related functions `np.hsplit` and `np.vsplit` are similar:

```
In[51]: grid = np.arange(16).reshape((4, 4))
        grid

Out[51]: array([[ 0,  1,  2,  3],
                [ 4,  5,  6,  7],
                [ 8,  9, 10, 11],
                [12, 13, 14, 15]])

In[52]: upper, lower = np.vsplit(grid, [2])
        print(upper)
        print(lower)

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

```
[[ 8  9 10 11]
 [12 13 14 15]]
```

```
In[53]: left, right = np.hsplit(grid, [2])
        print(left)
        print(right)
```

```
[[ 0  1]
 [ 4  5]
 [ 8  9]
 [12 13]]
[[ 2  3]
 [ 6  7]
 [10 11]
 [14 15]]
```

Similarly, `np.dsplit` will split arrays along the third axis.

Computation on NumPy Arrays: Universal Functions

Up until now, we have been discussing some of the basic nuts and bolts of NumPy; in the next few sections, we will dive into the reasons that NumPy is so important in the Python data science world. Namely, it provides an easy and flexible interface to optimized computation with arrays of data.

Computation on NumPy arrays can be very fast, or it can be very slow. The key to making it fast is to use *vectorized* operations, generally implemented through NumPy's *universal functions* (ufuncs). This section motivates the need for NumPy's ufuncs, which can be used to make repeated calculations on array elements much more efficient. It then introduces many of the most common and useful arithmetic ufuncs available in the NumPy package.

The Slowness of Loops

Python's default implementation (known as CPython) does some operations very slowly. This is in part due to the dynamic, interpreted nature of the language: the fact that types are flexible, so that sequences of operations cannot be compiled down to efficient machine code as in languages like C and Fortran. Recently there have been various attempts to address this weakness: well-known examples are the PyPy project, a just-in-time compiled implementation of Python; the Cython project, which converts Python code to compilable C code; and the Numba project, which converts snippets of Python code to fast LLVM bytecode. Each of these has its strengths and weaknesses, but it is safe to say that none of the three approaches has yet surpassed the reach and popularity of the standard CPython engine.

The relative sluggishness of Python generally manifests itself in situations where many small operations are being repeated—for instance, looping over arrays to oper-