NumPy Basics: Arrays and Vectorized Computation

NumPy, short for Numerical Python, is one of the most important foundational packages for numerical computing in Python. Most computational packages providing scientific functionality use NumPy's array objects as the *lingua franca* for data exchange.

Here are some of the things you'll find in NumPy:

- ndarray, an efficient multidimensional array providing fast array-oriented arithmetic operations and flexible *broadcasting* capabilities.
- Mathematical functions for fast operations on entire arrays of data without having to write loops.
- Tools for reading/writing array data to disk and working with memory-mapped files.
- Linear algebra, random number generation, and Fourier transform capabilities.
- A C API for connecting NumPy with libraries written in C, C++, or FORTRAN.

Because NumPy provides an easy-to-use C API, it is straightforward to pass data to external libraries written in a low-level language and also for external libraries to return data to Python as NumPy arrays. This feature has made Python a language of choice for wrapping legacy C/C++/Fortran codebases and giving them a dynamic and easy-to-use interface.

While NumPy by itself does not provide modeling or scientific functionality, having an understanding of NumPy arrays and array-oriented computing will help you use tools with array-oriented semantics, like pandas, much more effectively. Since

NumPy is a large topic, I will cover many advanced NumPy features like broadcasting in more depth later (see Appendix A).

For most data analysis applications, the main areas of functionality I'll focus on are:

- Fast vectorized array operations for data munging and cleaning, subsetting and filtering, transformation, and any other kinds of computations
- Common array algorithms like sorting, unique, and set operations
- Efficient descriptive statistics and aggregating/summarizing data
- Data alignment and relational data manipulations for merging and joining together heterogeneous datasets
- Expressing conditional logic as array expressions instead of loops with `if-elif-else` branches
- Group-wise data manipulations (aggregation, transformation, function application)

While NumPy provides a computational foundation for general numerical data processing, many readers will want to use pandas as the basis for most kinds of statistics or analytics, especially on tabular data. pandas also provides some more domain-specific functionality like time series manipulation, which is not present in NumPy.

Array-oriented computing in Python traces its roots back to 1995, when Jim Hugunin created the Numeric library. Over the next 10 years, many scientific programming communities began doing array programming in Python, but the library ecosystem had become fragmented in the early 2000s. In 2005, Travis Oliphant was able to forge the NumPy project from the then Numeric and Numarray projects to bring the community together around a single array computing framework.

One of the reasons NumPy is so important for numerical computations in Python is because it is designed for efficiency on large arrays of data. There are a number of reasons for this:

- NumPy internally stores data in a contiguous block of memory, independent of other built-in Python objects. NumPy's library of algorithms written in the C language can operate on this memory without any type checking or other overhead. NumPy arrays also use much less memory than built-in Python sequences.
- NumPy operations perform complex computations on entire arrays without the need for Python `for` loops.

To give you an idea of the performance difference, consider a NumPy array of one million integers, and the equivalent Python list:

```
In [7]: import numpy as np

In [8]: my_arr = np.arange(1000000)

In [9]: my_list = list(range(1000000))
```

Now let's multiply each sequence by 2:

```
In [10]: %time for _ in range(10): my_arr2 = my_arr * 2
CPU times: user 20 ms, sys: 50 ms, total: 70 ms
Wall time: 72.4 ms

In [11]: %time for _ in range(10): my_list2 = [x * 2 for x in my_list]
CPU times: user 760 ms, sys: 290 ms, total: 1.05 s
Wall time: 1.05 s
```

NumPy-based algorithms are generally 10 to 100 times faster (or more) than their pure Python counterparts and use significantly less memory.

4.1 The NumPy ndarray: A Multidimensional Array Object

One of the key features of NumPy is its N-dimensional array object, or ndarray, which is a fast, flexible container for large datasets in Python. Arrays enable you to perform mathematical operations on whole blocks of data using similar syntax to the equivalent operations between scalar elements.

To give you a flavor of how NumPy enables batch computations with similar syntax to scalar values on built-in Python objects, I first import NumPy and generate a small array of random data:

```
In [12]: import numpy as np

# Generate some random data
In [13]: data = np.random.randn(2, 3)

In [14]: data
Out[14]:
array([[-0.2047,  0.4789, -0.5194],
       [-0.5557,  1.9658,  1.3934]])
```

I then write mathematical operations with `data`:

```
In [15]: data * 10
Out[15]:
array([[ -2.0471,   4.7894,  -5.1944],
       [ -5.5573,  19.6578,  13.9341]])

In [16]: data + data
Out[16]:
```

```
array([[-0.4094,  0.9579, -1.0389],
       [-1.1115,  3.9316,  2.7868]])
```

In the first example, all of the elements have been multiplied by 10. In the second, the corresponding values in each "cell" in the array have been added to each other.

> In this chapter and throughout the book, I use the standard NumPy convention of always using `import numpy as np`. You are, of course, welcome to put `from numpy import *` in your code to avoid having to write `np.`, but I advise against making a habit of this. The `numpy` namespace is large and contains a number of functions whose names conflict with built-in Python functions (like `min` and `max`).

An ndarray is a generic multidimensional container for homogeneous data; that is, all of the elements must be the same type. Every array has a `shape`, a tuple indicating the size of each dimension, and a `dtype`, an object describing the *data type* of the array:

```
In [17]: data.shape
Out[17]: (2, 3)

In [18]: data.dtype
Out[18]: dtype('float64')
```

This chapter will introduce you to the basics of using NumPy arrays, and should be sufficient for following along with the rest of the book. While it's not necessary to have a deep understanding of NumPy for many data analytical applications, becoming proficient in array-oriented programming and thinking is a key step along the way to becoming a scientific Python guru.

> Whenever you see "array," "NumPy array," or "ndarray" in the text, with few exceptions they all refer to the same thing: the ndarray object.

Creating ndarrays

The easiest way to create an array is to use the `array` function. This accepts any sequence-like object (including other arrays) and produces a new NumPy array containing the passed data. For example, a list is a good candidate for conversion:

```
In [19]: data1 = [6, 7.5, 8, 0, 1]

In [20]: arr1 = np.array(data1)

In [21]: arr1
Out[21]: array([ 6. ,  7.5,  8. ,  0. ,  1. ])
```

Nested sequences, like a list of equal-length lists, will be converted into a multidimensional array:

```
In [22]: data2 = [[1, 2, 3, 4], [5, 6, 7, 8]]

In [23]: arr2 = np.array(data2)

In [24]: arr2
Out[24]:
array([[1, 2, 3, 4],
       [5, 6, 7, 8]])
```

Since `data2` was a list of lists, the NumPy array `arr2` has two dimensions with shape inferred from the data. We can confirm this by inspecting the `ndim` and `shape` attributes:

```
In [25]: arr2.ndim
Out[25]: 2

In [26]: arr2.shape
Out[26]: (2, 4)
```

Unless explicitly specified (more on this later), `np.array` tries to infer a good data type for the array that it creates. The data type is stored in a special `dtype` metadata object; for example, in the previous two examples we have:

```
In [27]: arr1.dtype
Out[27]: dtype('float64')

In [28]: arr2.dtype
Out[28]: dtype('int64')
```

In addition to `np.array`, there are a number of other functions for creating new arrays. As examples, `zeros` and `ones` create arrays of 0s or 1s, respectively, with a given length or shape. `empty` creates an array without initializing its values to any particular value. To create a higher dimensional array with these methods, pass a tuple for the shape:

```
In [29]: np.zeros(10)
Out[29]: array([ 0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.])

In [30]: np.zeros((3, 6))
Out[30]:
array([[ 0.,  0.,  0.,  0.,  0.,  0.],
       [ 0.,  0.,  0.,  0.,  0.,  0.],
       [ 0.,  0.,  0.,  0.,  0.,  0.]])

In [31]: np.empty((2, 3, 2))
Out[31]:
array([[[ 0.,  0.],
        [ 0.,  0.],
        [ 0.,  0.]],
```

```
       [[ 0.,  0.],
        [ 0.,  0.],
        [ 0.,  0.]]])
```

It's not safe to assume that `np.empty` will return an array of all zeros. In some cases, it may return uninitialized "garbage" values.

`arange` is an array-valued version of the built-in Python `range` function:

```
In [32]: np.arange(15)
Out[32]: array([ 0,  1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11, 12, 13, 14])
```

See Table 4-1 for a short list of standard array creation functions. Since NumPy is focused on numerical computing, the data type, if not specified, will in many cases be `float64` (floating point).

Table 4-1. Array creation functions

Function	Description
`array`	Convert input data (list, tuple, array, or other sequence type) to an ndarray either by inferring a dtype or explicitly specifying a dtype; copies the input data by default
`asarray`	Convert input to ndarray, but do not copy if the input is already an ndarray
`arange`	Like the built-in `range` but returns an ndarray instead of a list
`ones,` `ones_like`	Produce an array of all 1s with the given shape and dtype; `ones_like` takes another array and produces a ones array of the same shape and dtype
`zeros,` `zeros_like`	Like `ones` and `ones_like` but producing arrays of 0s instead
`empty,` `empty_like`	Create new arrays by allocating new memory, but do not populate with any values like `ones` and `zeros`
`full,` `full_like`	Produce an array of the given shape and dtype with all values set to the indicated "fill value" `full_like` takes another array and produces a filled array of the same shape and dtype
`eye, identity`	Create a square N × N identity matrix (1s on the diagonal and 0s elsewhere)

Data Types for ndarrays

The *data type* or `dtype` is a special object containing the information (or *metadata*, data about data) the ndarray needs to interpret a chunk of memory as a particular type of data:

```
In [33]: arr1 = np.array([1, 2, 3], dtype=np.float64)

In [34]: arr2 = np.array([1, 2, 3], dtype=np.int32)

In [35]: arr1.dtype
Out[35]: dtype('float64')
```

```
In [36]: arr2.dtype
Out[36]: dtype('int32')
```

dtypes are a source of NumPy's flexibility for interacting with data coming from other systems. In most cases they provide a mapping directly onto an underlying disk or memory representation, which makes it easy to read and write binary streams of data to disk and also to connect to code written in a low-level language like C or Fortran. The numerical dtypes are named the same way: a type name, like `float` or `int`, followed by a number indicating the number of bits per element. A standard double-precision floating-point value (what's used under the hood in Python's `float` object) takes up 8 bytes or 64 bits. Thus, this type is known in NumPy as `float64`. See Table 4-2 for a full listing of NumPy's supported data types.

> Don't worry about memorizing the NumPy dtypes, especially if you're a new user. It's often only necessary to care about the general *kind* of data you're dealing with, whether floating point, complex, integer, boolean, string, or general Python object. When you need more control over how data are stored in memory and on disk, especially large datasets, it is good to know that you have control over the storage type.

Table 4-2. NumPy data types

Type	Type code	Description
int8, uint8	i1, u1	Signed and unsigned 8-bit (1 byte) integer types
int16, uint16	i2, u2	Signed and unsigned 16-bit integer types
int32, uint32	i4, u4	Signed and unsigned 32-bit integer types
int64, uint64	i8, u8	Signed and unsigned 64-bit integer types
float16	f2	Half-precision floating point
float32	f4 or f	Standard single-precision floating point; compatible with C float
float64	f8 or d	Standard double-precision floating point; compatible with C double and Python `float` object
float128	f16 or g	Extended-precision floating point
complex64, complex128, complex256	c8, c16, c32	Complex numbers represented by two 32, 64, or 128 floats, respectively
bool	?	Boolean type storing `True` and `False` values
object	0	Python object type; a value can be any Python object
string_	S	Fixed-length ASCII string type (1 byte per character); for example, to create a string dtype with length 10, use `'S10'`
unicode_	U	Fixed-length Unicode type (number of bytes platform specific); same specification semantics as `string_` (e.g., `'U10'`)

You can explicitly convert or *cast* an array from one dtype to another using ndarray's `astype` method:

```
In [37]: arr = np.array([1, 2, 3, 4, 5])

In [38]: arr.dtype
Out[38]: dtype('int64')

In [39]: float_arr = arr.astype(np.float64)

In [40]: float_arr.dtype
Out[40]: dtype('float64')
```

In this example, integers were cast to floating point. If I cast some floating-point numbers to be of integer dtype, the decimal part will be truncated:

```
In [41]: arr = np.array([3.7, -1.2, -2.6, 0.5, 12.9, 10.1])

In [42]: arr
Out[42]: array([  3.7,  -1.2,  -2.6,   0.5,  12.9,  10.1])

In [43]: arr.astype(np.int32)
Out[43]: array([ 3, -1, -2,  0, 12, 10], dtype=int32)
```

If you have an array of strings representing numbers, you can use `astype` to convert them to numeric form:

```
In [44]: numeric_strings = np.array(['1.25', '-9.6', '42'], dtype=np.string_)

In [45]: numeric_strings.astype(float)
Out[45]: array([  1.25,  -9.6 ,  42.  ])
```

> It's important to be cautious when using the `numpy.string_` type, as string data in NumPy is fixed size and may truncate input without warning. pandas has more intuitive out-of-the-box behavior on non-numeric data.

If casting were to fail for some reason (like a string that cannot be converted to `float64`), a `ValueError` will be raised. Here I was a bit lazy and wrote `float` instead of `np.float64`; NumPy aliases the Python types to its own equivalent data dtypes.

You can also use another array's dtype attribute:

```
In [46]: int_array = np.arange(10)

In [47]: calibers = np.array([.22, .270, .357, .380, .44, .50], dtype=np.float64)

In [48]: int_array.astype(calibers.dtype)
Out[48]: array([ 0.,  1.,  2.,  3.,  4.,  5.,  6.,  7.,  8.,  9.])
```

There are shorthand type code strings you can also use to refer to a dtype:

```
In [49]: empty_uint32 = np.empty(8, dtype='u4')

In [50]: empty_uint32
Out[50]:
array([         0, 1075314688,          0, 1075707904,          0,
       1075838976,          0, 1072693248], dtype=uint32)
```

Calling `astype` *always* creates a new array (a copy of the data), even if the new dtype is the same as the old dtype.

Arithmetic with NumPy Arrays

Arrays are important because they enable you to express batch operations on data without writing any `for` loops. NumPy users call this *vectorization*. Any arithmetic operations between equal-size arrays applies the operation element-wise:

```
In [51]: arr = np.array([[1., 2., 3.], [4., 5., 6.]])

In [52]: arr
Out[52]:
array([[ 1.,  2.,  3.],
       [ 4.,  5.,  6.]])

In [53]: arr * arr
Out[53]:
array([[  1.,   4.,   9.],
       [ 16.,  25.,  36.]])

In [54]: arr - arr
Out[54]:
array([[ 0.,  0.,  0.],
       [ 0.,  0.,  0.]])
```

Arithmetic operations with scalars propagate the scalar argument to each element in the array:

```
In [55]: 1 / arr
Out[55]:
array([[ 1.    ,  0.5   ,  0.3333],
       [ 0.25  ,  0.2   ,  0.1667]])

In [56]: arr ** 0.5
Out[56]:
array([[ 1.    ,  1.4142,  1.7321],
       [ 2.    ,  2.2361,  2.4495]])
```

Comparisons between arrays of the same size yield boolean arrays:

```
In [57]: arr2 = np.array([[0., 4., 1.], [7., 2., 12.]])

In [58]: arr2
Out[58]:
array([[  0.,   4.,   1.],
       [  7.,   2.,  12.]])

In [59]: arr2 > arr
Out[59]:
array([[False,  True, False],
       [ True, False,  True]], dtype=bool)
```

Operations between differently sized arrays is called *broadcasting* and will be discussed in more detail in Appendix A. Having a deep understanding of broadcasting is not necessary for most of this book.

Basic Indexing and Slicing

NumPy array indexing is a rich topic, as there are many ways you may want to select a subset of your data or individual elements. One-dimensional arrays are simple; on the surface they act similarly to Python lists:

```
In [60]: arr = np.arange(10)

In [61]: arr
Out[61]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])

In [62]: arr[5]
Out[62]: 5

In [63]: arr[5:8]
Out[63]: array([5, 6, 7])

In [64]: arr[5:8] = 12

In [65]: arr
Out[65]: array([ 0,  1,  2,  3,  4, 12, 12, 12,  8,  9])
```

As you can see, if you assign a scalar value to a slice, as in `arr[5:8] = 12`, the value is propagated (or *broadcasted* henceforth) to the entire selection. An important first distinction from Python's built-in lists is that array slices are *views* on the original array. This means that the data is not copied, and any modifications to the view will be reflected in the source array.

To give an example of this, I first create a slice of `arr`:

```
In [66]: arr_slice = arr[5:8]

In [67]: arr_slice
Out[67]: array([12, 12, 12])
```

Now, when I change values in `arr_slice`, the mutations are reflected in the original array `arr`:

```
In [68]: arr_slice[1] = 12345

In [69]: arr
Out[69]: array([    0,     1,     2,     3,     4,    12, 12345,    12,     8,
    9])
```

The "bare" slice `[:]` will assign to all values in an array:

```
In [70]: arr_slice[:] = 64

In [71]: arr
Out[71]: array([ 0,  1,  2,  3,  4, 64, 64, 64,  8,  9])
```

If you are new to NumPy, you might be surprised by this, especially if you have used other array programming languages that copy data more eagerly. As NumPy has been designed to be able to work with very large arrays, you could imagine performance and memory problems if NumPy insisted on always copying data.

If you want a copy of a slice of an ndarray instead of a view, you will need to explicitly copy the array—for example, `arr[5:8].copy()`.

With higher dimensional arrays, you have many more options. In a two-dimensional array, the elements at each index are no longer scalars but rather one-dimensional arrays:

```
In [72]: arr2d = np.array([[1, 2, 3], [4, 5, 6], [7, 8, 9]])

In [73]: arr2d[2]
Out[73]: array([7, 8, 9])
```

Thus, individual elements can be accessed recursively. But that is a bit too much work, so you can pass a comma-separated list of indices to select individual elements. So these are equivalent:

```
In [74]: arr2d[0][2]
Out[74]: 3

In [75]: arr2d[0, 2]
Out[75]: 3
```

See Figure 4-1 for an illustration of indexing on a two-dimensional array. I find it helpful to think of axis 0 as the "rows" of the array and axis 1 as the "columns."

Figure 4-1. Indexing elements in a NumPy array

In multidimensional arrays, if you omit later indices, the returned object will be a lower dimensional ndarray consisting of all the data along the higher dimensions. So in the 2 × 2 × 3 array `arr3d`:

```
In [76]: arr3d = np.array([[[1, 2, 3], [4, 5, 6]], [[7, 8, 9], [10, 11, 12]]])

In [77]: arr3d
Out[77]:
array([[[ 1,  2,  3],
        [ 4,  5,  6]],
       [[ 7,  8,  9],
        [10, 11, 12]]])
```

`arr3d[0]` is a 2 × 3 array:

```
In [78]: arr3d[0]
Out[78]:
array([[1, 2, 3],
       [4, 5, 6]])
```

Both scalar values and arrays can be assigned to `arr3d[0]`:

```
In [79]: old_values = arr3d[0].copy()

In [80]: arr3d[0] = 42

In [81]: arr3d
Out[81]:
array([[[42, 42, 42],
        [42, 42, 42]],
       [[ 7,  8,  9],
        [10, 11, 12]]])

In [82]: arr3d[0] = old_values
```

```
In [83]: arr3d
Out[83]:
array([[[ 1,  2,  3],
        [ 4,  5,  6]],
       [[ 7,  8,  9],
        [10, 11, 12]]])
```

Similarly, `arr3d[1, 0]` gives you all of the values whose indices start with `(1, 0)`, forming a 1-dimensional array:

```
In [84]: arr3d[1, 0]
Out[84]: array([7, 8, 9])
```

This expression is the same as though we had indexed in two steps:

```
In [85]: x = arr3d[1]

In [86]: x
Out[86]:
array([[ 7,  8,  9],
       [10, 11, 12]])

In [87]: x[0]
Out[87]: array([7, 8, 9])
```

Note that in all of these cases where subsections of the array have been selected, the returned arrays are views.

Indexing with slices

Like one-dimensional objects such as Python lists, ndarrays can be sliced with the familiar syntax:

```
In [88]: arr
Out[88]: array([ 0,  1,  2,  3,  4, 64, 64, 64,  8,  9])

In [89]: arr[1:6]
Out[89]: array([ 1,  2,  3,  4, 64])
```

Consider the two-dimensional array from before, `arr2d`. Slicing this array is a bit different:

```
In [90]: arr2d
Out[90]:
array([[1, 2, 3],
       [4, 5, 6],
       [7, 8, 9]])

In [91]: arr2d[:2]
Out[91]:
array([[1, 2, 3],
       [4, 5, 6]])
```

As you can see, it has sliced along axis 0, the first axis. A slice, therefore, selects a range of elements along an axis. It can be helpful to read the expression `arr2d[:2]` as "select the first two rows of `arr2d`."

You can pass multiple slices just like you can pass multiple indexes:

```
In [92]: arr2d[:2, 1:]
Out[92]:
array([[2, 3],
       [5, 6]])
```

When slicing like this, you always obtain array views of the same number of dimensions. By mixing integer indexes and slices, you get lower dimensional slices.

For example, I can select the second row but only the first two columns like so:

```
In [93]: arr2d[1, :2]
Out[93]: array([4, 5])
```

Similarly, I can select the third column but only the first two rows like so:

```
In [94]: arr2d[:2, 2]
Out[94]: array([3, 6])
```

See Figure 4-2 for an illustration. Note that a colon by itself means to take the entire axis, so you can slice only higher dimensional axes by doing:

```
In [95]: arr2d[:, :1]
Out[95]:
array([[1],
       [4],
       [7]])
```

Of course, assigning to a slice expression assigns to the whole selection:

```
In [96]: arr2d[:2, 1:] = 0

In [97]: arr2d
Out[97]:
array([[1, 0, 0],
       [4, 0, 0],
       [7, 8, 9]])
```
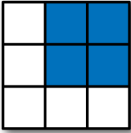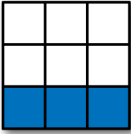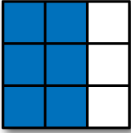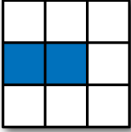
Expression	Shape
arr[:2, 1:]	(2, 2)
arr[2]	(3,)
arr[2, :]	(3,)
arr[2:, :]	(1, 3)
arr[:, :2]	(3, 2)
arr[1, :2]	(2,)
arr[1:2, :2]	(1, 2)

Figure 4-2. Two-dimensional array slicing

Boolean Indexing

Let's consider an example where we have some data in an array and an array of names with duplicates. I'm going to use here the randn function in numpy.random to generate some random normally distributed data:

```
In [98]: names = np.array(['Bob', 'Joe', 'Will', 'Bob', 'Will', 'Joe', 'Joe'])

In [99]: data = np.random.randn(7, 4)

In [100]: names
Out[100]:
array(['Bob', 'Joe', 'Will', 'Bob', 'Will', 'Joe', 'Joe'],
      dtype='<U4')

In [101]: data
Out[101]:
array([[ 0.0929,  0.2817,  0.769 ,  1.2464],
       [ 1.0072, -1.2962,  0.275 ,  0.2289],
       [ 1.3529,  0.8864, -2.0016, -0.3718],
       [ 1.669 , -0.4386, -0.5397,  0.477 ],
       [ 3.2489, -1.0212, -0.5771,  0.1241],
```

```
        [ 0.3026,  0.5238,  0.0009,  1.3438],
        [-0.7135, -0.8312, -2.3702, -1.8608]])
```

Suppose each name corresponds to a row in the `data` array and we wanted to select all the rows with corresponding name `'Bob'`. Like arithmetic operations, comparisons (such as ==) with arrays are also vectorized. Thus, comparing `names` with the string `'Bob'` yields a boolean array:

```
In [102]: names == 'Bob'
Out[102]: array([ True, False, False,  True, False, False, False], dtype=bool)
```

This boolean array can be passed when indexing the array:

```
In [103]: data[names == 'Bob']
Out[103]:
array([[ 0.0929,  0.2817,  0.769 ,  1.2464],
       [ 1.669 , -0.4386, -0.5397,  0.477 ]])
```

The boolean array must be of the same length as the array axis it's indexing. You can even mix and match boolean arrays with slices or integers (or sequences of integers; more on this later).

Boolean selection will not fail if the boolean array is not the correct length, so I recommend care when using this feature.

In these examples, I select from the rows where `names == 'Bob'` and index the columns, too:

```
In [104]: data[names == 'Bob', 2:]
Out[104]:
array([[ 0.769 ,  1.2464],
       [-0.5397,  0.477 ]])

In [105]: data[names == 'Bob', 3]
Out[105]: array([ 1.2464,  0.477 ])
```

To select everything but `'Bob'`, you can either use != or negate the condition using ~:

```
In [106]: names != 'Bob'
Out[106]: array([False,  True,  True, False,  True,  True,  True], dtype=bool)

In [107]: data[~(names == 'Bob')]
Out[107]:
array([[ 1.0072, -1.2962,  0.275 ,  0.2289],
       [ 1.3529,  0.8864, -2.0016, -0.3718],
       [ 3.2489, -1.0212, -0.5771,  0.1241],
       [ 0.3026,  0.5238,  0.0009,  1.3438],
       [-0.7135, -0.8312, -2.3702, -1.8608]])
```

The ~ operator can be useful when you want to invert a general condition:

```
In [108]: cond = names == 'Bob'

In [109]: data[~cond]
Out[109]:
array([[ 1.0072, -1.2962,  0.275 ,  0.2289],
       [ 1.3529,  0.8864, -2.0016, -0.3718],
       [ 3.2489, -1.0212, -0.5771,  0.1241],
       [ 0.3026,  0.5238,  0.0009,  1.3438],
       [-0.7135, -0.8312, -2.3702, -1.8608]])
```

Selecting two of the three names to combine multiple boolean conditions, use boolean arithmetic operators like & (and) and | (or):

```
In [110]: mask = (names == 'Bob') | (names == 'Will')

In [111]: mask
Out[111]: array([ True, False,  True,  True,  True, False, False], dtype=bool)

In [112]: data[mask]
Out[112]:
array([[ 0.0929,  0.2817,  0.769 ,  1.2464],
       [ 1.3529,  0.8864, -2.0016, -0.3718],
       [ 1.669 , -0.4386, -0.5397,  0.477 ],
       [ 3.2489, -1.0212, -0.5771,  0.1241]])
```

Selecting data from an array by boolean indexing *always* creates a copy of the data, even if the returned array is unchanged.

The Python keywords and and or do not work with boolean arrays.
Use & (and) and | (or) instead.

Setting values with boolean arrays works in a common-sense way. To set all of the negative values in data to 0 we need only do:

```
In [113]: data[data < 0] = 0

In [114]: data
Out[114]:
array([[ 0.0929,  0.2817,  0.769 ,  1.2464],
       [ 1.0072,  0.    ,  0.275 ,  0.2289],
       [ 1.3529,  0.8864,  0.    ,  0.    ],
       [ 1.669 ,  0.    ,  0.    ,  0.477 ],
       [ 3.2489,  0.    ,  0.    ,  0.1241],
       [ 0.3026,  0.5238,  0.0009,  1.3438],
       [ 0.    ,  0.    ,  0.    ,  0.    ]])
```

Setting whole rows or columns using a one-dimensional boolean array is also easy:

```
In [115]: data[names != 'Joe'] = 7
```

```
In [116]: data
Out[116]:
array([[ 7.    , 7.    , 7.    , 7.    ],
       [ 1.0072, 0.    , 0.275 , 0.2289],
       [ 7.    , 7.    , 7.    , 7.    ],
       [ 7.    , 7.    , 7.    , 7.    ],
       [ 7.    , 7.    , 7.    , 7.    ],
       [ 0.3026, 0.5238, 0.0009, 1.3438],
       [ 0.    , 0.    , 0.    , 0.    ]])
```

As we will see later, these types of operations on two-dimensional data are convenient to do with pandas.

Fancy Indexing

Fancy indexing is a term adopted by NumPy to describe indexing using integer arrays. Suppose we had an 8 × 4 array:

```
In [117]: arr = np.empty((8, 4))
```

```
In [118]: for i in range(8):
   .....:     arr[i] = i
```

```
In [119]: arr
Out[119]:
array([[ 0., 0., 0., 0.],
       [ 1., 1., 1., 1.],
       [ 2., 2., 2., 2.],
       [ 3., 3., 3., 3.],
       [ 4., 4., 4., 4.],
       [ 5., 5., 5., 5.],
       [ 6., 6., 6., 6.],
       [ 7., 7., 7., 7.]])
```

To select out a subset of the rows in a particular order, you can simply pass a list or ndarray of integers specifying the desired order:

```
In [120]: arr[[4, 3, 0, 6]]
Out[120]:
array([[ 4., 4., 4., 4.],
       [ 3., 3., 3., 3.],
       [ 0., 0., 0., 0.],
       [ 6., 6., 6., 6.]])
```

Hopefully this code did what you expected! Using negative indices selects rows from the end:

```
In [121]: arr[[-3, -5, -7]]
Out[121]:
```

```
array([[ 5.,  5.,  5.,  5.],
       [ 3.,  3.,  3.,  3.],
       [ 1.,  1.,  1.,  1.]])
```

Passing multiple index arrays does something slightly different; it selects a one-dimensional array of elements corresponding to each tuple of indices:

```
In [122]: arr = np.arange(32).reshape((8, 4))

In [123]: arr
Out[123]:
array([[ 0,  1,  2,  3],
       [ 4,  5,  6,  7],
       [ 8,  9, 10, 11],
       [12, 13, 14, 15],
       [16, 17, 18, 19],
       [20, 21, 22, 23],
       [24, 25, 26, 27],
       [28, 29, 30, 31]])

In [124]: arr[[1, 5, 7, 2], [0, 3, 1, 2]]
Out[124]: array([ 4, 23, 29, 10])
```

We'll look at the `reshape` method in more detail in Appendix A.

Here the elements `(1, 0)`, `(5, 3)`, `(7, 1)`, and `(2, 2)` were selected. Regardless of how many dimensions the array has (here, only 2), the result of fancy indexing is always one-dimensional.

The behavior of fancy indexing in this case is a bit different from what some users might have expected (myself included), which is the rectangular region formed by selecting a subset of the matrix's rows and columns. Here is one way to get that:

```
In [125]: arr[[1, 5, 7, 2]][:, [0, 3, 1, 2]]
Out[125]:
array([[ 4,  7,  5,  6],
       [20, 23, 21, 22],
       [28, 31, 29, 30],
       [ 8, 11,  9, 10]])
```

Keep in mind that fancy indexing, unlike slicing, always copies the data into a new array.

Transposing Arrays and Swapping Axes

Transposing is a special form of reshaping that similarly returns a view on the underlying data without copying anything. Arrays have the `transpose` method and also the special `T` attribute:

```
In [126]: arr = np.arange(15).reshape((3, 5))

In [127]: arr
```

```
Out[127]:
array([[ 0,  1,  2,  3,  4],
       [ 5,  6,  7,  8,  9],
       [10, 11, 12, 13, 14]])

In [128]: arr.T
Out[128]:
array([[ 0,  5, 10],
       [ 1,  6, 11],
       [ 2,  7, 12],
       [ 3,  8, 13],
       [ 4,  9, 14]])
```

When doing matrix computations, you may do this very often—for example, when computing the inner matrix product using `np.dot`:

```
In [129]: arr = np.random.randn(6, 3)

In [130]: arr
Out[130]:
array([[-0.8608,  0.5601, -1.2659],
       [ 0.1198, -1.0635,  0.3329],
       [-2.3594, -0.1995, -1.542 ],
       [-0.9707, -1.307 ,  0.2863],
       [ 0.378 , -0.7539,  0.3313],
       [ 1.3497,  0.0699,  0.2467]])

In [131]: np.dot(arr.T, arr)
Out[131]:
array([[ 9.2291,  0.9394,  4.948 ],
       [ 0.9394,  3.7662, -1.3622],
       [ 4.948 , -1.3622,  4.3437]])
```

For higher dimensional arrays, `transpose` will accept a tuple of axis numbers to permute the axes (for extra mind bending):

```
In [132]: arr = np.arange(16).reshape((2, 2, 4))

In [133]: arr
Out[133]:
array([[[ 0,  1,  2,  3],
        [ 4,  5,  6,  7]],
       [[ 8,  9, 10, 11],
        [12, 13, 14, 15]]])

In [134]: arr.transpose((1, 0, 2))
Out[134]:
array([[[ 0,  1,  2,  3],
        [ 8,  9, 10, 11]],
       [[ 4,  5,  6,  7],
        [12, 13, 14, 15]]])
```

Here, the axes have been reordered with the second axis first, the first axis second, and the last axis unchanged.

Simple transposing with `.T` is a special case of swapping axes. ndarray has the method `swapaxes`, which takes a pair of axis numbers and switches the indicated axes to rearrange the data:

```
In [135]: arr
Out[135]:
array([[[ 0,  1,  2,  3],
        [ 4,  5,  6,  7]],

       [[ 8,  9, 10, 11],
        [12, 13, 14, 15]]])

In [136]: arr.swapaxes(1, 2)
Out[136]:
array([[[ 0,  4],
        [ 1,  5],
        [ 2,  6],
        [ 3,  7]],

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

`swapaxes` similarly returns a view on the data without making a copy.

4.2 Universal Functions: Fast Element-Wise Array Functions

A universal function, or *ufunc*, is a function that performs element-wise operations on data in ndarrays. You can think of them as fast vectorized wrappers for simple functions that take one or more scalar values and produce one or more scalar results.

Many ufuncs are simple element-wise transformations, like `sqrt` or `exp`:

```
In [137]: arr = np.arange(10)

In [138]: arr
Out[138]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])

In [139]: np.sqrt(arr)
Out[139]:
array([ 0.    ,  1.    ,  1.4142,  1.7321,  2.    ,  2.2361,  2.4495,
        2.6458,  2.8284,  3.    ])

In [140]: np.exp(arr)
Out[140]:
array([    1.    ,     2.7183,     7.3891,    20.0855,    54.5982,
         148.4132,   403.4288,  1096.6332,  2980.958 ,  8103.0839])
```

These are referred to as *unary* ufuncs. Others, such as add or maximum, take two arrays (thus, *binary* ufuncs) and return a single array as the result:

```
In [141]: x = np.random.randn(8)

In [142]: y = np.random.randn(8)

In [143]: x
Out[143]:
array([-0.0119,  1.0048,  1.3272, -0.9193, -1.5491,  0.0222,  0.7584,
       -0.6605])

In [144]: y
Out[144]:
array([ 0.8626, -0.01  ,  0.05  ,  0.6702,  0.853 , -0.9559, -0.0235,
       -2.3042])

In [145]: np.maximum(x, y)
Out[145]:
array([ 0.8626,  1.0048,  1.3272,  0.6702,  0.853 ,  0.0222,  0.7584,
       -0.6605])
```

Here, numpy.maximum computed the element-wise maximum of the elements in x and y.

While not common, a ufunc can return multiple arrays. modf is one example, a vectorized version of the built-in Python divmod; it returns the fractional and integral parts of a floating-point array:

```
In [146]: arr = np.random.randn(7) * 5

In [147]: arr
Out[147]: array([-3.2623, -6.0915, -6.663 ,  5.3731,  3.6182,  3.45  ,  5.0077])

In [148]: remainder, whole_part = np.modf(arr)

In [149]: remainder
Out[149]: array([-0.2623, -0.0915, -0.663 ,  0.3731,  0.6182,  0.45  ,  0.0077])

In [150]: whole_part
Out[150]: array([-3., -6., -6.,  5.,  3.,  3.,  5.])
```

Ufuncs accept an optional out argument that allows them to operate in-place on arrays:

```
In [151]: arr
Out[151]: array([-3.2623, -6.0915, -6.663 ,  5.3731,  3.6182,  3.45  ,  5.0077])

In [152]: np.sqrt(arr)
Out[152]: array([   nan,    nan,    nan,  2.318 ,  1.9022,  1.8574,  2.2378])

In [153]: np.sqrt(arr, arr)
```

```
Out[153]: array([    nan,    nan,    nan, 2.318 , 1.9022, 1.8574, 2.2378])

In [154]: arr
Out[154]: array([    nan,    nan,    nan, 2.318 , 1.9022, 1.8574, 2.2378])
```

See Tables 4-3 and 4-4 for a listing of available ufuncs.

Table 4-3. Unary ufuncs

Function	Description
abs, fabs	Compute the absolute value element-wise for integer, floating-point, or complex values
sqrt	Compute the square root of each element (equivalent to `arr ** 0.5`)
square	Compute the square of each element (equivalent to `arr ** 2`)
exp	Compute the exponent e^x of each element
log, log10, log2, log1p	Natural logarithm (base e), log base 10, log base 2, and log(1 + x), respectively
sign	Compute the sign of each element: 1 (positive), 0 (zero), or −1 (negative)
ceil	Compute the ceiling of each element (i.e., the smallest integer greater than or equal to that number)
floor	Compute the floor of each element (i.e., the largest integer less than or equal to each element)
rint	Round elements to the nearest integer, preserving the `dtype`
modf	Return fractional and integral parts of array as a separate array
isnan	Return boolean array indicating whether each value is NaN (Not a Number)
isfinite, isinf	Return boolean array indicating whether each element is finite (non-`inf`, non-NaN) or infinite, respectively
cos, cosh, sin, sinh, tan, tanh	Regular and hyperbolic trigonometric functions
arccos, arccosh, arcsin, arcsinh, arctan, arctanh	Inverse trigonometric functions
logical_not	Compute truth value of `not x` element-wise (equivalent to `~arr`).

Table 4-4. Binary universal functions

Function	Description
add	Add corresponding elements in arrays
subtract	Subtract elements in second array from first array
multiply	Multiply array elements
divide, floor_divide	Divide or floor divide (truncating the remainder)
power	Raise elements in first array to powers indicated in second array
maximum, fmax	Element-wise maximum; `fmax` ignores NaN
minimum, fmin	Element-wise minimum; `fmin` ignores NaN
mod	Element-wise modulus (remainder of division)
copysign	Copy sign of values in second argument to values in first argument

Function	Description
`greater, greater_equal, less, less_equal, equal, not_equal`	Perform element-wise comparison, yielding boolean array (equivalent to infix operators `>`, `>=`, `<`, `<=`, `==`, `!=`)
`logical_and, logical_or, logical_xor`	Compute element-wise truth value of logical operation (equivalent to infix operators `&` `|`, `^`)

4.3 Array-Oriented Programming with Arrays

Using NumPy arrays enables you to express many kinds of data processing tasks as concise array expressions that might otherwise require writing loops. This practice of replacing explicit loops with array expressions is commonly referred to as *vectorization*. In general, vectorized array operations will often be one or two (or more) orders of magnitude faster than their pure Python equivalents, with the biggest impact in any kind of numerical computations. Later, in Appendix A, I explain *broadcasting*, a powerful method for vectorizing computations.

As a simple example, suppose we wished to evaluate the function `sqrt(x^2 + y^2)` across a regular grid of values. The `np.meshgrid` function takes two 1D arrays and produces two 2D matrices corresponding to all pairs of `(x, y)` in the two arrays:

```
In [155]: points = np.arange(-5, 5, 0.01) # 1000 equally spaced points

In [156]: xs, ys = np.meshgrid(points, points)

In [157]: ys
Out[157]:
array([[-5.  , -5.  , -5.  , ..., -5.  , -5.  , -5.  ],
       [-4.99, -4.99, -4.99, ..., -4.99, -4.99, -4.99],
       [-4.98, -4.98, -4.98, ..., -4.98, -4.98, -4.98],
       ...,
       [ 4.97,  4.97,  4.97, ...,  4.97,  4.97,  4.97],
       [ 4.98,  4.98,  4.98, ...,  4.98,  4.98,  4.98],
       [ 4.99,  4.99,  4.99, ...,  4.99,  4.99,  4.99]])
```

Now, evaluating the function is a matter of writing the same expression you would write with two points:

```
In [158]: z = np.sqrt(xs ** 2 + ys ** 2)

In [159]: z
Out[159]:
array([[ 7.0711,  7.064 ,  7.0569, ...,  7.0499,  7.0569,  7.064 ],
       [ 7.064 ,  7.0569,  7.0499, ...,  7.0428,  7.0499,  7.0569],
       [ 7.0569,  7.0499,  7.0428, ...,  7.0357,  7.0428,  7.0499],
       ...,
       [ 7.0499,  7.0428,  7.0357, ...,  7.0286,  7.0357,  7.0428],
       [ 7.0569,  7.0499,  7.0428, ...,  7.0357,  7.0428,  7.0499],
       [ 7.064 ,  7.0569,  7.0499, ...,  7.0428,  7.0499,  7.0569]])
```

As a preview of Chapter 9, I use matplotlib to create visualizations of this two-dimensional array:

```
In [160]: import matplotlib.pyplot as plt

In [161]: plt.imshow(z, cmap=plt.cm.gray); plt.colorbar()
Out[161]: <matplotlib.colorbar.Colorbar at 0x7f715e3fa630>

In [162]: plt.title("Image plot of $\sqrt{x^2 + y^2}$ for a grid of values")
Out[162]: <matplotlib.text.Text at 0x7f715d2de748>
```

See Figure 4-3. Here I used the matplotlib function `imshow` to create an image plot from a two-dimensional array of function values.
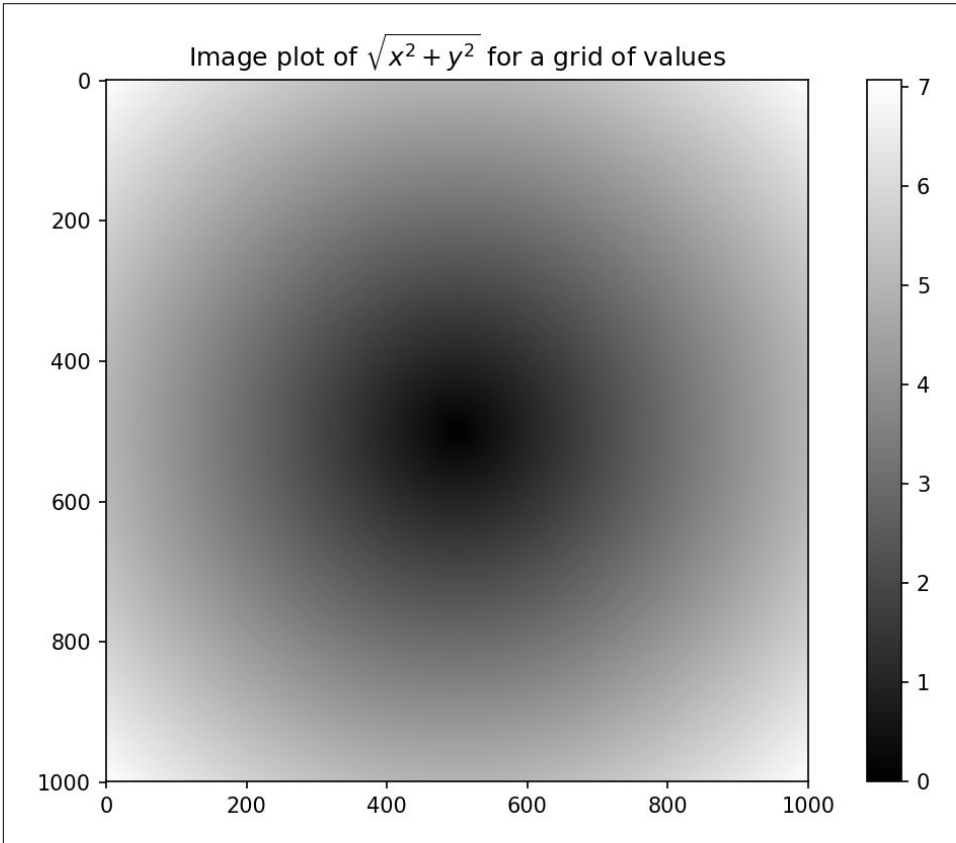

Figure 4-3. Plot of function evaluated on grid

Expressing Conditional Logic as Array Operations

The `numpy.where` function is a vectorized version of the ternary expression `x if condition else y`. Suppose we had a boolean array and two arrays of values:

```
In [165]: xarr = np.array([1.1, 1.2, 1.3, 1.4, 1.5])

In [166]: yarr = np.array([2.1, 2.2, 2.3, 2.4, 2.5])

In [167]: cond = np.array([True, False, True, True, False])
```

Suppose we wanted to take a value from `xarr` whenever the corresponding value in `cond` is `True`, and otherwise take the value from `yarr`. A list comprehension doing this might look like:

```
In [168]: result = [(x if c else y)
   .....:           for x, y, c in zip(xarr, yarr, cond)]

In [169]: result
Out[169]: [1.1000000000000001, 2.2000000000000002, 1.3, 1.3999999999999999, 2.5]
```

This has multiple problems. First, it will not be very fast for large arrays (because all the work is being done in interpreted Python code). Second, it will not work with multidimensional arrays. With `np.where` you can write this very concisely:

```
In [170]: result = np.where(cond, xarr, yarr)

In [171]: result
Out[171]: array([ 1.1,  2.2,  1.3,  1.4,  2.5])
```

The second and third arguments to `np.where` don't need to be arrays; one or both of them can be scalars. A typical use of `where` in data analysis is to produce a new array of values based on another array. Suppose you had a matrix of randomly generated data and you wanted to replace all positive values with 2 and all negative values with –2. This is very easy to do with `np.where`:

```
In [172]: arr = np.random.randn(4, 4)

In [173]: arr
Out[173]:
array([[-0.5031, -0.6223, -0.9212, -0.7262],
       [ 0.2229,  0.0513, -1.1577,  0.8167],
       [ 0.4336,  1.0107,  1.8249, -0.9975],
       [ 0.8506, -0.1316,  0.9124,  0.1882]])

In [174]: arr > 0
Out[174]:
array([[False, False, False, False],
       [ True,  True, False,  True],
       [ True,  True,  True, False],
       [ True, False,  True,  True]], dtype=bool)

In [175]: np.where(arr > 0, 2, -2)
Out[175]:
array([[-2, -2, -2, -2],
       [ 2,  2, -2,  2],
```

```
       [ 2,  2,  2, -2],
       [ 2, -2,  2,  2]])
```

You can combine scalars and arrays when using `np.where`. For example, I can replace all positive values in `arr` with the constant 2 like so:

```
In [176]: np.where(arr > 0, 2, arr) # set only positive values to 2
Out[176]:
array([[-0.5031, -0.6223, -0.9212, -0.7262],
       [ 2.    ,  2.    , -1.1577,  2.    ],
       [ 2.    ,  2.    ,  2.    , -0.9975],
       [ 2.    , -0.1316,  2.    ,  2.    ]])
```

The arrays passed to `np.where` can be more than just equal-sized arrays or scalars.

Mathematical and Statistical Methods

A set of mathematical functions that compute statistics about an entire array or about the data along an axis are accessible as methods of the array class. You can use aggregations (often called *reductions*) like `sum`, `mean`, and `std` (standard deviation) either by calling the array instance method or using the top-level NumPy function.

Here I generate some normally distributed random data and compute some aggregate statistics:

```
In [177]: arr = np.random.randn(5, 4)

In [178]: arr
Out[178]:
array([[ 2.1695, -0.1149,  2.0037,  0.0296],
       [ 0.7953,  0.1181, -0.7485,  0.585 ],
       [ 0.1527, -1.5657, -0.5625, -0.0327],
       [-0.929 , -0.4826, -0.0363,  1.0954],
       [ 0.9809, -0.5895,  1.5817, -0.5287]])

In [179]: arr.mean()
Out[179]: 0.19607051119998253

In [180]: np.mean(arr)
Out[180]: 0.19607051119998253

In [181]: arr.sum()
Out[181]: 3.9214102239996507
```

Functions like `mean` and `sum` take an optional `axis` argument that computes the statistic over the given axis, resulting in an array with one fewer dimension:

```
In [182]: arr.mean(axis=1)
Out[182]: array([ 1.022 ,  0.1875, -0.502 , -0.0881,  0.3611])

In [183]: arr.sum(axis=0)
Out[183]: array([ 3.1693, -2.6345,  2.2381,  1.1486])
```

Here, `arr.mean(1)` means "compute mean across the columns" where `arr.sum(0)` means "compute sum down the rows."

Other methods like `cumsum` and `cumprod` do not aggregate, instead producing an array of the intermediate results:

```
In [184]: arr = np.array([0, 1, 2, 3, 4, 5, 6, 7])

In [185]: arr.cumsum()
Out[185]: array([ 0,  1,  3,  6, 10, 15, 21, 28])
```

In multidimensional arrays, accumulation functions like `cumsum` return an array of the same size, but with the partial aggregates computed along the indicated axis according to each lower dimensional slice:

```
In [186]: arr = np.array([[0, 1, 2], [3, 4, 5], [6, 7, 8]])

In [187]: arr
Out[187]:
array([[0, 1, 2],
       [3, 4, 5],
       [6, 7, 8]])

In [188]: arr.cumsum(axis=0)
Out[188]:
array([[ 0,  1,  2],
       [ 3,  5,  7],
       [ 9, 12, 15]])

In [189]: arr.cumprod(axis=1)
Out[189]:
array([[  0,   0,   0],
       [  3,  12,  60],
       [  6,  42, 336]])
```

See Table 4-5 for a full listing. We'll see many examples of these methods in action in later chapters.

Table 4-5. Basic array statistical methods

Method	Description
sum	Sum of all the elements in the array or along an axis; zero-length arrays have sum 0
mean	Arithmetic mean; zero-length arrays have NaN mean
std, var	Standard deviation and variance, respectively, with optional degrees of freedom adjustment (default denominator n)
min, max	Minimum and maximum
argmin, argmax	Indices of minimum and maximum elements, respectively
cumsum	Cumulative sum of elements starting from 0
cumprod	Cumulative product of elements starting from 1

Methods for Boolean Arrays

Boolean values are coerced to 1 (`True`) and 0 (`False`) in the preceding methods. Thus, `sum` is often used as a means of counting `True` values in a boolean array:

```
In [190]: arr = np.random.randn(100)

In [191]: (arr > 0).sum() # Number of positive values
Out[191]: 42
```

There are two additional methods, `any` and `all`, useful especially for boolean arrays. `any` tests whether one or more values in an array is `True`, while `all` checks if every value is `True`:

```
In [192]: bools = np.array([False, False, True, False])

In [193]: bools.any()
Out[193]: True

In [194]: bools.all()
Out[194]: False
```

These methods also work with non-boolean arrays, where non-zero elements evaluate to `True`.

Sorting

Like Python's built-in list type, NumPy arrays can be sorted in-place with the `sort` method:

```
In [195]: arr = np.random.randn(6)

In [196]: arr
Out[196]: array([ 0.6095, -0.4938,  1.24  , -0.1357,  1.43  , -0.8469])

In [197]: arr.sort()

In [198]: arr
Out[198]: array([-0.8469, -0.4938, -0.1357,  0.6095,  1.24  ,  1.43  ])
```

You can sort each one-dimensional section of values in a multidimensional array in-place along an axis by passing the axis number to `sort`:

```
In [199]: arr = np.random.randn(5, 3)

In [200]: arr
Out[200]:
array([[ 0.6033,  1.2636, -0.2555],
       [-0.4457,  0.4684, -0.9616],
       [-1.8245,  0.6254,  1.0229],
       [ 1.1074,  0.0909, -0.3501],
       [ 0.218 , -0.8948, -1.7415]])
```

```
In [201]: arr.sort(1)

In [202]: arr
Out[202]:
array([[-0.2555,  0.6033,  1.2636],
       [-0.9616, -0.4457,  0.4684],
       [-1.8245,  0.6254,  1.0229],
       [-0.3501,  0.0909,  1.1074],
       [-1.7415, -0.8948,  0.218 ]])
```

The top-level method `np.sort` returns a sorted copy of an array instead of modifying the array in-place. A quick-and-dirty way to compute the quantiles of an array is to sort it and select the value at a particular rank:

```
In [203]: large_arr = np.random.randn(1000)

In [204]: large_arr.sort()

In [205]: large_arr[int(0.05 * len(large_arr))] # 5% quantile
Out[205]: -1.5311513550102103
```

For more details on using NumPy's sorting methods, and more advanced techniques like indirect sorts, see Appendix A. Several other kinds of data manipulations related to sorting (e.g., sorting a table of data by one or more columns) can also be found in pandas.

Unique and Other Set Logic

NumPy has some basic set operations for one-dimensional ndarrays. A commonly used one is `np.unique`, which returns the sorted unique values in an array:

```
In [206]: names = np.array(['Bob', 'Joe', 'Will', 'Bob', 'Will', 'Joe', 'Joe'])

In [207]: np.unique(names)
Out[207]:
array(['Bob', 'Joe', 'Will'],
      dtype='<U4')

In [208]: ints = np.array([3, 3, 3, 2, 2, 1, 1, 4, 4])

In [209]: np.unique(ints)
Out[209]: array([1, 2, 3, 4])
```

Contrast `np.unique` with the pure Python alternative:

```
In [210]: sorted(set(names))
Out[210]: ['Bob', 'Joe', 'Will']
```

Another function, `np.in1d`, tests membership of the values in one array in another, returning a boolean array:

```
In [211]: values = np.array([6, 0, 0, 3, 2, 5, 6])

In [212]: np.in1d(values, [2, 3, 6])
Out[212]: array([ True, False, False,  True,  True, False,  True], dtype=bool)
```

See Table 4-6 for a listing of set functions in NumPy.

Table 4-6. Array set operations

Method	Description
unique(x)	Compute the sorted, unique elements in x
intersect1d(x, y)	Compute the sorted, common elements in x and y
union1d(x, y)	Compute the sorted union of elements
in1d(x, y)	Compute a boolean array indicating whether each element of x is contained in y
setdiff1d(x, y)	Set difference, elements in x that are not in y
setxor1d(x, y)	Set symmetric differences; elements that are in either of the arrays, but not both

4.4 File Input and Output with Arrays

NumPy is able to save and load data to and from disk either in text or binary format. In this section I only discuss NumPy's built-in binary format, since most users will prefer pandas and other tools for loading text or tabular data (see Chapter 6 for much more).

`np.save` and `np.load` are the two workhorse functions for efficiently saving and load-ing array data on disk. Arrays are saved by default in an uncompressed raw binary format with file extension *.npy*:

```
In [213]: arr = np.arange(10)

In [214]: np.save('some_array', arr)
```

If the file path does not already end in *.npy*, the extension will be appended. The array on disk can then be loaded with `np.load`:

```
In [215]: np.load('some_array.npy')
Out[215]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

You save multiple arrays in an uncompressed archive using `np.savez` and passing the arrays as keyword arguments:

```
In [216]: np.savez('array_archive.npz', a=arr, b=arr)
```

When loading an *.npz* file, you get back a dict-like object that loads the individual arrays lazily:

```
In [217]: arch = np.load('array_archive.npz')

In [218]: arch['b']
Out[218]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

If your data compresses well, you may wish to use `numpy.savez_compressed` instead:

```
In [219]: np.savez_compressed('arrays_compressed.npz', a=arr, b=arr)
```

4.5 Linear Algebra

Linear algebra, like matrix multiplication, decompositions, determinants, and other square matrix math, is an important part of any array library. Unlike some languages like MATLAB, multiplying two two-dimensional arrays with * is an element-wise product instead of a matrix dot product. Thus, there is a function `dot`, both an array method and a function in the `numpy` namespace, for matrix multiplication:

```
In [223]: x = np.array([[1., 2., 3.], [4., 5., 6.]])

In [224]: y = np.array([[6., 23.], [-1, 7], [8, 9]])

In [225]: x
Out[225]:
array([[ 1.,  2.,  3.],
       [ 4.,  5.,  6.]])

In [226]: y
Out[226]:
array([[  6.,  23.],
       [ -1.,   7.],
       [  8.,   9.]])

In [227]: x.dot(y)
Out[227]:
array([[  28.,   64.],
       [  67.,  181.]])
```

`x.dot(y)` is equivalent to `np.dot(x, y)`:

```
In [228]: np.dot(x, y)
Out[228]:
array([[  28.,   64.],
       [  67.,  181.]])
```

A matrix product between a two-dimensional array and a suitably sized one-dimensional array results in a one-dimensional array:

```
In [229]: np.dot(x, np.ones(3))
Out[229]: array([  6.,  15.])
```

The `@` symbol (as of Python 3.5) also works as an infix operator that performs matrix multiplication:

```
In [230]: x @ np.ones(3)
Out[230]: array([  6.,  15.])
```

`numpy.linalg` has a standard set of matrix decompositions and things like inverse and determinant. These are implemented under the hood via the same industry-standard linear algebra libraries used in other languages like MATLAB and R, such as BLAS, LAPACK, or possibly (depending on your NumPy build) the proprietary Intel MKL (Math Kernel Library):

```
In [231]: from numpy.linalg import inv, qr

In [232]: X = np.random.randn(5, 5)

In [233]: mat = X.T.dot(X)

In [234]: inv(mat)
Out[234]:
array([[  933.1189,   871.8258, -1417.6902, -1460.4005,  1782.1391],
       [  871.8258,   815.3929, -1325.9965, -1365.9242,  1666.9347],
       [-1417.6902, -1325.9965,  2158.4424,  2222.0191, -2711.6822],
       [-1460.4005, -1365.9242,  2222.0191,  2289.0575, -2793.422 ],
       [ 1782.1391,  1666.9347, -2711.6822, -2793.422 ,  3409.5128]])

In [235]: mat.dot(inv(mat))
Out[235]:
array([[ 1.,  0., -0., -0., -0.],
       [-0.,  1.,  0.,  0.,  0.],
       [ 0.,  0.,  1.,  0.,  0.],
       [-0.,  0.,  0.,  1., -0.],
       [-0.,  0.,  0.,  0.,  1.]])

In [236]: q, r = qr(mat)

In [237]: r
Out[237]:
array([[-1.6914,  4.38  ,  0.1757,  0.4075, -0.7838],
       [ 0.    , -2.6436,  0.1939, -3.072 , -1.0702],
       [ 0.    ,  0.    , -0.8138,  1.5414,  0.6155],
       [ 0.    ,  0.    ,  0.    , -2.6445, -2.1669],
       [ 0.    ,  0.    ,  0.    ,  0.    ,  0.0002]])
```

The expression `X.T.dot(X)` computes the dot product of `X` with its transpose `X.T`.

See Table 4-7 for a list of some of the most commonly used linear algebra functions.

Table 4-7. Commonly used numpy.linalg functions

Function	Description
diag	Return the diagonal (or off-diagonal) elements of a square matrix as a 1D array, or convert a 1D array into a square matrix with zeros on the off-diagonal
dot	Matrix multiplication
trace	Compute the sum of the diagonal elements
det	Compute the matrix determinant

Function	Description
eig	Compute the eigenvalues and eigenvectors of a square matrix
inv	Compute the inverse of a square matrix
pinv	Compute the Moore-Penrose pseudo-inverse of a matrix
qr	Compute the QR decomposition
svd	Compute the singular value decomposition (SVD)
solve	Solve the linear system Ax = b for x, where A is a square matrix
lstsq	Compute the least-squares solution to Ax = b

4.6 Pseudorandom Number Generation

The `numpy.random` module supplements the built-in Python `random` with functions for efficiently generating whole arrays of sample values from many kinds of probability distributions. For example, you can get a 4 × 4 array of samples from the standard normal distribution using `normal`:

```
In [238]: samples = np.random.normal(size=(4, 4))

In [239]: samples
Out[239]:
array([[ 0.5732,  0.1933,  0.4429,  1.2796],
       [ 0.575 ,  0.4339, -0.7658, -1.237 ],
       [-0.5367,  1.8545, -0.92  , -0.1082],
       [ 0.1525,  0.9435, -1.0953, -0.144 ]])
```

Python's built-in `random` module, by contrast, only samples one value at a time. As you can see from this benchmark, `numpy.random` is well over an order of magnitude faster for generating very large samples:

```
In [240]: from random import normalvariate

In [241]: N = 1000000

In [242]: %timeit samples = [normalvariate(0, 1) for _ in range(N)]
1.77 s +- 126 ms per loop (mean +- std. dev. of 7 runs, 1 loop each)

In [243]: %timeit np.random.normal(size=N)
61.7 ms +- 1.32 ms per loop (mean +- std. dev. of 7 runs, 10 loops each)
```

We say that these are *pseudorandom* numbers because they are generated by an algorithm with deterministic behavior based on the *seed* of the random number generator. You can change NumPy's random number generation seed using `np.random.seed`:

```
In [244]: np.random.seed(1234)
```

The data generation functions in `numpy.random` use a global random seed. To avoid global state, you can use `numpy.random.RandomState` to create a random number generator isolated from others:

```
In [245]: rng = np.random.RandomState(1234)

In [246]: rng.randn(10)
Out[246]:
array([ 0.4714, -1.191 ,  1.4327, -0.3127, -0.7206,  0.8872,  0.8596,
        -0.6365,  0.0157, -2.2427])
```

See Table 4-8 for a partial list of functions available in `numpy.random`. I'll give some examples of leveraging these functions' ability to generate large arrays of samples all at once in the next section.

Table 4-8. Partial list of numpy.random functions

Function	Description
seed	Seed the random number generator
permutation	Return a random permutation of a sequence, or return a permuted range
shuffle	Randomly permute a sequence in-place
rand	Draw samples from a uniform distribution
randint	Draw random integers from a given low-to-high range
randn	Draw samples from a normal distribution with mean 0 and standard deviation 1 (MATLAB-like interface)
binomial	Draw samples from a binomial distribution
normal	Draw samples from a normal (Gaussian) distribution
beta	Draw samples from a beta distribution
chisquare	Draw samples from a chi-square distribution
gamma	Draw samples from a gamma distribution
uniform	Draw samples from a uniform [0, 1) distribution

4.7 Example: Random Walks

The simulation of random walks provides an illustrative application of utilizing array operations. Let's first consider a simple random walk starting at 0 with steps of 1 and −1 occurring with equal probability.
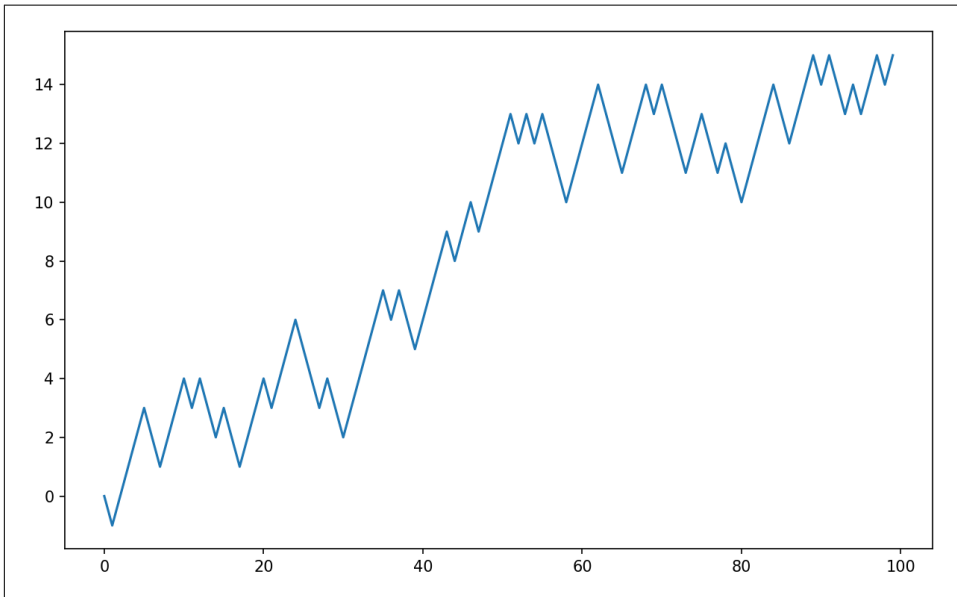
Here is a pure Python way to implement a single random walk with 1,000 steps using the built-in `random` module:

```
In [247]: import random
     ...: position = 0
     ...: walk = [position]
     ...: steps = 1000
     ...: for i in range(steps):
     ...:     step = 1 if random.randint(0, 1) else -1
     ...:     position += step
```

```
.....:         walk.append(position)
.....:
```

See Figure 4-4 for an example plot of the first 100 values on one of these random walks:

```
In [249]: plt.plot(walk[:100])
```


Figure 4-4. A simple random walk

You might make the observation that `walk` is simply the cumulative sum of the random steps and could be evaluated as an array expression. Thus, I use the `np.random` module to draw 1,000 coin flips at once, set these to 1 and –1, and compute the cumulative sum:

```
In [251]: nsteps = 1000

In [252]: draws = np.random.randint(0, 2, size=nsteps)

In [253]: steps = np.where(draws > 0, 1, -1)

In [254]: walk = steps.cumsum()
```

From this we can begin to extract statistics like the minimum and maximum value along the walk's trajectory:

```
In [255]: walk.min()
Out[255]: -3
```

```
In [256]: walk.max()
Out[256]: 31
```

A more complicated statistic is the *first crossing time*, the step at which the random walk reaches a particular value. Here we might want to know how long it took the random walk to get at least 10 steps away from the origin 0 in either direction. `np.abs(walk) >= 10` gives us a boolean array indicating where the walk has reached or exceeded 10, but we want the index of the *first* 10 or –10. Turns out, we can compute this using `argmax`, which returns the first index of the maximum value in the boolean array (`True` is the maximum value):

```
In [257]: (np.abs(walk) >= 10).argmax()
Out[257]: 37
```

Note that using `argmax` here is not always efficient because it always makes a full scan of the array. In this special case, once a `True` is observed we know it to be the maximum value.

Simulating Many Random Walks at Once

If your goal was to simulate many random walks, say 5,000 of them, you can generate all of the random walks with minor modifications to the preceding code. If passed a 2-tuple, the `numpy.random` functions will generate a two-dimensional array of draws, and we can compute the cumulative sum across the rows to compute all 5,000 random walks in one shot:

```
In [258]: nwalks = 5000

In [259]: nsteps = 1000

In [260]: draws = np.random.randint(0, 2, size=(nwalks, nsteps)) # 0 or 1

In [261]: steps = np.where(draws > 0, 1, -1)

In [262]: walks = steps.cumsum(1)

In [263]: walks
Out[263]:
array([[  1,    0,    1, ...,    8,    7,    8],
       [  1,    0,   -1, ...,   34,   33,   32],
       [  1,    0,   -1, ...,    4,    5,    4],
       ...,
       [  1,    2,    1, ...,   24,   25,   26],
       [  1,    2,    3, ...,   14,   13,   14],
       [ -1,   -2,   -3, ...,  -24,  -23,  -22]])
```

Now, we can compute the maximum and minimum values obtained over all of the walks:

```
In [264]: walks.max()
Out[264]: 138

In [265]: walks.min()
Out[265]: -133
```

Out of these walks, let's compute the minimum crossing time to 30 or –30. This is slightly tricky because not all 5,000 of them reach 30. We can check this using the `any` method:

```
In [266]: hits30 = (np.abs(walks) >= 30).any(1)

In [267]: hits30
Out[267]: array([False,  True, False, ..., False,  True, False], dtype=bool)

In [268]: hits30.sum() # Number that hit 30 or -30
Out[268]: 3410
```

We can use this boolean array to select out the rows of `walks` that actually cross the absolute 30 level and call `argmax` across axis 1 to get the crossing times:

```
In [269]: crossing_times = (np.abs(walks[hits30]) >= 30).argmax(1)

In [270]: crossing_times.mean()
Out[270]: 498.88973607038122
```

Feel free to experiment with other distributions for the steps other than equal-sized coin flips. You need only use a different random number generation function, like `normal` to generate normally distributed steps with some mean and standard deviation:

```
In [271]: steps = np.random.normal(loc=0, scale=0.25,
    .....:                          size=(nwalks, nsteps))
```

4.8 Conclusion

While much of the rest of the book will focus on building data wrangling skills with pandas, we will continue to work in a similar array-based style. In Appendix A, we will dig deeper into NumPy features to help you further develop your array computing skills.