NEXT NumPy Basics: Arrays and Vectorized Computation









Chapter 3. Built-in Data Structures, Functions, and Files

This chapter discusses capabilities built into the Python language that will be used ubiquitously throughout the book. While add-on libraries like pandas and NumPy add advanced computational functionality for larger datasets, they are designed to be used together with Python's built-in data manipulation tools.

We'll start with Python's workhorse data structures: tuples, lists, dicts, and sets. Then, we'll discuss creating your own reusable Python functions. Finally, we'll look at the mechanics of Python file objects and interacting with your local hard

3.1 Data Structures and Sequences

Python's data structures are simple but powerful. Mastering their use is a critical part of becoming a proficient Python programmer.

Tuple

A tuple is a fixed-length, immutable sequence of Python objects. The easiest way to create one is with a comma-separated sequence of values:

```
In (1): tup = 4, 5, 6

In (2): tup
Out(2): (4, 5, 6)
```

When you're defining tuples in more complicated expressions, it's often necessary to enclose the values in parentheses, as in this example of creating a tuple of tuples:

```
In [3]: nested_tup = (4, 5, 6), (7, 8)

In [4]: nested_tup

Out[4]: ((4, 5, 6), (7, 8))
```

You can convert any sequence or iterator to a tuple by invoking tuple:

```
In [5]: tuple([4, 0, 2])
Out(5): (4, 0, 2)
In [6]: tup = tuple('string')
In [7]: tup
Out(7): ('s', 't', 'r', 'i', 'n', 'g')
```

Elements can be accessed with square brackets [] as with most other sequence types. As in C, C++, Java, and many other languages, sequences are 0-indexed in Python:

```
In [8]: tup[0]
Out[8]: 's'
```

While the objects stored in a tuple may be mutable themselves, once the tuple is created it's not possible to modify which object is stored in each slot:

If an object inside a tuple is mutable, such as a list, you can modify it in-place:

```
In (11): tup(1).append(3)

In (12): tup
Out(12): ('foo', (1, 2, 3), True)
```

You can concatenate tuples using the + operator to produce longer tuples:

```
In [13]: (4, None, 'foo') + (6, 0) + ('bar',)
Out[13]: (4, None, 'foo', 6, 0, 'bar')
```

Multiplying a tuple by an integer, as with lists, has the effect of concatenating together that many copies of the tuple:

```
In [14]: ('foo', 'bar') * 4
Out[14]: ('foo', 'bar', 'foo', 'bar', 'foo', 'bar', 'foo', 'bar')
```

Note that the objects themselves are not copied, only the references to them.

UNPACKING TUPLES

If you try to assign to a tuple-like expression of variables, Python will attempt to unpack the value on the righthand side of the equals sign:

```
In [15]: tup = (4, 5, 6)

In [16]: a, b, c = tup

In [17]: b

Out[17]: 5
```

Even sequences with nested tuples can be unpacked:

```
In [18]: tup = 4, 5, (6, 7)

In [19]: a, b, (c, d) = tup

In [20]: d
Out[20]: 7
```

Using this functionality you can easily swap variable names, a task which in many languages might look like:

```
tm\rho = a
a = b
b = tmp
```

But, in Python, the swap can be done like this:

```
In (21): a, b = 1, 2

In (22): a
Out(22): 1

In (23): b
Out(23): 2

In (24): b, a = a, b

In (25): a
Out(25): 2

In (26): b
Out(26): 1
```

A common use of variable unpacking is iterating over sequences of tuples or liere:

```
In [27]: seq = [(1, 2, 3), (4, 5, 6), (7, 8, 9)]

In [28]: for a, b, c in seq:
....: print('a=(0), b=(1), c=(2)'.format(a, b, c))
a=1, b=2, c=3
a=4, b=5, c=6
a=7, b=8, c=9
```

Another common use is returning multiple values from a function. I'll cover this in more detail later.

The Python language recently acquired some more advanced tuple unpacking to help with situations where you may want to "pluck" a few elements from the beginning of a tuple. This uses the special syntax "rest, which is also used in function signatures to capture an arbitrarily long list of positional arguments:

```
In (29): values = 1, 2, 3, 4, 5
In (30): a, b, *rest = values
In (31): a, b
Out(31): (1, 2)
In (32): rest
Out(32): (3, 4, 5)
```

This rest bit is sometimes something you want to discard; there is nothing special about the rest name. As a matter of convention, many Python programmers will use the underscore (_) for unwanted variables:

```
In [33]: a, b, *_ = values
```

TUPLE METHODS

Since the size and contents of a tuple cannot be modified, it is very light on instance methods. A particularly useful one (also available on lists) is count, which counts the number of occurrences of a value:

```
In [34]: a = (1, 2, 2, 2, 3, 4, 2)
In [35]: a.count(2)
Out(35]: 4
```

List

In contrast with tuples, lists are variable-length and their contents can be modified in-place. You can define them using square brackets [] or using the list type function:

```
In (36): a_list = (2, 3, 7, None)
In (37): tup = ('foo', 'bar', 'baz')
In (38): b_list = list(tup)
In (39): b_list
Out(39): ('foo', 'bar', 'baz')
In (40): b_list[1] = 'peekaboo'
In (41): b_list
Out(41): ('foo', 'peekaboo', 'baz')
```

Lists and tuples are semantically similar (though tuples cannot be modified) and can be used interchangeably in many functions.

The list function is frequently used in data processing as a way to materialize an iterator or generator expression:

```
In [42]: gen = range(10)
In [43]: gen
Out(43]: range(0, 10)
In [44]: list(gen)
Out(44): [0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
```

ADDING AND REMOVING ELEMENTS

Elements can be appended to the end of the list with the append method:

```
In [45]: b_list.append('dwarf')
In [46]: b_list
Out[46]: ['foo', 'peekaboo', 'baz', 'dwarf']
```

Using insert you can insert an element at a specific location in the list:

```
In [47]: b_list.insert(1, 'red')
In [48]: b_list
Out[48]: ('foo', 'red', 'peekaboo', 'baz', 'dwarf')
```

The insertion index must be between 0 and the length of the list, inclusive.

WARNING

insert is computationally expensive compared with append, because references to subsequent elements have to be shifted internally to make room for the new element. If you need to insert elements at both the beginning and end of a sequence, you may wish to explore collections.deque, a double-ended queue, for this purpose.

The inverse operation to insert is pop, which removes and returns an element at a particular index:

```
In [49]: b_list.pop(2)
Out[49]: 'peekaboo'

In [50]: b_list
Out[50]: ['foo', 'red', 'baz', 'dwarf']
```

Elements can be removed by value with remove, which locates the first such value and removes it from the last:

```
In (51): b_list.append('foo')
In (52): b_list
Out(52): ('foo', 'red', 'baz', 'dwarf', 'foo')
In (53): b_list.remove('foo')
In (54): b_list
Out(54): ('red', 'baz', 'dwarf', 'foo')
```

If performance is not a concern, by using append and remove, you can use a Python list as a perfectly suitable "multiset" data structure.

Check if a list contains a value using the in keyword:

```
In [55]: 'dwarf' in b_list
Out[55]: True
```

The keyword not can be used to negate in:

```
In [56]: 'dwarf' not in b_list
Out[56]: False
```

Checking whether a list contains a value is a lot slower than doing so with dicts and sets (to be introduced shortly), as Python makes a linear scan across the values of the list, whereas it can check the others (based on hash tables) in constant time.

CONCATENATING AND COMBINING LISTS

Similar to tuples, adding two lists together with + concatenates them:

```
In [57]: [4, None, 'foo'] + [7, 8, (2, 3)]
Out[57]: [4, None, 'foo', 7, 8, (2, 3)]
```

If you have a list already defined, you can append multiple elements to it using the ${\tt extend}$ method:

```
In [58]: x = [4, None, 'foo']
In [59]: x.extend([7, 8, (2, 3)])
In [68]: x
Out[68]: [4, None, 'foo', 7, 8, (2, 3)]
```

Note that list concatenation by addition is a comparatively expensive operation since a new list must be created and the objects copied over. Using extend to append elements to an existing list, especially if you are building up a large list, is usually preferable. Thus,

```
everything = []
for chunk in list_of_lists:
```

is faster than the concatenative alternative:

```
everything = []
for chunk in list_of_lists:
    everything = everything + chunk
```

SORTING

You can sort a list in-place (without creating a new object) by calling its sort function:

```
In [61]: a = {7, 2, 5, 1, 3}
In [62]: a.sort()
In [63]: a
Out[63]: {1, 2, 3, 5, 7}
```

sort has a few options that will occasionally come in handy. One is the ability to pass a secondary *sort key*—that is, a function that produces a value to use to sort the objects. For example, we could sort a collection of strings by their lengths:

```
In (64): b = ('saw', 'small', 'He', 'foxes', 'six')
In (65): b.sort(key=len)
In (66): b
Out(66): ['He', 'saw', 'six', 'small', 'foxes']
```

Soon, we'll look at the sorted function, which can produce a sorted copy of a general sequence.

BINARY SEARCH AND MAINTAINING A SORTED LIST

The built-in bisect module implements binary search and insertion into a sorted list. bisect. bisect finds the location where an element should be inserted to keep it sorted, while bisect.insort actually inserts the element into that location:

```
In (67): import bisect
In (68): c = (1, 2, 2, 2, 3, 4, 7]
In (69): bisect.bisect(c, 2)
Out(69): 4
In (78): bisect.bisect(c, 5)
Out(78): 6
In (71): bisect.insort(c, 6)
In (72): c
Out(72): (1, 2, 2, 2, 3, 4, 6, 7]
```

CAUTION

The bisect module functions do not check whether the list is sorted, as doing so would be computationally expensive. Thus, using them with an unsorted list will succeed without error but may lead to incorrect results.

SLICING

You can select sections of most sequence types by using slice notation, which in its basic form consists of start:stop passed to the indexing operator []:

```
In [73]: seq = [7, 2, 3, 7, 5, 6, 8, 1]
In [74]: seq[1:5]
Out[74]: [2, 3, 7, 5]
```

Slices can also be assigned to with a sequence:

```
In [75]: seq[3:4] = [6, 3]
In [76]: seq
Out[76]: [7, 2, 3, 6, 3, 5, 6, 8, 1]
```

While the element at the start index is included, the stop index is *not* included, so that the number of elements in the result is stop - start.

Either the \mathtt{start} or \mathtt{stop} can be omitted, in which case they default to the start of the sequence and the end of the sequence, respectively:

```
In [77]: seq::5]
Out[77]: [7, 2, 3, 6, 3]
In [78]: seq[3:]
Out[78]: [6, 3, 5, 6, 0, 1]
```

Negative indices slice the sequence relative to the end:

```
In [79]: seq[-4:]
Out[79]: [5, 6, 0, 1]
In [80]: seq[-6:-2]
Out[80]: [6, 3, 5, 6]
```

Slicing semantics takes a bit of getting used to, especially if you're coming from R or MATLAB. See Figure 3-1 for a helpful illustration of slicing with positive and negative integers. In the figure, the indices are shown at the "bin edges" to help show where the slice selections start and stop using positive or negative

A step can also be used after a second colon to, say, take every other element:

```
In [81]: seq[::2]
Out[81]: [7, 3, 3, 6, 1]
```

A clever use of this is to pass -1, which has the useful effect of reversing a list or timle.

Figure 3-1. Illustration of Python slicing conventions

Built-in Sequence Functions

Python has a handful of useful sequence functions that you should familiarize yourself with and use at any opportunity.

ENUMERATE

It's common when iterating over a sequence to want to keep track of the index of the current item. A do-it-yourself approach would look like:

```
i = 0
for value in collection:
  # do something with value
  i += 1
```

Since this is so common, Python has a built-in function, enumerate, which returns a sequence of (i, value) tuples:

```
for i, value in enumerate(collection):
    # do something with value
```

When you are indexing data, a helpful pattern that uses enumerate is computing a dict mapping the values of a sequence (which are assumed to be unique) to their locations in the sequence:

SORTE

The sorted function returns a new sorted list from the elements of any sequence:

```
In (87): sorted({7, 1, 2, 6, 0, 3, 2})
Out(87): (0, 1, 2, 2, 3, 6, 7)
In (88): sorted('horse race')
Out(88): ('', 'a', 'c', 'e', 'e', 'h', 'o', 'n', 'n', 's')
```

The sorted function accepts the same arguments as the sort method on lists.

ZII

zip "pairs" up the elements of a number of lists, tuples, or other sequences to create a list of tuples:

```
In (89): seq1 = ('foo', 'bar', 'baz')
In (90): seq2 = ('one', 'two', 'three')
In (91): zipped = zip(seq1, seq2)
In (92): list(zipped)
Out(92): (('foo', 'one'), ('bar', 'two'), ('baz', 'three'))
```

zip can take an arbitrary number of sequences, and the number of elements it produces is determined by the *shortest* sequence:

```
In [93]: seq3 = [False, True]
In [94]: list(zip(seq1, seq2, seq3))
Out[94]: [('foo', 'one', False), ('bar', 'two', True)]
```

A very common use of zip is simultaneously iterating over multiple sequences, possibly also combined with enumerate:

```
In [95]: for i, (a, b) in enumerate(zip(seq1, seq2)):
....: print('(0): (1), (2)'.format(i, a, b))
....:
0: foo, one
1: bar, two
2: baz, three
```

Given a "zipped" sequence, zip can be applied in a clever way to "unzip" the sequence. Another way to think about this is converting a list of rows into a list of columns. The syntax, which looks a bit magical, is:

```
In [98]: first_names
Out[98]: ('Nolan', 'Roger', 'Schilling')
In [99]: last_names
Out[99]: ('Ryan', 'Clemens', 'Curt')
```

REVERSED

reversed iterates over the elements of a sequence in reverse order:

```
In [100]: list(reversed(range(10)))
Out[100]: [9, 8, 7, 6, 5, 4, 3, 2, 1, 0]
```

Keep in mind that reversed is a generator (to be discussed in some more detail later), so it does not create the reversed sequence until materialized (e.g., with list or a for loop).

dict

dict is likely the most important built-in Python data structure. A more common name for it is hash map or associative array. It is a flexibly sized collection of key-value pairs, where key and value are Python objects. One approach for creating one is to use curly braces {} and colons to separate keys and values:

```
In [101]: empty_dict = ()

In [102]: d1 = {'a' : 'some value', 'b' : {1, 2, 3, 4}}

In [103]: d1

Out[103]: {'a': 'some value', 'b': {1, 2, 3, 4}}
```

You can access, insert, or set elements using the same syntax as for accessing elements of a list or tuple:

```
In [104]: d1[7] = 'an integer'
In [185]: d1
Out[185]: [7: 'an integer', 'a': 'some value', 'b': [1, 2, 3, 4])
In [106]: d1['b']
Out[186]: [1, 2, 3, 4]
```

You can check if a dict contains a key using the same syntax used for checking whether a list or tuple contains a value:

```
In [107]: 'b' in d1
Out[107]: True
```

You can delete values either using the del keyword or the pop method (which simultaneously returns the value and deletes the key):

The keys and values method give you iterators of the dict's keys and values, respectively. While the key-value pairs are not in any particular order, these functions output the keys and values in the same order:

```
In (117]: list(d1.keys())
Out[117]: ['a', 'b', 7]
In (118]: list(d1.values())
Out[118]: ['some value', [1, 2, 3, 4], 'an integer']
```

You can merge one dict into another using the $\ensuremath{\mathsf{update}}$ method:

```
In [119]: dl.update({'b' : 'foo', 'c' : 12})

In [128]: dl
Out[120]: (7: 'an integer', 'a': 'some value', 'b': 'foo', 'c': 12)
```

The update method changes dicts in-place, so any existing keys in the data passed to update will have their old values discarded.

CREATING DICTS FROM SEQUENCES

It's common to occasionally end up with two sequences that you want to pair up element-wise in a dict. As a first cut, you might write code like this:

```
mapping = ()
for key, value in zip(key_list, value_list):
    mapping(key) = value
```

Since a dict is essentially a collection of 2-tuples, the dict function accepts a list of 2-tuples:

```
In (121): mapping = dict(zip(range(5), reversed(range(5))))
In (122): mapping
Out(122): (0: 4, 1: 3, 2: 2, 3: 1, 4: 0)
```

Later we'll talk about dict comprehensions, another elegant way to construct

DEFAULT VALUES

It's very common to have logic like:

```
if key in some_dict:
    value = some_dict[key]
else:
    value = default_value
```

Thus, the dict methods get and pop can take a default value to be returned, so that the above if-else block can be written simply as:

```
value = some_dict.get(key, default_value)
```

get by default will return None if the key is not present, while pop will raise an exception. With setting values, a common case is for the values in a diet to be other collections, like lists. For example, you could imagine categorizing a list of words by their first letters as a diet of lists:

The setdefault dict method is for precisely this purpose. The preceding for loop can be rewritten as:

```
for word in words:

letter = word[0]

by_letter.setdefault(letter, []).append(word)
```

The built-in collections module has a useful class, defaultdict, which makes this even easier. To create one, you pass a type or function for generating the default value for each slot in the dict:

```
from collections import defaultdict
by_letter = defaultdict(list)
for word in words:
    by_letter(word[8]].append(word)
```

VALID DICT KEY TYPES

While the values of a dict can be any Python object, the keys generally have to be immutable objects like scalar types (int, float, string) or tuples (all the objects in the tuple need to be immutable, too). The technical term here is hashability. You can check whether an object is hashable (can be used as a key in a dict) with the hash function:

```
In (127): hash('string')
Out(127): -385472831944956388

In (128): hash((1, 2, (2, 3)))
Out(128): 1897636582276347782

In (129): hash((1, 2, (2, 3))) # foils because lists are mutable

TypeError
clapython-input-129-473c35a62c0b in (module)()
----> 1 hash((1, 2, (2, 3))) # foils because lists are mutable

TypeError: unhashable type: 'list'
```

To use a list as a key, one option is to convert it to a tuple, which can be hashed as long as its elements also can:

```
In (130): d = {}
In (131]: d[tuple([1, 2, 3])] = 5
In (132]: d
Out(132): {(1, 2, 3): 5}
```

set

A set is an unordered collection of unique elements. You can think of them like dicts, but keys only, no values. A set can be created in two ways: via the set function or via a set literal with curly braces:

```
In [133]: set([2, 2, 2, 1, 3, 3])
Out(133]: (1, 2, 3)
In [134]: {2, 2, 2, 1, 3, 3}
Out(134]: {1, 2, 3}
```

Sets support mathematical set operations like union, intersection, difference, and symmetric difference. Consider these two example sets:

```
In (135): a = {1, 2, 3, 4, 5}
In (136): b = {3, 4, 5, 6, 7, 8}
```

The union of these two sets is the set of distinct elements occurring in either set. This can be computed with either the union method or the | binary operator:

```
In [137]: a.union(b)
Out[137]: {1, 2, 3, 4, 5, 6, 7, 8}

In [138]: a | b
Out[138]: {1, 2, 3, 4, 5, 6, 7, 8}
```

The intersection contains the elements occurring in both sets. The & operator or the intersection method can be used:

```
In [139]: a.intersection(b)
Out(139]: {3, 4, 5}

In [140]: a & b
Out(140]: {3, 4, 5}
```

See \underline{Table} $\underline{3}$ - $\underline{1}$ for a list of commonly used set methods.

Table 3-1. Python set operations

Function	Alternative syntax	Description
a.add(x)	N/A	Add element x to the set a
a.clear()	N/A	Reset the set a to an empty state, discarding all of its elements
a.remove(x)	N/A	Remove element x from the set a
a.pop()	N/A	Remove an arbitrary element from the set a, raising KeyError if the set is empty
a.union(b)	a b	All of the unique elements in a and b
a.update(b)	a = b	Set the contents of a to be the union of the elements in a and b
a.intersection(b)	a & b	All of the elements in <i>both</i> a and b
a.intersection_update(b)	a &= b	Set the contents of a to be the intersection of the elements in a and b
a.difference(b)	a - b	The elements in a that are not in b
a.difference_update(b)	a -= b	Set a to the elements in a that are not in b
a.symmetric_difference(b)	a ^ b	All of the elements in either a or b but <i>not both</i>
a.symmetric_difference_update(b)	a ^= b	Set a to contain the elements in either a or b but not both
a.issubset(b)	N/A	True if the elements of a are all contained in b
a.issuperset(b)	N/A	True if the elements of b are all contained in a
a.isdisjoint(b)	N/A	True if a and b have no elements in common

All of the logical set operations have in-place counterparts, which enable you to replace the contents of the set on the left side of the operation with the result. For very large sets, this may be more efficient:

```
In [141]: c = a.copy()

In [142]: c |= b

In [143]: c

Out[143]: {1, 2, 3, 4, 5, 6, 7, 8}
```

```
In [144]: d = a.copy()

In [145]: d &= b

In [146]: d
Out[146]: (3, 4, 5)
```

Like dicts, set elements generally must be immutable. To have list-like elements, you must convert it to a tuple:

```
In [147]: my_data = [1, 2, 3, 4]
In [148]: my_set = {tuple(my_data)}
In [149]: my_set
Out[149]: {(1, 2, 3, 4)}
```

You can also check if a set is a subset of (is contained in) or a superset of (contains all elements of) another set:

```
In (150): a_set = (1, 2, 3, 4, 5)
In (151): (1, 2, 3).issubset(a_set)
Out[151]: True
In (152): a_set.issuperset((1, 2, 3))
Out[152]: True
```

Sets are equal if and only if their contents are equal:

```
In [153]: {1, 2, 3} == {3, 2, 1}
Out[153]: True
```

List, Set, and Dict Comprehensions

List comprehensions are one of the most-loved Python language features. They allow you to concisely form a new list by filtering the elements of a collection, transforming the elements passing the filter in one concise expression. They take the basic form:

```
[expr for val in collection if condition]
```

This is equivalent to the following for loop:

```
result = ()
for val in collection:
   if condition:
      result.append(expr)
```

The filter condition can be omitted, leaving only the expression. For example, given a list of strings, we could filter out strings with length 2 or less and also convert them to uppercase like this:

```
In (154): strings = ('a', 'as', 'bat', 'car', 'dove', 'python')
In (155): (x.upper() for x in strings if len(x) > 2)
Out(155): ('8AT', 'CAR', 'DOVE', 'PYTHON')
```

Set and dict comprehensions are a natural extension, producing sets and dicts in an idiomatically similar way instead of lists. A dict comprehension looks like this:

A set comprehension looks like the equivalent list comprehension except with curly braces instead of square brackets:

```
set_comp = {expr for value in collection if condition}
```

Like list comprehensions, set and dict comprehensions are mostly conveniences, but they similarly can make code both easier to write and read. Consider the list of strings from before. Suppose we wanted a set containing just the lengths of the strings contained in the collection; we could easily compute this using a set comprehension:

```
In [156]: unique_lengths = (len(x) for x in strings)

In [157]: unique_lengths
Out[157]: (1, 2, 3, 4, 6)
```

We could also express this more functionally using the $map\ \mbox{function},$ introduced shortly:

```
In [158]: set(map(len, strings))
Out(158]: {1, 2, 3, 4, 6}
```

As a simple dict comprehension example, we could create a lookup map of these strings to their locations in the list:

NESTED LIST COMPREHENSIONS

Suppose we have a list of lists containing some English and Spanish names:

You might have gotten these names from a couple of files and decided to organize them by language. Now, suppose we wanted to get a single list containing all names with two or more e's in them. We could certainly do this with a simple for loop:

```
names_of_interest = []
for names in all_data:
       enough_es = [name for name in names if name.count('e') >= 2]
names_of_interest.extend(enough_es)
```

You can actually wrap this whole operation up in a single nested list comprehension, which will look like:

```
In [162]: result = [name for names in all_data for name in names
                    if name.count('e') >= 2]
In [163]: result
```

At first, nested list comprehensions are a bit hard to wrap your head around. The for parts of the list comprehension are arranged according to the order of nesting, and any filter condition is put at the end as before. Here is another example where we "flatten" a list of tuples of integers into a simple list of

```
In [164]: some_tuples = [(1, 2, 3), (4, 5, 6), (7, 8, 9)]
In [165]: flattened = [x for tup in some_tuples for x in tup]
In [166]: flattened
Out[166]: [1, 2, 3, 4, 5, 6, 7, 8, 9]
```

Keep in mind that the order of the for expressions would be the same if you wrote a nested for loop instead of a list comprehension:

```
flattened = []
for tup in some_tuples:
    for x in tup:
        flattened.append(x)
```

You can have arbitrarily many levels of nesting, though if you have more than two or three levels of nesting you should probably start to question whether this makes sense from a code readability standpoint. It's important to distinguish the syntax just shown from a list comprehension inside a list comprehension, which

```
In [167]: [[x for x in tup] for tup in some_tuples]
Out[167]: [[1, 2, 3], [4, 5, 6], [7, 8, 9]]
```

This produces a list of lists, rather than a flattened list of all of the inner elements.

3.2 Functions

Functions are the primary and most important method of code organization and reuse in Python. As a rule of thumb, if you anticipate needing to repeat the same or very similar code more than once, it may be worth writing a reusable function Functions can also help make your code more readable by giving a name to a

Functions are declared with the def keyword and returned from with the return

```
def my_function(x, y, z=1.5):
    if z > 1:
        return z * (x + y)
    else:
        return z / (x + y)
```

There is no issue with having multiple return statements. If Python reaches the end of a function without encountering a ${\tt return}$ statement, None is returned automatically.

Each function can have positional arguments and keyword arguments. Keyword arguments are most commonly used to specify default values or optional arguments. In the preceding function, \boldsymbol{x} and \boldsymbol{y} are positional arguments while \boldsymbol{z} is a keyword argument. This means that the function can be called in any of these ways:

```
my_function(5, 6, z=0.7)
my_function(3.14, 7, 3.5)
my_function(10, 20)
```

The main restriction on function arguments is that the keyword arguments must follow the positional arguments (if any). You can specify keyword arguments in any order; this frees you from having to remember which order the function arguments were specified in and only what their names are.

NOTE

It is possible to use keywords for passing positional arguments as well. In the preceding example, we could also have written:

```
my_function(x=5, y=6, z=7)
my_function(y=6, x=5, z=7)
In some cases this can help with readability.
```

Namespaces, Scope, and Local Functions

Functions can access variables in two different scopes: global and local. An alternative and more descriptive name describing a variable scope in Python is a namespace. Any variables that are assigned within a function by default are assigned to the local namespace. The local namespace is created when the function is called and immediately populated by the function's arguments. After the function is finished, the local namespace is destroyed (with some exceptions that are outside the purview of this chapter). Consider the following function:

```
def func():
```

```
for i in range(5):
    a.append(i)
```

When func() is called, the empty list a is created, five elements are appended, and then a is destroyed when the function exits. Suppose instead we had declared a as follows:

```
a = []
def func():
    for i in range(5):
        a.append(i)
```

Assigning variables outside of the function's scope is possible, but those variables must be declared as global via the global keyword:

CAUTION

I generally discourage use of the global keyword.
Typically global variables are used to store some kind of
state in a system. If you find yourself using a lot of them, it
may indicate a need for object-oriented programming (using
classes).

Returning Multiple Values

When I first programmed in Python after having programmed in Java and C++, one of my favorite features was the ability to return multiple values from a function with simple syntax. Here's an example:

```
def f():
    a = 5
    b = 6
    c = 7
    return a, b, c
a, b, c = f()
```

In data analysis and other scientific applications, you may find yourself doing this often. What's happening here is that the function is actually just returning one object, namely a tuple, which is then being unpacked into the result variables. In the preceding example, we could have done this instead:

```
return_value = f()
```

In this case, return_value would be a 3-tuple with the three returned variables. A potentially attractive alternative to returning multiple values like before might be to return a dict instead:

```
def f():
    a = 5
    b = 6
    c = 7
    return ('a' : a, 'b' : b, 'c' : c)
```

This alternative technique can be useful depending on what you are trying to do.

Functions Are Objects

Since Python functions are objects, many constructs can be easily expressed that are difficult to do in other languages. Suppose we were doing some data cleaning and needed to apply a bunch of transformations to the following list of strings:

```
In [171]: states = [' Alabama', 'Georgia', 'Georgia', 'georgia', ....:

'south carolina##', 'West virginia?']
```

Anyone who has ever worked with user-submitted survey data has seen messy results like these. Lots of things need to happen to make this list of strings uniform and ready for analysis: stripping whitespace, removing punctuation symbols, and standardizing on proper capitalization. One way to do this is to use built-in string methods along with the re standard library module for regular expressions:

```
import re

def clean_strings(strings):
    result = {|
    for value in strings:
        value = value.strip()
        value = re.sub('[!e?]', '', value)
        value = value.ttile()
        result.append(value)
    return result
```

The result looks like this:

```
In [173]: cleam_strings(states)
Out[173]:
['Alabama',
'Georgia',
'Georgia',
'Georgia',
'Florida',
'South Carolina',
'Mest Virginia']
```

An alternative approach that you may find useful is to make a list of the operations you want to apply to a particular set of strings:

```
def remove_punctuation(value):
    return re.sub('[!e?]', '', value)

clean_ops = [str.strip, remove_punctuation, str.title]

def clean_strings(strings, ops):
    result = []
    for value in strings:
        for function in ops:
            value = function(value)
        result.append(value)
    return result
```

Then we have the following:

```
In [175]: clean_strings(states, clean_ops)
Out(175]:
('Alabama',
    'Georgia',
    'Georgia',
    'Georgia',
    'Florida',
    'South Carolina',
    'West Virginia']
```

A more functional pattern like this enables you to easily modify how the strings are transformed at a very high level. The clean_strings function is also now more reusable and generic.

You can use functions as arguments to other functions like the built-in map function, which applies a function to a sequence of some kind:

```
In [176]: for x im map(remove_punctuation, states):
.....: print(x)
Alabama
Georgia
Georgia
Georgia
georgia
stOrtida
South carolina
West virginia
```

Anonymous (Lambda) Functions

Python has support for so-called *anonymous* or *lambda* functions, which are a way of writing functions consisting of a single statement, the result of which is the return value. They are defined with the lambda keyword, which has no meaning other than "we are declaring an anonymous function":

```
def short_function(x):
    return x * 2
equiv_anon = lambda x: x * 2
```

I usually refer to these as lambda functions in the rest of the book. They are especially convenient in data analysis because, as you'll see, there are many cases where data transformation functions will take functions as arguments. It's often less typing (and clearer) to pass a lambda function as opposed to writing a full-out function declaration or even assigning the lambda function to a local variable. For example, consider this silly example:

```
def apply_to_list(some_list, f):
    return (f(x) for x in some_list)

ints = [4, 0, 1, 5, 6]
apply_to_list(ints, lambda x: x * 2)
```

You could also have written [x * 2 for x in ints], but here we were able to succinctly pass a custom operator to the $apply_to_list$ function.

As another example, suppose you wanted to sort a collection of strings by the number of distinct letters in each string:

```
In [177]: strings = ['foo', 'card', 'bar', 'aaaa', 'abab']
```

Here we could pass a lambda function to the list's sort method:

```
In [178]: strings.sort(key=lambda x: len(set(list(x))))
In [179]: strings
Out[179]: ('aaaa', 'foo', 'abab', 'bar', 'card')
```

NOTE

One reason lambda functions are called anonymous functions is that, unlike functions declared with the def keyword, the function object itself is never given an explicit __name__ attribute.

Currying: Partial Argument Application

Currying is computer science jargon (named after the mathematician Haskell Curry) that means deriving new functions from existing ones by partial argument application. For example, suppose we had a trivial function that adds two numbers together.

```
def add_numbers(x, y):
    return x + y
```

Using this function, we could derive a new function of one variable, add_five, that adds 5 to its argument:

```
add_five = lambda y: add_numbers(5, y)
```

The second argument to add_numbers is said to be curried. There's nothing very fancy here, as all we've really done is define a new function that calls an existing function. The built-in functools module can simplify this process using the partial function:

```
from functools import partial
add_five = partial(add_numbers, 5)
```

Generators

Having a consistent way to iterate over sequences, like objects in a list or lines in a file, is an important Python feature. This is accomplished by means of the *iterator protocol*, a generic way to make objects iterable. For example, iterating over a dict yields the dict keys:

When you write for key in some_dict, the Python interpreter first attempts to create an iterator out of some dict:

```
In [182]: dict_iterator = iter(some_dict)

In [183]: dict_iterator

Out[183]: dict_keyiterator at 0x7ff84e90ee58>
```

An iterator is any object that will yield objects to the Python interpreter when used in a context like a for loop. Most methods expecting a list or list-like object will also accept any iterable object. This includes built-in methods such as min, max, and sum, and type constructors like list and tuple:

```
In [184]: list(dict_iterator)
Out(184): ('a', 'b', 'c')
```

A generator is a concise way to construct a new iterable object. Whereas normal functions execute and return a single result at a time, generators return a sequence of multiple results lazily, pausing after each one until the next one is requested. To create a generator, use the yield keyword instead of return in a function:

```
def squares(n=10):
    print('Generating squares from 1 to (0)'.format(n ** 2))
    for i in range(1, n + 1):
        yield i ** 2
```

When you actually call the generator, no code is immediately executed:

```
In [186]: gen = squares()

In [187]: gen
Out[187]: cgenerator object squares at 0x7ff84e92bbf8>
```

It is not until you request elements from the generator that it begins executing its code:

```
In [188]: for x in gen:
....: print(x, end=' ')
Generating squares from 1 to 100
1 4 9 16 25 36 49 64 81 100
```

GENERATOR EXPRESSSIONS

Another even more concise way to make a generator is by using a generator expression. This is a generator analogue to list, diet, and set comprehensions; to create one, enclose what would otherwise be a list comprehension within parentheses instead of brackets:

```
In [189]: gen = (x ** 2 for x in range(100))

In [190]: gen
Out[190]: <generator object <genexpr> at 0x7ff84e92b150>
```

This is completely equivalent to the following more verbose generator:

Generator expressions can be used instead of list comprehensions as function arguments in many cases:

```
In [191]: sum(x ** 2 for x in range(100))
Out(191]: 328350
In [192]: dict(i, i **2) for i in range(5))
Out(192]: {0: 0, 1: 1, 2: 4, 3: 9, 4: 16}
```

ITERTOOLS MODULE

The standard library itertools module has a collection of generators for many common data algorithms. For example, groupby takes any sequence and a function, grouping consecutive elements in the sequence by return value of the function. Here's an example:

```
In [193]: import itertools

In [194]: first_letter = lambda x: x[0]

In [195]: names = ['Alan', 'Adam', 'Wes', 'Will', 'Albert', 'Steven']

In [196]: for letter, names in itertools.groupby(names, first_letter):
....: print(letter, list(names)) # names is a generator

A ['Alan', 'Adam']

W ('Wes', 'Will')
```

```
A ('Albert')
S ('Steven')
```

See Table 3-2 for a list of a few other itertools functions I've frequently found helpful. You may like to check out the official Python documentation for more on this useful built-in utility module.

Table 3-2. Some useful itertools functions

Function	Description
combinations(iterable,	Generates a sequence of all possible k-tuples of elements in the iterable, ignoring order an without replacement (see also the companion function combinations_with_replacement)
permutations(iterable,	Generates a sequence of all possible k-tuples of elements in the iterable, respecting order
groupby(iterable[, keyfunc])	Generates (key, sub-iterator) for each unique key
product(*iterables, repeat=1)	Generates the Cartesian product of the input iterables as tuples, similar to a nested for loop

Errors and Exception Handling

Handling Python errors or exceptions gracefully is an important part of building robust programs. In data analysis applications, many functions only work on certain kinds of input. As an example, Python's float function is capable of casting a string to a floating-point number, but fails with ValueError on improper inputs:

```
In [197]: float('1.2345')
Out[197]: 1.2345

In [198]: float('something')

ValueError Traceback (most recent cal cipython-input-198-2649e4ade8e6) in <module>()
---> 1 float('something')
ValueError: could not convert string to float: 'something'
```

Suppose we wanted a version of float that fails gracefully, returning the input argument. We can do this by writing a function that encloses the call to float in a try/except block:

```
def attempt_float(x):
    try:
        return float(x)
    except:
        return x
```

The code in the except part of the block will only be executed if float(x) raises an exception:

```
In (200): attempt_float('1.2345')
Out[200]: 1.2345
In (201): attempt_float('something')
Out[201]: 'something'
```

You might notice that ${\tt float}$ can raise exceptions other than ${\tt ValueError}$:

```
In [202]: float((1, 2))

TypeError Traceback (most recent cal cyphon-input-202-82f777b0e564> in cmodule>()
----> 1 float((1, 2))

TypeError: float() argument must be a string or a number, not 'tuple'
```

You might want to only suppress ValueError, since a TypeError (the input was not a string or numeric value) might indicate a legitimate bug in your program. To do that, write the exception type after except:

```
def attempt_float(x):
    try:
        return float(x)
    except ValueError:
        return x
```

We have then:

You can catch multiple exception types by writing a tuple of exception types instead (the parentheses are required):

```
def attempt_float(x):
    try:
    return float(x)
```

```
except (TypeError, ValueError):
    return x
```

In some cases, you may not want to suppress an exception, but you want some code to be executed regardless of whether the code in the try block succeeds or not. To do this, use finally:

```
f = open(path, 'w')
try:
    write_to_file(f)
finally:
    f.close()
```

Here, the file handle f will *always* get closed. Similarly, you can have code that executes only if the try: block succeeds using else:

```
f = open(path, 'w')
try:
    write_to_file(f)
except:
    print('failed')
else:
    print('Succeeded')
finally:
    f.close()
```

EXCEPTIONS IN IPYTHON

If an exception is raised while you are %run-ing a script or executing any statement, IPython will by default print a full call stack trace (traceback) with a few lines of context around the position at each point in the stack:

Having additional context by itself is a big advantage over the standard Python interpreter (which does not provide any additional context). You can control the amount of context shown using the %xmode magic command, from Plain (same as the standard Python interpreter) to Verbose (which inlines function argument values and more). As you will see later in the chapter, you can step into the stack (using the %debug or %pdb magics) after an error has occurred for interactive post-mortem debugging.

3.3 Files and the Operating System

Most of this book uses high-level tools like pandas.read_csv to read data files from disk into Python data structures. However, it's important to understand the basics of how to work with files in Python. Fortunately, it's very simple, which is one reason why Python is so popular for text and file munging.

To open a file for reading or writing, use the built-in open function with either a relative or absolute file path:

```
In (207): path = 'examples/segismundo.txt'
In (208): f = open(path)
```

By default, the file is opened in read-only mode 'r'. We can then treat the file handle f like a list and iterate over the lines like so:

```
for line in f:
pass
```

The lines come out of the file with the end-of-line (EOL) markers intact, so you'll often see code to get an EOL-free list of lines in a file like:

```
In [209]: lines = [x.rstrip() for x in open(path)]

In [210]: lines
Out[210]:
[Suefia el rico en su riqueza,',
'que más cuidados le ofrece;',
'',
'suefia el pobre que padece',
'su miseria y su pobreza;',
'',
'suefia el que a medrar empieza,',
'suefia el que afana y pretende,',
'suefia el que afana y orfende,',
'',
'y en el mundo, en conclusión,',
'todos suefian lo que son,',
'aunque ninguno lo entiende.',
'']
```

When you use open to create file objects, it is important to explicitly close the file when you are finished with it. Closing the file releases its resources back to the operating system:

```
In [211]: f.close()
```

One of the ways to make it easier to clean up open files is to use the with statement:

```
In [212]: with open(path) as f:
    ....: lines = (x.rstrip() for x in f)
```

This will automatically close the file f when exiting the with block.

If we had typed f = open(path, 'w'), a new file at examples/segismundo.txl would have been created (be carefull), overwriting any one in its place. There is also the 'x' file mode, which creates a writable file but fails if the file path already exists. See Table 3-3 for a list of all valid file read/write modes.

For readable files, some of the most commonly used methods are read, seek, and tell. read returns a certain number of characters from the file. What constitutes a "character" is determined by the file's encoding (e.g., UTF-8) or simply raw bytes if the file is opened in binary mode:

```
In (213): f = open(path)
In (214): f.read(18)
Out(214): 'Sueña el r'
In (215): f2 = open(path, 'rb') # Binary mode
In (216): f2.read(18)
Out(216): b'Sue\xcl\xbla el '
```

The read method advances the file handle's position by the number of bytes read. tell gives you the current position:

```
In [217]: f.tell()
Out(217): 11
In [218]: f2.tell()
Out(218]: 10
```

Even though we read 10 characters from the file, the position is 11 because it took that many bytes to decode 10 characters using the default encoding. You can check the default encoding in the sys module:

```
In (219): import sys
In (220): sys.getdefaultencoding()
Out(220): 'utf-8'
```

seek changes the file position to the indicated byte in the file:

```
In [221]: f.seek(3)
Out[221]: 3

In [222]: f.read(1)
Out[222]: 'A'
```

Lastly, we remember to close the files:

```
In [223]: f.close()
In [224]: f2.close()
```

Table 3-3. Python file modes

Mode	Description
r	Read-only mode
W	Write-only mode; creates a new file (erasing the data for any file with the same name)
×	Write-only mode; creates a new file, but fails if the file path already exists
a	Append to existing file (create the file if it does not already exist)
r+	Read and write
b	Add to mode for binary files (i.e., 'rb' or 'wb')
t	Text mode for files (automatically decoding bytes to Unicode). This is the default if not specified. Add t to other modes to use this (i.e., 'rt' or 'xt')

To write text to a file, you can use the file's write or writelines methods. For example, we could create a version of $prof_mod.py$ with no blank lines like so:

```
In [225]: with open('tmp.txt', 'w') as handle:
.....: handle.writelines(x for x in open(path) if len(x) > 1)

In [226]: with open('tmp.txt') as f:
.....: lines of.readlines()

In [227]: lines
Out[227]:
['Sueña el rico en su riqueza,\n',
'que más cuidados le ofrece;\n',
'sum de le pober que padece\n',
'sum iseria y su pobreza;\n',
'sueña el que a medrar empieza,\n',
'sueña el que afana y pretende,\n',
'sueña el que agravia y ofende,\n',
'y en el mundo, en conclusión,\n',
'todos sueñan lo que son,\n',
'aunque ninguno lo entiende.\n')
```

See Table 3-4 for many of the most commonly used file methods.

Method	Description
read([size])	Return data from file as a string, with optional size argument indicating the number of bytes to read
readlines([size])	Return list of lines in the file, with optional size argument
write(str)	Write passed string to file
writelines(strings)	Write passed sequence of strings to the file
close()	Close the handle
flush()	Flush the internal I/O buffer to disk
seek(pos)	Move to indicated file position (integer)
tell()	Return current file position as integer
closed	True if the file is closed

Bytes and Unicode with Files

The default behavior for Python files (whether readable or writable) is text mode, which means that you intend to work with Python strings (i.e., Unicode). This contrasts with binary mode, which you can obtain by appending b onto the file mode. Let's look at the file (which contains non-ASCII characters with UTF-8 encoding) from the previous section:

```
In [230]: with open(path) as f:
....: chars = f.read(10)

In [231]: chars
Out[231]: 'Sueña el r'
```

UTF-8 is a variable-length Unicode encoding, so when I requested some number of characters from the file, Python reads enough bytes (which could be as few as 10 or as many as 40 bytes) from the file to decode that many characters. If I open the file in 'rb' mode instead, read requests exact numbers of bytes:

```
In [232]: with open(path, 'rb') as f:
....: data = f.read(10)

In [233]: data
Out[233]: b'Sue\xc3\xb1a el '
```

Depending on the text encoding, you may be able to decode the bytes to a str object yourself, but only if each of the encoded Unicode characters is fully formed:

Text mode, combined with the encoding option of open, provides a convenient way to convert from one Unicode encoding to another:

Beware using seek when opening files in any mode other than binary. If the file position falls in the middle of the bytes defining a Unicode character, then subsequent reads will result in an error:

```
In [240]: f = open(path)

In [241]: f.read(5)

Out[241]: 'Sueña'

In [242]: f.seek(4)

Out[242]: 4

In [243]: f.read(1)

UnicodeDecodeError

Cipython-input-243-59354f952aa4> in <module>()

---> 1 f.read(1)

//miniconda/erws/book-erw/lib/python3.6/codecs.py in decode (self, input, 319 # decode input (taking the buffer into account)

320 data = self.buffer + input

--> 321 (result, consumed) = self_buffer_decode (data, self.e)

322 # heep undecoded input until the next call

323 self.buffer = data(consumed);

UnicodeDecodeError: 'utf-8' codec can't decode byte 0xb1 in position 0: tart byte

In [244]: f.close()
```

If you find yourself regularly doing data analysis on non-ASCII text data, mastering Python's Unicode functionality will prove valuable. See Python's online documentation for much more.

3.4 Conclusion

With some of the basics and the Python environment and language now under our belt, it's time to move on and learn about NumPy and array-oriented computing in Python.

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