Scientific Computing 272

Section 4: Lists in Python

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Section Outline



Data Collections

- ▶ Up to now, we have put a single value into a single variable
- ▶ But what if we want to work with collections of data?

Example (Data collection)

The number of whales sighted near a research station, counted each day for a two-week period, is given in the next table.

Day : 1	2	3	4	5	6	7	8	9	10	11	12	13	14
Whales: 5	4	7	3	2	3	2	6	4	2	1	7	1	3

- ► Without a collection data type, we need fourteen variables to store these values
- ► This is still manageable, but what if have data for a year, or a decade, or a century?

Lists

- ► Solution: Use a list
- Put the values, separated by commas, inside (square) brackets

Example (List)

```
>>> [5, 4, 7, 3, 2, 3, 2, 6, 4, 2, 1, 7, 1, 3]
[5, 4, 7, 3, 2, 3, 2, 6, 4, 2, 1, 7, 1, 3]
```

- ▶ list is a Python data type
- Therefore, we can have objects of type list
- ► A list can be assigned to a variable
- ► A list object owns methods
- ► There are standard functions that operate on lists

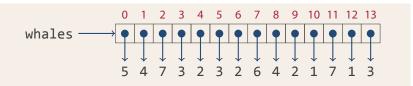
List Assignment

Example (Assign a list to a variable)

```
>>> whales = [5, 4, 7, 3, 2, 3, 2, 6, 4, 2, 1, 7, 1, 3]
>>> whales
[5, 4, 7, 3, 2, 3, 2, 6, 4, 2, 1, 7, 1, 3]
```

- ► The variable whales contains a **reference** to the list
- ► Each of the indices in the list contains a reference to a number

List Memory Model



List Indices

- Think of a list as a vector: Just as we can index over the vector components, we index over the elements in a list
- ► The first index is 0: Think of this as saying, "We are x positions from the front." Or: "There are x elements before this one."
- ► To refer to a particular item, put the index in brackets after a reference to the list, such as the name of a variable

Example (List indexing)

```
>>> whales = [5, 4, 7, 3, 2, 3, 2, 6, 4, 2, 1, 7, 1, 3]
>>> whales[0]
5
>>> whales[11]
7
>>> [2, 3, 5, 7, 11, 13, 17, 19, 23, 29][5]
13
```

Legal Indices

- For a list of length n, a legal index i is an integer in the set $\{0 \le i < n\}$
- ► Trying to use an out-of-range index is an error

Indexing out of range

```
>>> whales = [5, 4, 7, 3, 2, 3, 2, 6, 4, 2, 1, 7, 1, 3]
>>> whales[23]
Traceback (most recent call last):
   File "<stdin>", line 1, in <module>
IndexError: list index out of range
```

Indexing Backwards

- Python also lets us index backwards from the end of a list
- ▶ Since 0 = -0, index -1 refers to the last item, and so on
- ▶ We can also assign the values in a list to other variables

Example (Indexing backwards)

```
>>> whales = [5, 4, 7, 3, 2, 3, 2, 6, 4, 2, 1, 7, 1, 3]
>>> whales[-1]
3
>>> whales[-14]
5
>>> third = whales[2]
>>> print('On the third day', third, 'whales were seen.')
On the third day 7 whales were seen.
```

The Empty List

- In maths and computer science, we note identity elements
- For example, 0 for arithmetic, and the empty string for strings
- ► There is also an empty list, written [], with no elements

An empty list has no legal indices

```
>>> whales = []
>>> whales[0]
Traceback (most recent call last):
   File "<stdin>", line 1, in <module>
IndexError: list index out of range
>>> whales[-1]
Traceback (most recent call last):
   File "<stdin>", line 1, in <module>
IndexError: list index out of range
```

Legal Indices for the Empty List

- ► Trying to index into an empty list is always an error
- ▶ Legal indices *i* for a list of length *n* are in the set $\{i \in \mathbb{Z} \mid -n \le i < n\}$
- For an empty list, n = 0
- ► So, a legal index *i* must be in $\{0 \le i < 0\}$
- This set is empty
- So, there are no legal indices into an empty list

Lists Are Heterogeneous

- Lists can contain any type of data
- ► We can also "mix" different data types in one list
- ► Therefore, lists are called **heterogeneous**

Example (List heterogeneity)

```
>>> kr = ['Krypton', 'Kr', -157.2, -153.4]
>>> print(kr[0], 'boiling point is', kr[3], 'centigrade')
Krypton boiling point is -153.4 centigrade
```

- Using a list to aggregate data is not a good idea
- ► (We shall see better ways later)
- Besides, many list functions assume all items have the same type, and these functions fail if the items do not

Modifying Lists

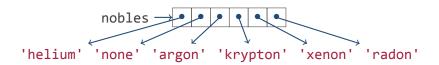
- Lists are mutable
- ▶ We can modify a list after it has been declared

Example (List mutation)

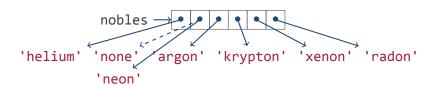
```
>>> nobles = ['helium', 'none', 'argon', 'krypton',
... 'xenon', 'radon']
>>> nobles
['helium', 'none', 'argon', 'krypton', 'xenon', 'radon']
>>> nobles[1] = 'neon'
>>> nobles
['helium', 'neon', 'argon', 'krypton', 'xenon', 'radon']
```

List Mutation

Before mutation



After mutation



Strings Are Immutable

- ► The expression L[i], where L is a list and i an index, behaves just like a normal variable
- On the right: "Get the value of the item at i in L"
- ► On the left: "Figure out where item i is in L so that we can overwrite it"
- Compare this to strings, where we cannot change a letter after the string has been created
- ► For example, upper() actually creates a new string

Example (Strings are immutable)

```
>>> name = 'Mendeleev'
>>> capitalized = name.upper()
>>> print(name, capitalized)
Mendeleev MENDELEEV
```

Built-In List Functions

Table: Built-in list functions

Function	Description
len(L)	Returns the number of items in list L
max(L)	Returns the maximum value in list L
min(L)	Returns the minimum value in list L
sum(L)	Returns the sum of the values in list L

- max and min use the natural order of the list elements, which have to be mutually comparable
- ▶ Note that we have seen some of these functions before
- ▶ 1en, for example, has previously been applied to strings

List Functions and Range Checking

Example (Half-lives of Plutonium)

```
>>> half lives = [87.74, 24110.0, 6537.0, 14.4, 376000.0]
>>> len(half lives)
5
>>> max(half lives)
376000.0
>>> min(half lives)
14.4
>>> sum(half lives)
406749,140000000001
>>> i = 2
>>> 0 <= i < len(half lives)
True
```

Note how we check whether an index is in range.

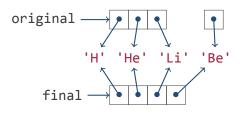
List Operations

Inappropriate list concatenation

```
>>> ['H', 'He', 'Li'] + 'Be'
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: can only concatenate list (not "str") to list
```

- Python complains if we try to combine a list with other types in inappropriate ways
- ▶ It is not possible to append a string to a list with the + operator
- But the + operator is overloaded for lists, so we can concatenate lists just like we can concatenate strings...

Memory Model for List Concatenation



Example (List concatenation)

```
>>> original = ['H', 'He', 'Li']
>>> final = original + ['Be']
>>> final
['H', 'He', 'Li', 'Be']
```

List Functions and Methods

Example

```
>>> 1 + 2 + 3
6
>>> sum([1, 2, 3])
6
>>> sum(['a', 'b', 'c'])
Traceback (most recent call last):
   File "<stdin>", line 1, in <module>
TypeError: unsupported operand type(s) for +: 'int' and 'str'
>>> metals = 'Fi Ni'.split()
>>> metals * 3
['Fi', 'Ni', 'Fi', 'Ni', 'Fi', 'Ni']
```

- sum requires its argument list to contain numbers
- ► Note how we use the split method of a string to turn the string 'Fe Ni' into a two-element list ['Fe', 'Ni']

Iteration and for Loops

- ▶ Python has lists so that we don't need to create *n* variables to store *n* values
- ► A for loop lets us **iterate** over a list, without having to write one statement per element
- We call it a loop, because it repeats a block of statements

General Form of a for Loop

- ► (iterable) is an iterable object like a list
- (variable) is a variable that takes on each of the values in the iterable object in turn
- ▶ **(block)** is a block of statements

What Happens in a for Loop

- ▶ Python executes the loop block once for each value in the iterable object
- Each pass through the block is called an iteration
- At the start of each iteration, Python assigns the next value in the iterable object to the variable
- So, we can do something with each value in turn
- ▶ Remember that the block statements must be indented
- ► In English, we would say: "For each element in the iterable object, perform the block of statements"

Looping with for

Example (for loop)

- Note that v functions like a normal variable
- ► So, we can perform arithmetic, etc.
- After the for loop has completed, the variable refers to the value it was assigned during the last execution of the loop

Nested Loops

Example (Nested Loops)

```
>>> outer = ['Li', 'Na', 'K']
>>> inner = ['F', 'Cl', 'Br']
>>> for metal in outer:
... for gas in inner:
            print(metal + gas, end=' ')
... print()
. . .
LiF LiCl LiBr
NaF NaCl NaBr
KF KCl KBr
>>> print('metal = {}, gas = {}'.format(metal, gas))
metal = K, gas = Br
```

The Basic Counting Principle: Number of Loop Iterations

If the outer loop runs n_{outer} times and the inner loop runs n_{inner} times for each of them, the inner loop executes $n_{\text{outer}} \times n_{\text{inner}}$ times.

Ranges

Use the range function to generate integer values in a specified range; it works only for ints. Of course, these statements don't necessarily have to do anything with either the iterable object or the values...

Example (Repetition)

```
>>> for i in range(3): # 0 <= i < 3
   print(i)
0
2
>>> for i in range(3): # 0 <= i < 3
       print('Hi there!')
Hi there!
Hi there!
Hi there!
```

Ranges

The range function can be called in three ways:

- ▶ range(n) for the values $0 \le i < n$ with step size 1
- range(m, n) for the values $m \le i < n$ with step size 1
- ▶ range(m, n, s) for the values $0 \le i < n$ with step size s

Example (Repetition)

```
>>> for i in range(-3, 0):
         print(i)
. . .
-3
-2
-1
>>> for i in range(4, 13, 3):
         print(i)
. . .
10
```

Nested Loops

Example (multiplication_table.py)

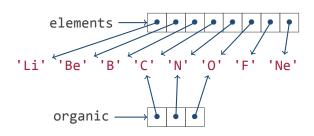
```
def print table(n):
    """Print the multiplication table for numbers 1 to n."""
    # print the headers row
    for i in range(1, n + 1):
        print('\t{}'.format(i))
    print() # end the header row
    # print the column number and the contents of the table
    for i in range(1, n + 1):
        print(i, end=' ')
        for j in range(1, n + 1):
            print('\t{}'.format(i * j), end=' ')
```

Slicing

- We can create a new list from an existing list by taking a slice
- For list, list[i:j] is the slice of the original list, from index i (inclusive) to index j (exclusive)

Example (List slicing)

Slicing Memory Model



- Slicing does not modify lists
- ► That means: Slicing leaves the original list intact
- ► And slicing returns a new list

List Slicing and Copying

- ► We may omit the first or last indices if we want to slice from the beginning or end, respectively
- ▶ We may omit both indices to obtain a copy of the original

Example (List slicing and copying)

```
>>> elements = ['Li', 'Be', 'B', 'C', 'N', 'O', 'F', 'Ne']
>>> elements[3:]
['C', 'N', 'O', 'F', 'Ne']
>>> elements[:5]
['Li', 'Be', 'B', 'C', 'N']
>>> copy = elements[:]
>>> elements.append('Na')
>>> elements
['Li', 'Be', 'B', 'C', 'N', 'O', 'F', 'Ne', 'Na']
>>> copy
['Li', 'Be', 'B', 'C', 'N', 'O', 'F', 'Ne']
```

Aliasing

- ► An alias is an alternative for something
- ► In Python, two variables are said be **aliased** if they refer to the same object, that is, contain the same reference
- ► If two variables contain a reference to the same list, modifying the list using one variable will be "seen" by the other

Example (Aliasing)

```
>>> elements = ['Li', 'Be', 'B', 'C', 'N', 'O', 'F', 'N']
>>> elements_copy = elements
>>> elements[7] = 'Ne'
>>> elements
['Li', 'Be', 'B', 'C', 'N', 'O', 'F', 'Ne']
>>> elements_copy
['Li', 'Be', 'B', 'C', 'N', 'O', 'F', 'Ne']
```

Aliasing in Function Calls

Example (List aliasing in functions)

```
>>> def sort and reverse(L):
        '''Return list L sorted and reversed.'''
... L.sort()
... L.reverse()
... return L
. . .
>>> elements = ['Li', 'Be', 'B', 'C', 'N', 'O', 'F', 'N']
>>> e2 = sort and reverse(elements)
>>> e2
['O', 'N', 'N', 'Li', 'F', 'C', 'Be', 'B']
>>> elements
['O', 'N', 'N', 'Li', 'F', 'C', 'Be', 'B']
>>> e2[3] = 'Oops'
>>> e2
['O', 'N', 'N', 'Oops', 'F', 'C', 'Be', 'B']
>>> elements
['O', 'N', 'N', 'Oops', 'F', 'C', 'Be', 'B']
```

List Methods

Method	Description
L.append(v)	Appends value v to list L, i.e. $L[len(L):] = [v]$
L.extend(M)	Appends all items in the iterable object M to the end of list L, i.e. L[len(L):] = M
L.index(v)	Returns the index of the first item whose value is v
L.insert(i, v)	Inserts value v at index i in list L, shifting following items to make room
L.pop()	Removes and returns the last element of L, which must be nonempty; L.pop(i) removes and returns the item at index i
L.remove(v)	Removes the first occurrence of value v from list L
L.reverse()	Reverses the order of the values in list L
L.sort()	Sorts the values in list L in ascending order

For sorting, Python uses **Timsort**, which is **adaptive**, meaning sorting is faster if list elements are sorted or almost sorted, and **stable**, meaning equal elements appear in the same order in the sorted list as they did in the unsorted list.

List Methods

Example (List methods)

```
>>> colours = 'red orange green black blue'.split()
>>> colours
['red', 'orange', 'green', 'black', 'blue']
>>> colours.remove('black')
>>> colours
['red', 'orange', 'green', 'blue']
>>> colours.insert(2, 'yellow')
>>> colours
['red', 'orange', 'yellow', 'green', 'blue']
>>> colours.append('purple')
>>> colours
['red', 'orange', 'yellow', 'green', 'blue', 'purple']
```

List Methods

- Remember that a list method modifies a list—it does not return a new list
- List methods may return the special value None; Python does not display anything when asked to evaluate None

Example (The special value None)

```
>>> x = None
>>> x
>>> print(x)
None
>>> colours = 'red yellow blue green'.split()
>>> colours
['red', 'yellow', 'blue', 'green']
>>> sorted_colours = colours.sort()
>>> colours
['blue', 'green', 'red', 'yellow']
```

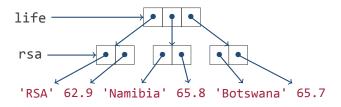
Nested Lists

- ► Since lists are heterogeneous, they can contain other lists
- ► We can also assign sublists to variables

Example (Nested lists)

```
>>> life = [['South Africa', 62.9],
... ['Namibia', 65.8],
           ['Botswana', 65.7]]
>>> life[0]
['South Africa', 62.9]
>>> print('Life expectancy in', life[1][0], 'is', life[1][1])
Life expectancy in Namibia is 65.8
>>> botswana = life[2]
>>> botswana[0]
'Botswana'
>>> botswana[1]
65.7
```

Aliasing in Nested Lists



Assigning a sublist to a variable creates an alias, so changes show up in the main list.

Example (Aliasing in nested lists)

```
>>> life = [['ZA', 62.9], ['NA', 65.8], ['BW', 65.7]]
>>> rsa = life[0]
>>> rsa[1] = 63
>>> life
[['RSA', 63], ['NA', 65.8], ['BW', 65.7]]
```

Other Sequences: Strings

- Formally, a string is an **immutable sequence** of characters
- ▶ Being a sequence, a string can be indexed and sliced

Example (Strings as sequences)

```
>>> rock = 'anthracite'
>>> rock[9]
'e'
>>> rock[0:3]
'ant'
>>> for character in rock[:5]:
... print(character, end=' ')
...
a n t h r
```

Other sequences: Tuples

- ► A **tuple** is a general sequence like a list, but unlike lists, they are immutable
- ► Tuples are written with parentheses instead of brackets
- ► The empty tuple is written ()
- ightharpoonup To avoid ambiguity, a tuple with one element x is written (x,)

Example (Tuples)

```
>>> bases = ('A', 'C', 'G', 'T')
>>> for base in bases:
... print(base, end=' ')
...
A C G T
```

Immutability of Tuples

Although tuples cannot be changed once created, the objects they refer to can still be changed—if these referenced objects are, themselves, mutable.

Tuples are immutable

```
>>> life = [['ZA', 62.9], ['NA', 65.8], ['BW', 65.7]]
>>> life[0] = life[1]
>>> life = (['ZA', 62.9], ['NA', 65.8], ['BW', 65.7])
>>> life[0] = life[1]
Traceback (most recent call last):
   File "<stdin>", line 1, in <module>
TypeError: 'tuple' object does not support item assignment
>>> life[0][1] = 63
>>> life
(['ZA', 63], ['NA', 65.8], ['BW', 65.7])
```

The sys Module and Command-Line Arguments

- ► The sys module provides access to variables used and maintained by the Python interpreter
- ► It also contains functions that interact "strongly" with the interpreter
- sys.argv is the list of command arguments passed to a Python script
- This means we don't have to run Python interactively or use input to get input from a user
- Careful: All items in sys.argv are strings, so convert them to appropriate numeric types if necessary
- ► Also, sys.argv[0] always contains the name of the script, including the .py extension if present

The sys Module and Command-Line Arguments

Example (print_cmd.py)

```
import sys

if __name__ == '__main__':
    for i in range(len(sys.argv)):
        print(i, sys.argv[i], type(sys.argv[i]))
```

Example (Use of sys.argv)

```
whkbester@h00:~$ python print_cmd.py calculate math.sqrt 22.0
0 print_cmd.py <type 'str'>
1 calculate <type 'str'>
2 math.sqrt <type 'str'>
3 22.0 <type 'str'>
```