Foundations of Data Science for Biologists

Introduction to Python

BIO 724D

10-JAN-2024

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Announcements

Please welcome new students who will be joining us

Class schedule for the next two weeks:

- Today is our first lecture/lab session (10 Jan)
- We will *not* meet tomorrow for a lunch session (11 Jan)
- No class on Monday (15 Jan)
- We will meet for our first lunch session next Thursday (18 Jan)
- After that, the regular pattern: lecture/lab on Mondays, lunch on Thursdays

Changes to assignments and grading:

- No more exit tickets on Thursdays; instead, include in the weekly problem set
- Earlier feedback on your notebooks and include in the weekly problem set

Why learn another programming language?

Why learn Python?

To expand your computing skills

- Work with non-tabular data (e.g., images, sound, text, results of simulations)
- Carry out modeling and simulations
- Use machine learning and artificial intelligence approaches to process data
- Automate tasks and instruments (e.g., use Arduino or Raspberry Pi to capture data)
- Carry out signal processing
- “Glue” code from multiple languages into a single workflow (bash, C, SQL, R, etc.)

To increase your value to future employers, collaborators, and mentees

What is Python?

A **general programming language** (GPL)

Python was designed by computer scientists to be as broadly applicable as possible

R is a more specialized language, designed by statisticians for statisticians

Python shares several familiar features with R:

very high-level language (VHLL): abstracted from hardware, highly portable

interpreted language: commands are read one at a time while the program executes

supports multiple programming paradigms: object-oriented, functional, and others

professionally maintained: ongoing bug fixes, feature expansions, library support

supports reproducible research: free, open-source, cross-platform, widely adopted

huge code base: covers a mind-boggling range of applications

extensive learning materials: videos, books, and websites

What makes Python different from R?

A general programming language

- Includes a greater diversity of data structures optimized for different purposes
- Object-oriented programming features are more extensive and especially powerful
- Scalable to enterprise level (used by Facebook, Instagram, YouTube, Reddit, etc.)

An emphasis on readability of code

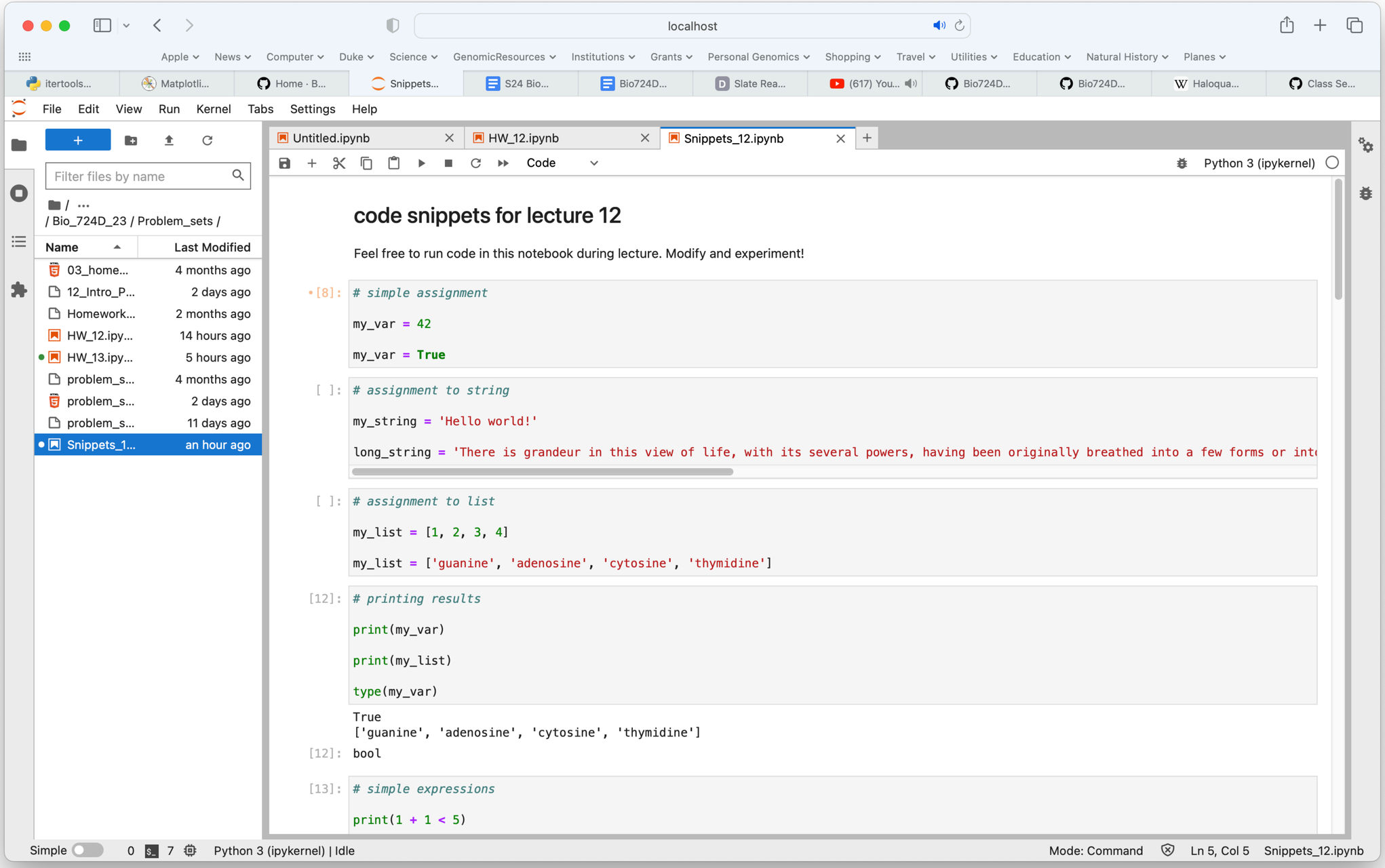
- Syntax is very clear, more so than just about any other language
- Uses numerous functional programming features to simplify code

An emphasis on ease of writing and debugging code

- Much larger set of standard libraries (“batteries included” philosophy)
- Exception handlers and error reporting are powerful and customizable
- Widely considered the best language for collaborative coding

JupyterLab notebooks

The JupyterLab interface



Introduction to Python for R programmers

Starting out with a new language

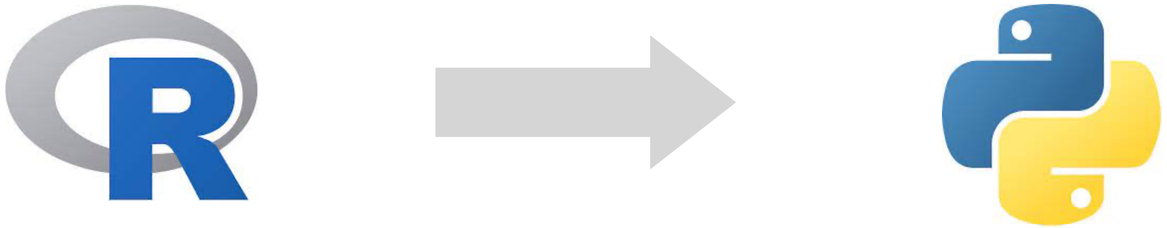
The good news: your experience with R will help (a lot!)

- Basic programming concepts remain the same
- Python and R share many features that some other languages do not

The challenge: differences between them can create unexpected errors and results

Today's goals:

- Get you working with Python code as quickly as possible
- Minimize the frustration caused by differences between the two languages



Similarities between R and Python

Many of the same **data types** are available: integer, float, boolean, string, list

Assignment and updating data objects is very similar

Square-bracket and name-based **indexing** are both available

Flow control works similarly, including how test conditions are defined

Defining and using basic **functions** is similar

Functional and object-oriented programming **paradigms** are available

However: there are important differences to be aware of in each case!

Assignment and operators

Basic assignment works similarly to R

- Data types are inferred from values (*dynamic typing*)
- Variable names can be re-assigned to new values / types (*re-binding*)
- Data types can be converted where sensible (called *casting* in Python)

Most of the common **operators** work similarly to R

- Arithmetic: `+`, `-`, `*`, `/`, `%`, `//` (but use `**` for exponentiation, not `^`)
- String: `+` (concatenate)
- Comparison: `==`, `!=`, `>`, `<`, `>=`, `<=`
- Logical: `and`, `or`, `not`
- Membership: `in`, `not in`

`red text = key differences from R`

Six key differences between R and Python

1. Larger set of standard data types and data structures
2. How data types and data structures are implemented
3. How indexing works
4. How some functions are implemented
5. How code is formatted
6. How libraries are used

These differences will cause most of your challenges in transitioning to Python

However: most are straightforward once you understand them

1 Diversity of data types and data structures

The **four common** data types in Python are: `int, float, str, bool`

Similar to R, except that they hold single values, not vectors of values

The **four common** data structures in Python are: `list, tuple, set, dictionary`

`list` is similar to R

The others are containers with no direct parallels in base R or the Tidyverse

Many **additional** standard data types / structures are available

A few commonly used data types are available through **third-party libraries**

NumPy: `ndarray` (n-dimensional arrays built from many different base data types)

Pandas: `Series` (named list) and `DataFrame` (enhanced data frame)

1.1 Identifying standard data types and data structures

Atomic types can be distinguished by their values (similar to R atomic vectors):

integer: number with no decimal (dot)

float: number with a decimal (dot), even if followed by zero or no decimal values

bool: `True, False` (no quotes)

string: quotes surrounding characters (including only numerals)

Data structures can be distinguished as follows:

list: item(s) enclosed in square brackets `['a', 'b', 'c']`

tuple: item(s) enclosed in round brackets `('a', 'b', 'c')`

set: item(s) enclosed in curly braces `{'a', 'b', 'c'}`

dictionary: key:value pair(s) in curly braces `{'a': 1, 'b': 2, 'c': 3 }`

Use `type()` to identify the type/class of any data object

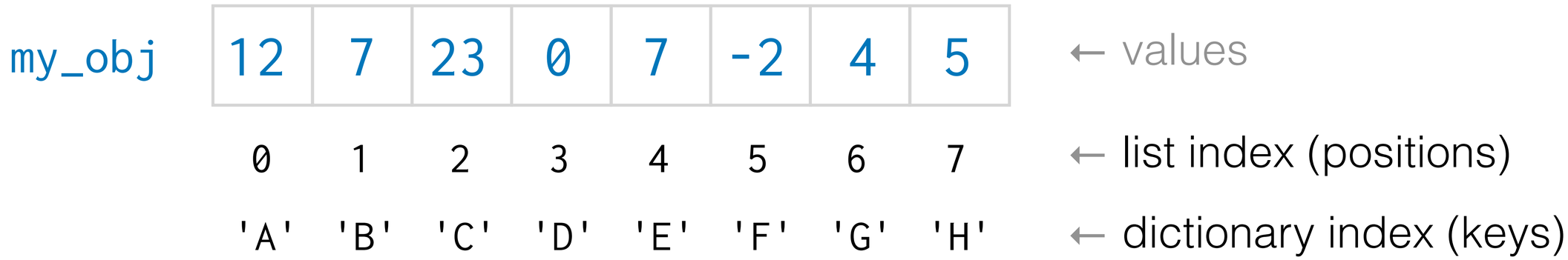
1.2 List and dictionary

These two data structures are common in Python programs

- Can hold a mix of any kind of objects and can be nested
- Provide many functions

Primary difference is how information is accessed

- Lists are indexed by **position**, dictionaries are indexed by **keys**
- Keys can be strings or numbers; each key must be unique but values can repeat



2 Implementation of data types and structures

Differences in how Python implements data types and structures are based on:

- Iterable data objects
- Mutable and immutable data objects

2.1 Iterables in Python

Only containers and strings are iterable

Iterable means that the object can return one value or item at a time

Unlike R, where almost every data type is iterable (because atomics are vectors)

Basic data types (`int`, `float`, `str`, `bool`, etc.) hold single values

Unlike R, where all "atomic" variables are actually vectors (even if of length 1)

Strings contain a single sequence of characters (including whitespaces)

Strings work differently in Python

Indexing and iterating is with reference to individual characters (not items, as in R)

All iterables (except strings) can hold a mix of data types

Unlike R, where only lists can contain items of different types

2.2 Mutable and immutable objects

Mutable data objects can be modified, **immutable** objects cannot

- Immutable data objects are useful as “read only” information
- Immutable data objects occupy less memory and provide much faster performance

Immutable objects *can* be deleted

- Re-binding the name of an immutable object to a different object deletes the data
- Mutability only refers to whether data contained in an object can be changed

2.3 Mutable and immutable objects, continued

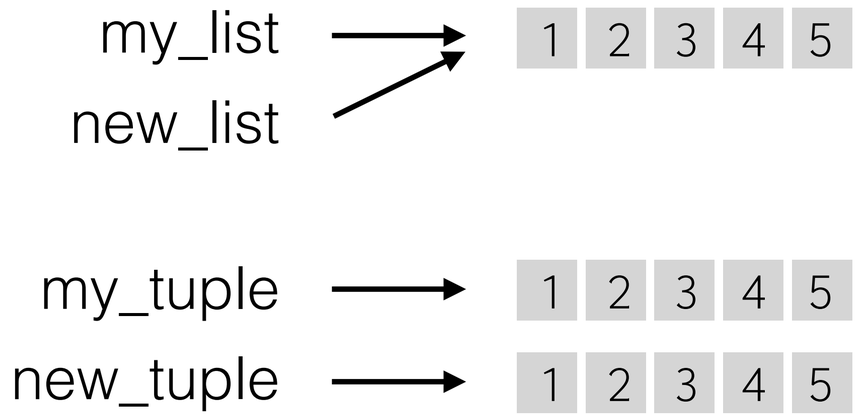
Assigning a mutable data object to a new identifier does not create a copy

This process creates an alias, but points to the same information in memory

Updating either the original or new identifier changes the data for *both*

This is not true for immutable objects; instead, a true copy is created

```
# assign an existing mutable object
my_list = [1, 2, 3,4, 5]
new_list = my_list
# now try with an immutable object
my_tuple = (1, 2, 3, 4, 5)
new_tuple = my_tuple
```

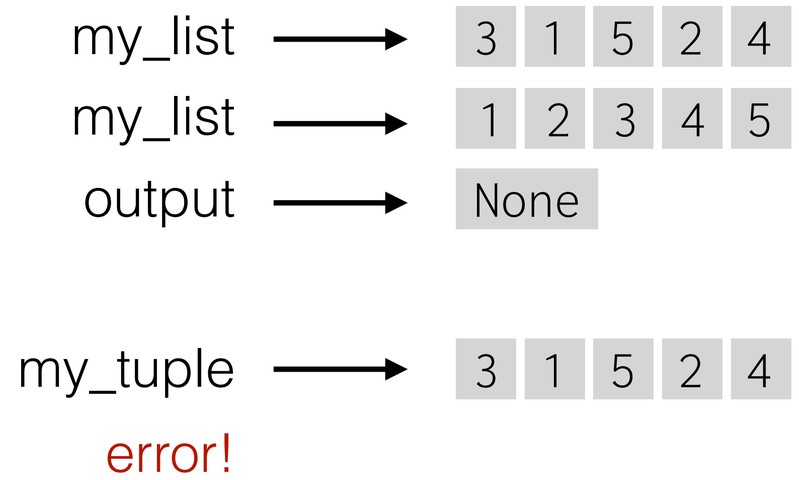


2.4 Mutable and immutable objects, continued

Many functions work differently when applied to mutable and immutable objects

- Mutable objects are typically altered *in place*
  - The function itself silently returns None
  - Assignment while applying a mutating function will create an undesirable result!
- Any function that alters contents cannot be applied to an immutable object

```
# apply sort to a mutable object
my_list = [3, 1, 5, 2, 4]
my_list.sort()
output = my_list.sort()
# now apply sort to an immutable object
my_tuple = (3, 1, 5, 2, 4)
my_tuple.sort()
```



3 Indexing

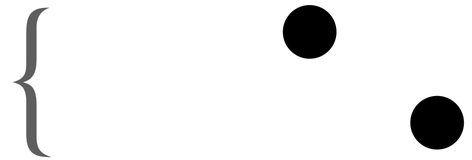
Square-bracket indexing in Python is different from R in two ways:

- zero-based
- slices do not include the end number

my_obj	12	7	23	0	8	-2	4	5	← values
	1	2	3	4	5	6	7	8	← R index
	0	1	2	3	4	5	6	7	← Python index

Examples:

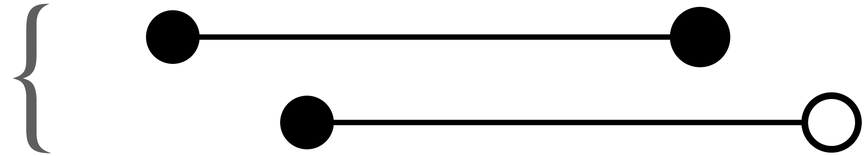
`my_obj[2]`



`[7]` R

`[23]` Py

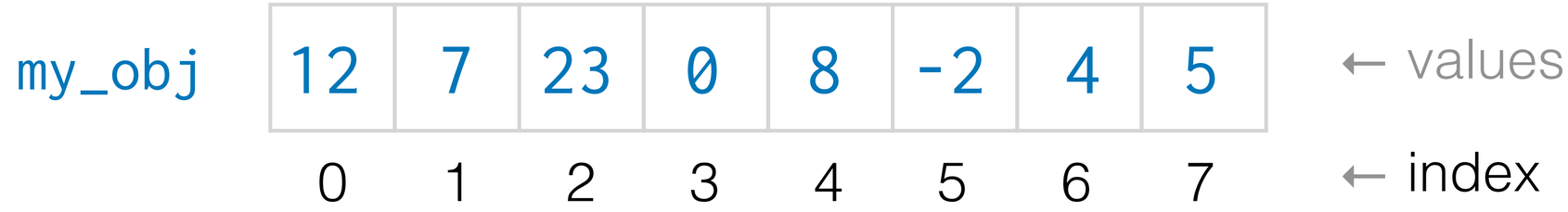
`my_obj[1:5]`



`[12, 7, 23, 0, 8]` R

`[7, 23, 0, 8]` Py

3.1 Examples of indexing



index	*return*	*notes*
`my_obj[1]`	`[7]`	single item
`my_obj[0:1]`	`[12]`	slice of length 1
`my_obj[3:]`	`[0, 8, -2, 4, 5]`	open slice to end
`my_obj[:2]`	`[12, 7]`	open slice from start
`my_obj[-1]`	`[5]`	last item
`my_obj[0:8:3]`	`[12, 0, 4]`	slice with step = 3
`my_obj[-1:0:-1]`	`[5, 4, -2, 8, 0, 23, 7]`	slice with reverse step
`my_obj[::-1]`	`[5, 4, -2, 8, 0, 23, 7, 12]`	reverse (“Martian smiley”)

4 Functions

Python has two representations of functions

Function: syntax and use are similar to functions in R

Method: function bound to a specific data class; they have a distinct syntax

```
# create a list
my_list = [5, 3, 1, 2, 4]
# call a function
function_result = len(my_list)        # functions take arguments
print(function_result)                # prints 5
# now call a method
my_list.sort()                        # methods are attached to objects
print(my_list)                        # returns [1, 2, 3, 4, 5]
my_string = 'hello world'
my_string.sort()                      # returns an AttributeError
```

5 Syntax and formatting

Python has a clear syntax

- Expressions often contain fewer characters than other programming languages
- Expressions mimic statements in English as much as possible
- Requires use of whitespace, unlike R and most other languages

Use indenting to indicate code code blocks

- Best practice is to use 4 spaces
- Any number of tabs or space is allowed, but must be consistent
- Indent 4 additional spaces to indicate a nested code blocks (no limit to nesting)

Use # to indicate comments (very similar to R)

- # at the beginning of a line makes the entire line a comment
- # in the middle of a line makes everything after it a comment

5.1 Syntax for flow control

Python provides `if`, `for`, and `while` flow control structures

- The basic syntax is similar to R, although a few additional options are available
- Test conditions are expressed in a similar way

To create a control structure:

- Use colon and indenting rather than curly braces to define the code block
- Stop indenting to indicate the end of the code block

```
# test for life stage of frogs
if gills == True :
    cohort = 'tadpole'
else :
    cohort = 'adult'
print('Cohort is', cohort)
```

```
# print out names of study group
for x in study_group :
    print('name:', x)
num = len(study_group)
print('total individuals =', num)
```

5.2 Syntax for creating a function

Creating a function in Python uses different syntax from R

- Use the `def` keyword rather than calling the `function()` function
- Use colon and indenting rather than curly braces to define the code block
- Do not use an assignment operator

```
# create a function to test whether 7 is a factor
def is_div_by_7(input_value) :
    if input_value % 7 == 0 : return True
    else: return False
# call the function
result_1 = is_div_by_7(3)
result_2 = is_div_by_7(42)
print(result_1, result_2)                    # returns False True
```

6 Libraries

A vast constellation of useful libraries is available for Python (as for R)

Standard modules: these are built and maintained by the Python Software Organization

- Quite extensive and provide many functions and data classes (“batteries included”)
- Do not need to be installed: distributed with Python installations and updates

Third-party packages: these are built and maintained by others (like packages in R)

- Quality, reliability, and compatibility with updates varies enormously
- Some are widely used and extremely reliable (e.g., SciPy, NumPy, Matplotlib, Pandas)
- Packages need to be installed before use and manually updated

6.1 Importing libraries

To access a library, you first need to import it within your program:

```
import csv
```

Provides access to all data structures and functions in the `csv` module

Best practice: place import statements at the beginning of a program or module

Multiple libraries can be imported by separating names with commas:

```
import csv, math, timedate
```

Aliases provide a convenient way to abbreviate names:

```
import numpy as np, pandas as pd
```

6.2 Using functions or data structures in libraries

To use a function in a library, precede with the module name and a period:

```
my_result = factorial(3)          # generates NameError (factorial not defined)
import math                       # factorial() is part of the math module
my_result = factorial(3)          # still generates a NameError
my_result = math.factorial(3)     # correct syntax!
print(my_result)                  # now we have the result: 6
```

This requirement prevents “name collisions” between libraries

Resources for Python

Resources for learning Python

Textbooks

Downey (2015) *Think Python* (2ed). Green Tea Press: here

McKinney (2022) *Python for Data Analysis* (3ed). O'Reilly: here (NumPy and pandas)

Tutorials

Software Carpentry: here

Wikiversity: here

w3schools: here

Resources for Python programming

Official Python documentation

The Python Language Reference: here

The Python Standard Library: here

General Python programming reference

Martelli et al. (2017) *Python in a Nutshell* (3ed). O'Reilly: here

Glossaries of Python terminology

Official Python Glossary: here

Python Lingo from Fluent Python: here

Python style guide

PEP 8: here