# Labs for Foundations of Applied Mathematics

Python Essentials

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### Preface

This lab manual is designed to accompany the textbook Foundations of Applied Mathematics by Humpherys, Jarvis and Evans. This manual begins with an introduction to Python [VD10] from scratch, which only requires a basic understanding of general programming concepts (variables, functions, etc.). Later labs introduce several Python packages that are essential for mathematical and scientific computing in Python.

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Part I Labs

# Introduction to Python

Lab Objective: Python is a powerful, general-purpose programming language. It can be used interactively, allowing for very rapid development. Python has many powerful scientific computing tools, making it an ideal language for applied and computational mathematics. In this introductory lab we introduce Python syntax, data types, functions, and control flow tools. These Python basics are an essential part of almost every problem you will solve and almost every program you will write.

#### **Getting Started**

Python is quickly gaining momentum as a fundamental tool in scientific computing. Anaconda is a free distribution service by Continuum Analytics, Inc., that includes the cross-platform Python interpreter (the software that actually executes Python code) and many Python libraries that are commonly used for applied and computational mathematics. To install Python via Anaconda, go to https://www.anaconda.com/download/, download the installer for Python 3.7 corresponding to your operating system, and follow the on-screen instructions. Note that Python 2.7 is syntactically different than Python 3.7, and support for Python 2 will be phased out by the end of 2020.

#### Running Python

Python files are saved with a .py extension. For beginners, we strongly recommend using a simple text editor for writing Python files. However, many free IDEs (Integrated Development Environments—large applications that facilitate code development with some sophisticated tools) are also compatible with Python. For now, the simpler the coding environment, the better.

A plain Python file looks similar to the following code.

The # character creates a single-line *comment*. Comments are ignored by the interpreter and serve as annotations for the accompanying source code. A pair of three quotes, """ """ or '''', creates a multi-line string literal, which may also be used as a multi-line comment. A triple-quoted string literal at the top of the file serves as the *header* for the file. The header typically identifies the author and includes instructions on using the file. Executable Python code comes after the header.

**Problem 1.** Open the file named python\_intro.py (or create the file in a text editor if you don't have it). Add your information to the header at the top, then add the following code.

```
if __name__ == "__main__":
    print("Hello, world!")  # Indent with four spaces (NOT a tab).
```

Open a command prompt (Terminal on Linux or Mac and Command Prompt or GitBash on Windows) and navigate to the directory where the new file is saved. Use the command 1s (or DIR on Windows) to list the files and folders in the current directory, pwd (CD , on Windows) to print the working directory, and cd to change directories.

Now the Python file can be executed with the following command:

```
$ python python_intro.py
```

If Hello, world! is displayed on the screen, you have just successfully executed your first Python program!

#### **IPython**

Python can be run interactively using several interfaces. The most basic of these is the Python interpreter. In this and subsequent labs, the triple brackets >>> indicate that the given code is being executed one line at a time via the Python interpreter.

There are, however, more useful interfaces. Chief among these is *IPython*, [PG07, jup] which is included with the Anaconda distribution. To execute a script in IPython, use the "run command."

 $<sup>^1\</sup>mathrm{See}\ \mathrm{https://ipython.org/}\ \mathrm{and}\ \mathrm{https://jupyter.org/}.$ 

```
>>> exit()  # Exit the Python interpreter.
$ ipython  # Start IPython.

In [1]: print("This is IPython!")  # Execute some code.
This is IPython!

In [2]: %run python_intro.py  # Run a particular Python script.
Hello, world!
```

One of the biggest advantages of IPython is that it supports *object introspection*, whereas the regular Python interpreter does not. Object introspection quickly reveals all methods and attributes associated with an object. IPython also has a built-in help() function that provides interactive help.

```
# A list is a basic Python data structure. To see the methods associated with
# a list, type the object name (list), followed by a period, and press tab.
In [1]: list. # Press 'tab'.
              append() count()
                                insert() remove()
             clear() extend() mro()
                                           reverse()
              copy()
                       index() pop()
                                           sort()
# To learn more about a specific method, use a '?' and hit 'Enter'.
In [1]: list.append?
Docstring: L.append(object) -> None -- append object to end
          method_descriptor
Type:
In [2]: help()
                                    # Start IPython's interactive help utility.
help> list
                                    # Get documentation on the list class.
Help on class list in module __builtin__:
class list(object)
 list() -> new empty list
 # ...
                                   # Press 'q' to exit the info screen.
help> quit
                                    # End the interactive help session.
```

#### NOTE

Use IPython side-by-side with a text editor to quickly test syntax and small code snippets. Testing small pieces of code in IPython **before** putting it into a program reveals errors and greatly speeds up the coding process. Consult the internet with questions; **stackoverflow.com** is a particularly valuable resource for answering common programming questions.

The best way to learn a new coding language is by actually writing code. Follow along with the examples in the yellow code boxes in this lab by executing them in an IPython console. Avoid copy and paste for now; your fingers need to learn the language as well.

#### **Python Basics**

#### Arithmetic

Python can be used as a calculator with the regular +, -, \*, and / operators. Use \*\* for exponentiation and % for modular division.

In most Python interpreters, the underscore character \_ is a variable with the value of the previous command's output, like the ANS button on many calculators.

```
>>> 12 * 3
36
>>> _ / 4
9.0
```

Data comparisons like < and > act as expected. The == operator checks for numerical equality and the <= and >= operators correspond to  $\le$  and  $\ge$ , respectively. To connect multiple boolean expressions, use the operators and, or, and not.<sup>2</sup>

```
>>> 3 > 2.99
True
>>> 1.0 <= 1 or 2 > 3
True
>>> 7 == 7 and not 4 < 4
True

>>> True and True and True and True and False
False
>>> False or False or False or False or True
True
>>> True or not True
True
```

#### **Variables**

Variables are used to temporarily store data. A **single** equals sign = assigns one or more values (on the right) to one or more variable names (on the left). A **double** equals sign == is a comparison operator that returns **True** or **False**, as in the previous code block.

Unlike many programming languages, Python does not require a variable's data type to be specified upon initialization. Because of this, Python is called a *dynamically typed* language.

<sup>&</sup>lt;sup>2</sup>In many other programming languages, the and, or, and not operators are written as &&, ||, and !, respectively. Python's convention is much more readable and does not require parentheses.

#### **Functions**

To define a function, use the def keyword followed by the function name, a parenthesized list of parameters, and a colon. Then indent the function body using exactly four spaces.

```
>>> def add(x, y):
... return x + y # Indent with four spaces.
```

#### ACHTUNG!

Many other languages use the curly braces {} to delimit blocks, but Python uses whitespace indentation. In fact, whitespace is essentially the only thing that Python is particularly picky about compared to other languages: mixing tabs and spaces confuses the interpreter and causes problems. Most text editors have a setting to set the indentation type to spaces so you can use the tab key on your keyboard to insert four spaces (sometimes called *soft tabs*). For consistency, never use tabs; always use spaces.

Functions are defined with *parameters* and are called with *arguments*, although the terms are often used interchangeably. Below, width and height are parameters for the function area(). The values 2 and 5 are the arguments that are passed when calling the function.

```
>>> def area(width, height):  # Define the function.
... return width * height
...
>>> area(2, 5)  # Call the function.
10
```

Python functions can also return multiple values.

The keyword lambda is a shortcut for creating one-line functions. For example, the polynomials  $f(x) = 6x^3 + 4x^2 - x + 3$  and  $g(x, y, z) = x + y^2 - z^3$  can be defined as functions in one line each.

```
# Define the polynomials the usual way using 'def'.
>>> def f(x):
...    return 6*x**3 + 4*x**2 - x + 3
>>> def g(x, y, z):
...    return x + y**2 - z**3

# Equivalently, define the polynomials quickly using 'lambda'.
>>> f = lambda x: 6*x**3 + 4*x**2 - x + 3
>>> g = lambda x, y, z: x + y**2 - z**3
```

#### NOTE

Documentation is important in every programming language. Every function should have a docstring—a string literal in triple quotes just under the function declaration—that describes the purpose of the function, the expected inputs and return values, and any other notes that are important to the user. Short docstrings are acceptable for very simple functions, but more complicated functions require careful and detailed explanations.

```
>>> def add(x, y):
... """Return the sum of the two inputs."""
... return x + y

>>> def area(width, height):
... """Return the area of the rectangle with the specified width
... and height.
... """
... return width * height
...
>>> def arithmetic(a, b):
... """Return the difference and the product of the two inputs."""
... return a - b, a * b
```

Lambda functions cannot have custom docstrings, so the lambda keyword should only be used as a shortcut for very simple or intuitive functions that do not need additional labeling.

**Problem 2.** The volume of a sphere with radius r is  $V = \frac{4}{3}\pi r^3$ . In your Python file from Problem 1, define a function called **sphere\_volume()** that accepts a single parameter r. Return the volume of the sphere of radius r, using 3.14159 as an approximation for  $\pi$  (for now). Also write an appropriate docstring for your function.

To test your function, call it under the if \_\_name\_\_ == "\_\_main\_\_" clause and print the returned value. Run your file to see if your answer is what you expect it to be.

#### ACHTUNG!

The return statement instantly ends the function call and passes the return value to the function caller. However, functions are not required to have a return statement. A function without a return statement implicitly returns the Python constant None, which is similar to the special value null of many other languages. Calling print() at the end of a function does not cause a function to return any values.

If you have any intention of using the results of a function, use a return statement.

It is also possible to specify *default values* for a function's parameters. In the following example, the function pad() has three parameters, and the value of c defaults to 0. If it is not specified in the function call, the variable c will contain the value 0 when the function is executed.

```
>>> def pad(a, b, c=0):
... """Print the arguments, plus a zero if c is not specified."""
... print(a, b, c)
...
>>> pad(1, 2, 3)  # Specify each parameter.
1 2 3
>>> pad(1, 2)  # Specify only non-default parameters.
1 2 0
```

Arguments are passed to functions based on position or name, and positional arguments must be defined before named arguments. For example, a and b must come before c in the function definition of pad(). Examine the following code blocks demonstrating how positional and named arguments are used to call a function.

```
# Try defining printer with a named argument before a positional argument.
>>> def pad(c=0, a, b):
... print(a, b, c)
...
SyntaxError: non-default argument follows default argument
```

```
# Correctly define pad() with the named argument after positional arguments.
>>> def pad(a, b, c=0):
        """Print the arguments, plus a zero if c is not specified."""
        print(a, b, c)
# Call pad() with 3 positional arguments.
>>> pad(2, 4, 6)
2 4 6
# Call pad() with 3 named arguments. Note the change in order.
>>> pad(b=3, c=5, a=7)
7 3 5
# Call pad() with 2 named arguments, excluding c.
>>> pad(b=1, a=2)
2 1 0
# Call pad() with 1 positional argument and 2 named arguments.
>>> pad(1, c=2, b=3)
1 3 2
```

**Problem 3.** The built-in **print()** function has the useful keyword arguments **sep** and **end**. It accepts any number of positional arguments and prints them out with **sep** inserted between values (defaulting to a space), then prints **end** (defaulting to the *newline character* '\n').

Write a function called isolate() that accepts five arguments. Print the first three separated by 5 spaces, then print the rest with a single space between each output. For example,

```
>>> isolate(1, 2, 3, 4, 5)
1 2 3 4 5
```

#### **Data Types and Structures**

#### **Numerical Types**

Python has four numerical data types: int, long, float, and complex. Each stores a different kind of number. The built-in function type() identifies an object's data type.

Python has two types of division: integer and float. The / operator performs float division (true fractional division), and the // operator performs integer division, which rounds the result down to the next integer. If both operands for // are integers, the result will be an int. If one or both operands are floats, the result will be a float. Regular division with / always returns a float.

Python also supports computations of complex numbers by pairing two numbers as the real and imaginary parts. Use the letter j, not i, for the imaginary part.

#### Strings

In Python, strings are created with either single or double quotes. To concatenate two or more strings, use the + operator between string variables or literals.

```
>>> str1 = "Hello"
>>> str2 = 'world'
>>> my_string = str1 + " " + str2 + '!'
>>> my_string
'Hello world!'
```

Parts of a string can be accessed using *slicing*, which is indicated by square brackets [ ]. Slicing syntax is [start:stop:step]. The parameters start and stop default to the beginning and end of the string, respectively. The parameter step defaults to 1.

```
>>> my_string[6:]
'world!'

# Slice from the 3rd to the 8th character (not including the 8th character).
>>> my_string[3:8]
'lo wo'

# Get every other character in the string.
>>> my_string[::2]
'Hlowrd'
```

#### Problem 4. Write two new functions called first\_half() and backward().

- first\_half() should accept a parameter and return the first half of it, excluding the middle character if there is an odd number of characters.
   (Hint: the built-in function len() returns the length of the input.)
- 2. The backward() function should accept a parameter and reverse the order of its characters using slicing, then return the reversed string.

(Hint: The step parameter used in slicing can be negative.)

Use IPython to quickly test your syntax for each function.

#### Lists

A Python list is created by enclosing comma-separated values with square brackets [ ]. Entries of a list do **not** have to be of the same type. Access entries in a list by using the same indexing or slicing operations as used with strings.

```
>>> my_list = ["Hello", 93.8, "world", 10]
>>> my_list[0]
'Hello'
>>> my_list[-2]
'world'
>>> my_list[:2]
['Hello', 93.8]
```

Common list methods (functions) include append(), insert(), remove(), and pop(). Consult IPython for details on each of these methods using object introspection.

```
>>> my_list = [1, 2]  # Create a simple list of two integers.
>>> my_list.append(4)  # Append the integer 4 to the end.
>>> my_list.insert(2, 3)  # Insert 3 at location 2.
>>> my_list
[1, 2, 3, 4]
>>> my_list.remove(3)  # Remove 3 from the list.
>>> my_list.pop()  # Remove (and return) the last entry.
```

```
4
>>> my_list
[1, 2]
```

Slicing is also very useful for replacing values in a list.

```
>>> my_list = [10, 20, 30, 40, 50]

>>> my_list[0] = -1

>>> my_list[3:] = [8, 9]

>>> print(my_list)

[-1, 20, 30, 8, 9]
```

The in operator quickly checks if a given value is in a list (or another iterable, including strings).

```
>>> my_list = [1, 2, 3, 4, 5]
>>> 2 in my_list
True
>>> 6 in my_list
False
>>> 'a' in "xylophone" # 'in' also works on strings.
False
```

#### **Tuples**

A Python tuple is an ordered collection of elements, created by enclosing comma-separated values with parentheses (and ). Tuples are similar to lists, but they are much more rigid, have less built-in operations, and cannot be altered after creation. Therefore, lists are preferable for managing dynamic, ordered collections of objects.

When multiple objects are returned by a function, they are returned as a tuple. For example, recall that the arithmetic() function returns two values.

```
>>> x, y = arithmetic(5,2)  # Get each value individually,
>>> print(x, y)
3 10
>>> both = arithmetic(5,2)  # or get them both as a tuple.
>>> print(both)
(3, 10)
```

**Problem 5.** Write a function called list\_ops(). Define a list with the entries "bear", "ant", "cat", and "dog", in that order. Then perform the following operations on the list:

- 1. Append "eagle".
- 2. Replace the entry at index 2 with "fox".
- 3. Remove (or pop) the entry at index 1.

- 4. Sort the list in reverse alphabetical order.
- Replace "eagle" with "hawk".
   (Hint: the list's index() method may be helpful.)
- 6. Add the string "hunter" to the last entry in the list.

Return the resulting list.

Work out (on paper) what the result should be, then check that your function returns the correct list. Consider printing the list at each step to see the intermediate results.

#### Sets

A Python set is an unordered collection of distinct objects. Objects can be added to or removed from a set after its creation. Initialize a set with curly braces { } and separate the values by commas, or use set() to create an empty set. Like mathematical sets, Python sets have operations such as union, intersection, difference, and symmetric difference.

```
# Initialize some sets. Note that repeats are not added.
>>> gym_members = {"Doe, John", "Doe, John", "Smith, Jane", "Brown, Bob"}
>>> print(gym_members)
{'Doe, John', 'Brown, Bob', 'Smith, Jane'}

>>> gym_members.add("Lytle, Josh")  # Add an object to the set.
>>> gym_members.discard("Doe, John")  # Delete an object from the set.
>>> print(gym_members)
{'Lytle, Josh', 'Brown, Bob', 'Smith, Jane'}

>>> gym_members.intersection({"Lytle, Josh", "Henriksen, Ian", "Webb, Jared"})
{'Lytle, Josh'}
>>> gym_members.difference({"Brown, Bob", "Sharp, Sarah"})
{'Lytle, Josh', 'Smith, Jane'}
```

#### **Dictionaries**

Like a set, a Python dict (dictionary) is an unordered data type. A dictionary stores key-value pairs, called *items*. The values of a dictionary are indexed by its keys. Dictionaries are initialized with curly braces, colons, and commas. Use dict() or {} to create an empty dictionary.

```
>>> my_dictionary = {"business": 4121, "math": 2061, "visual arts": 7321}
>>> print(my_dictionary["math"])
2061

# Add a value indexed by 'science' and delete the 'business' keypair.
>>> my_dictionary["science"] = 6284
>>> my_dictionary.pop("business") # Use 'pop' or 'popitem' to remove.
4121
>>> print(my_dictionary)
```

```
{'math': 2061, 'visual arts': 7321, 'science': 6284}

# Display the keys and values.
>>> my_dictionary.keys()
dict_keys(['math', 'visual arts', 'science'])
>>> my_dictionary.values()
dict_values([2061, 7321, 6284])
```

As far as data access goes, lists are like dictionaries whose keys are the integers  $0, 1, \ldots, n-1$ , where n is the number of items in the list. The keys of a dictionary need not be integers, but they must be immutable, which means that they must be objects that cannot be modified after creation. We will discuss mutability more thoroughly in the Standard Library lab.

#### Type Casting

The names of each of Python's data types can be used as functions to cast a value as that type. This is particularly useful for converting between integers and floats.

```
# Cast numerical values as different kinds of numerical values.
>>> x = int(3.0)
>>> y = float(3)
>>> z = complex(3)
>>> print(x, y, z)
3 3.0 (3+0j)
# Cast a list as a set and vice versa.
>>> set([1, 2, 3, 4, 4])
{1, 2, 3, 4}
>>> list({'a', 'a', 'b', 'b', 'c'})
['a', 'c', 'b']
# Cast other objects as strings.
>>> str(['a', str(1), 'b', float(2)])
"['a', '1', 'b', 2.0]"
>>> str(list(set([complex(float(3))])))
'[(3+0j)]'
```

#### **Control Flow Tools**

Control flow blocks dictate the order in which code is executed. Python supports the usual control flow statements including if statements, while loops, and for loops.

#### The If Statement

An if statement executes the indented code if (and only if) the given condition holds. The elif statement is short for "else if" and can be used multiple times following an if statement, or not at all. The else keyword may be used at most once at the end of a series of if/elif statements.

```
>>> food = "bagel"
>>> if food == "apple":  # As with functions, the colon denotes
... print("72 calories")  # the start of each code block.
... elif food == "banana" or food == "carrot":
... print("105 calories")
... else:
... print("calorie count unavailable")
...
calorie count unavailable
```

**Problem 6.** Write a function called pig\_latin(). Accept a parameter word, translate it into Pig Latin, then return the translation. Specifically, if word starts with a vowel, add "hay" to the end; if word starts with a consonant, take the first character of word, move it to the end, and add "ay".

(Hint: use the in operator to check if the first letter is a vowel.)

#### The While Loop

A while loop executes an indented block of code while the given condition holds.

```
>>> i = 0
>>> while i < 10:
... print(i, end=' ')  # Print a space instead of a newline.
... i += 1  # Shortcut syntax for i = i+1.
...
0 1 2 3 4 5 6 7 8 9
```

There are two additional useful statements to use inside of loops:

- 1. break manually exits the loop, regardless of which iteration the loop is on or if the termination condition is met.
- 2. continue skips the current iteration and returns to the top of the loop block if the termination condition is still not met.

```
>>> while i < 10:
... i += 1
... if i % 3 == 0:
... continue  # Skip multiples of 3.
... print(i, end=' ')
1 2 4 5 7 8 10
```

#### The For Loop

A for loop iterates over the items in any *iterable*. Iterables include (but are not limited to) strings, lists, sets, and dictionaries.

```
>>> colors = ["red", "green", "blue", "yellow"]
>>> for entry in colors:
... print(entry + "!")
...
red!
green!
blue!
yellow!
```

The break and continue statements also work in for loops. A continue in a for loop will automatically increment the index or item, whereas a continue in a while loop makes no automatic changes to any variable.

```
>>> for word in ["It", "definitely", "looks", "pretty", "bad", "today"]:
...     if word == "definitely":
...         continue
...     elif word == "bad":
...         break
...     print(word, end=' ')
...
It looks pretty
```

In addition, Python has some very useful built-in functions that can be used in conjunction with the for statement:

- 1. range(start, stop, step): Produces a sequence of integers, following slicing syntax. If only one argument is specified, it produces a sequence of integers from 0 to the argument, incrementing by one. This function is used **very** often.
- 2. zip(): Joins multiple sequences so they can be iterated over simultaneously.
- 3. enumerate(): Yields both a count and a value from the sequence. Typically used to get both the index of an item and the actual item simultaneously.
- 4. reversed(): Reverses the order of the iteration.
- 5. sorted(): Returns a new list of sorted items that can then be used for iteration.

Each of these functions, except for sorted(), returns an *iterator*, an object that is built specifically for looping but not for creating actual lists. To put the items of the sequence in a collection, use list(), set(), or tuple().

```
# Strings and lists are both iterables.
>>> vowels = "aeiou"
>>> colors = ["red", "yellow", "white", "blue", "purple"]
# Iterate by index.
>>> for i in range(5):
      print(i, vowels[i], colors[i])
. . .
0 a red
1 e yellow
2 i white
3 o blue
4 u purple
# Iterate through both sequences at once.
>>> for letter, word in zip(vowels, colors):
        print(letter, word)
. . .
a red
e yellow
i white
o blue
u purple
# Get the index and the item simultaneously.
>>> for i, color in enumerate(colors):
       print(i, color)
. . .
. . .
0 red
1 yellow
2 white
3 blue
4 purple
# Iterate through the list in sorted (alphabetical) order.
>>> for item in sorted(colors):
        print(item, end=' ')
. . .
blue purple red white yellow
# Iterate through the list backward.
>>> for item in reversed(colors):
        print(item, end=' ')
. . .
purple blue white yellow red
```

**Problem 7.** This problem originates from https://projecteuler.net, an excellent resource for math-related coding problems.

A palindromic number reads the same both ways. The largest palindrome made from the product of two 2-digit numbers is  $9009 = 91 \times 99$ . Write a function called palindrome() that finds and returns the largest palindromic number made from the product of two 3-digit numbers.

#### List Comprehension

A list comprehension uses for loop syntax between square brackets to create a list. This is a powerful, efficient way to build lists. The code is concise and runs quickly.

```
>>> [float(n) for n in range(5)]
[0.0, 1.0, 2.0, 3.0, 4.0]
```

List comprehensions can be thought of as "inverted loops", meaning that the body of the loop comes before the looping condition. The following loop and list comprehension produce the same list, but the list comprehension takes only about two-thirds the time to execute.

```
>>> loop_output = []
>>> for i in range(5):
... loop_output.append(i**2)
...
>>> list_output = [i**2 for i in range(5)]
```

Tuple, set, and dictionary comprehensions can be done in the same way as list comprehensions by using the appropriate style of brackets on the end.

```
>>> colors = ["red", "blue", "yellow"]
>>> {c[0]:c for c in colors}
{'r': 'red', 'b': 'blue', 'y': 'yellow'}
>>> {"bright " + c for c in colors}
```

{'bright blue', 'bright red', 'bright yellow'}

**Problem 8.** The alternating harmonic series is defined as follows.

$$\sum_{n=1}^{\infty} \frac{(-1)^{(n+1)}}{n} = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \frac{1}{5} - \dots = \ln(2)$$

Write a function called  ${\tt alt\_harmonic}()$  that accepts an integer n. Use a list comprehension to quickly compute the sum of the first n terms of this series (be careful not to compute only n-1 terms). The sum of the first 500,000 terms of this series approximates  $\ln(2)$  to five decimal places.

(Hint: consider using Python's built-in sum() function.)

#### Additional Material

#### **Further Reading**

Refer back to this and other introductory labs often as you continue getting used to Python syntax and data types. As you continue your study of Python, we strongly recommend the following readings.

- The official Python tutorial: http://docs.python.org/3.6/tutorial/introduction.html (especially chapters 3, 4, and 5).
- Section 1.2 of the SciPy lecture notes: http://scipy-lectures.github.io/.
- PEP8 Python style guide: http://www.python.org/dev/peps/pep-0008/.

#### **Generalized Function Input**

On rare occasion, it is necessary to define a function without knowing exactly what the parameters will be like or how many there will be. This is usually done by defining the function with the parameters \*args and \*\*kwargs. Here \*args is a list of the positional arguments and \*\*kwargs is a dictionary mapping the keywords to their argument. This is the most general form of a function definition.

See https://docs.python.org/3.6/tutorial/controlflow.html for more on this topic.

#### **Function Decorators**

A function decorator is a special function that "wraps" other functions. It takes in a function as input and returns a new function that pre-processes the inputs or post-processes the outputs of the original function.

```
>>> def typewriter(func):
... """Decorator for printing the type of output a function returns"""
... def wrapper(*args, **kwargs):
... output = func(*args, **kwargs)  # Call the decorated function.
... print("output type:", type(output)) # Process before finishing.
... return output  # Return the function output.
... return wrapper
```

The outer function, typewriter(), returns the new function wrapper(). Since wrapper() accepts \*args and \*\*kwargs as arguments, the input function func() accepts any number of positional or keyword arguments.

Apply a decorator to a function by tagging the function's definition with an @ symbol and the decorator name.

```
>>> @typewriter
... def combine(a, b, c):
... return a*b // c
```

Placing the tag above the definition is equivalent to adding the following line of code after the function definition:

```
>>> combine = typewriter(combine)
```

Now, calling combine() actually calls wrapper(), which then calls the original combine().

```
>>> combine(3, 4, 6)
output type: <class 'int'>
2
>>> combine(3.0, 4, 6)
output type: <class 'float'>
2.0
```

Function decorators can also be customized with arguments. This requires another level of nesting: the outermost function must define and return a decorator that defines and returns a wrapper.

```
>>> def repeat(times):
        """Decorator for calling a function several times."""
        def decorator(func):
            def wrapper(*args, **kwargs):
                for _ in range(times):
                    output = func(*args, **kwargs)
                return output
            return wrapper
        return decorator
. . .
>>> @repeat(3)
... def hello_world():
        print("Hello, world!")
>>> hello_world()
Hello, world!
Hello, world!
Hello, world!
```

See https://www.python.org/dev/peps/pep-0318/ for more details.

# $\mathcal{I}$

# The Standard Library

Lab Objective: Python is designed to make it easy to implement complex tasks with little code. To that end, every Python distribution includes several built-in functions for accomplishing common tasks. In addition, Python is designed to import and reuse code written by others. A Python file with code that can be imported is called a module. All Python distributions include a collection of modules for accomplishing a variety of tasks, collectively called the Python Standard Library. In this lab we explore some built-in functions, learn how to create, import, and use modules, and become familiar with the standard library.

#### **Built-in Functions**

Python has several built-in functions that may be used at any time. IPython's object introspection feature makes it easy to learn about these functions: start IPython from the command line and use? to bring up technical details on each function.

```
In [1]: min?
Docstring:
min(iterable, *[, default=obj, key=func]) -> value
min(arg1, arg2, *args, *[, key=func]) -> value

With a single iterable argument, return its smallest item. The
default keyword-only argument specifies an object to return if
the provided iterable is empty.
With two or more arguments, return the smallest argument.
Type: builtin_function_or_method

In [2]: len?
Signature: len(obj, /)
Docstring: Return the number of items in a container.
Type: builtin_function_or_method
```

| Function         | Returns  |  |  |
|------------------|--|--|--|
| abs()            | The absolute value of a real number, or the magnitude      |  |  |
|                  | of a complex number.                                       |  |  |
| min()            | The smallest element of a single iterable, or the smallest |  |  |
|                  | of several arguments. Strings are compared based on        |  |  |
|                  | lexicographical order: numerical characters first, then    |  |  |
|                  | upper-case letters, then lower-case letters.               |  |  |
| <pre>max()</pre> | The largest element of a single iterable, or the largest   |  |  |
|                  | of several arguments.                                      |  |  |
| <pre>len()</pre> | The number of items of a sequence or collection.           |  |  |
| round()          | A float rounded to a given precision in decimal digits.    |  |  |
| <pre>sum()</pre> | The sum of a sequence of numbers.                          |  |  |

Table 2.1: Common built-in functions for numerical calculations.

```
# abs() can be used with real or complex numbers.
>>> print(abs(-7), abs(3 + 4j))
7 5.0
# min() and max() can be used on a list, string, or several arguments.
# String characters are ordered lexicographically.
>>> print(min([4, 2, 6]), min("aXbYcZ"), min('1', 'a', 'A'))
>>> print(max([4, 2, 6]), max("aXbYcZ"), max('1', 'a', 'A'))
6 c a
# len() can be used on a string, list, set, dict, tuple, or other iterable.
>>> print(len([2, 7, 1]), len("abcdef"), len({1, 'a', 'a'}))
3 6 2
# sum() can be used on iterables containing numbers, but not strings.
>>> my_list = [1, 2, 3]
>>> my_tuple = (4, 5, 6)
>>> my_set = \{7, 8, 9\}
>>> sum(my_list) + sum(my_tuple) + sum(my_set)
>>> sum([min(my_list), max(my_tuple), len(my_set)])
10
# round() is particularly useful for formatting data to be printed.
>>> round(3.14159265358979323, 2)
3.14
```

See https://docs.python.org/3/library/functions.html for more detailed documentation on all of Python's built-in functions.

**Problem 1.** Write a function that accepts a list L and returns the minimum, maximum, and average of the entries of L (in that order). Can you implement this function in a single line?

#### Namespaces

Whenever a Python object—a number, data structure, function, or other entity—is created, it is stored somewhere in computer memory. A *name* (or variable) is a reference to a Python object, and a *namespace* is a dictionary that maps names to Python objects.

```
# The number 4 is the object, 'number_of_students' is the name.
>>> number_of_sudents = 4

# The list is the object, and 'beatles' is the name.
>>> beatles = ["John", "Paul", "George", "Ringo"]

# Python statements defining a function also form an object.
# The name for this function is 'add_numbers'.
>>> def add_numbers(a, b):
... return a + b
...
```

A single equals sign assigns a name to an object. If a name is assigned to another name, that new name refers to the same object as the original name.

To see all of the names in the current namespace, use the built-in function dir(). To delete a name from the namespace, use the del keyword (with caution!).

```
# Add 'stem' to the namespace.
>>> stem = ["Science", "Technology", "Engineering", "Mathematics"]
>>> dir()
['__annotations__', '__builtins__', '__doc__', '__loader__', '__name__',
    '__package__', '__spec__', 'stem']

# Remove 'stem' from the namespace.
>>> del stem
>>> "stem" in dir()
False
>>> print(stem)
Traceback (most recent call last):
    File "<stdin>", line 1, in <module>
NameError: name 'stem' is not defined
```

#### Note

Many programming languages distinguish between *variables* and *pointers*. A pointer refers to a variable by storing the address in memory where the corresponding object is stored. Python names are essentially pointers, and traditional pointer operations and cleanup are done automatically. For example, Python automatically deletes objects in memory that have no names assigned to them (no pointers referring to them). This feature is called *garbage collection*.

#### Mutability

Every Python object type falls into one of two categories: a *mutable* object, which may be altered at any time, or an *immutable* object, which cannot be altered once created. Attempting to change an immutable object creates a new object in memory. If two names refer to the same mutable object, any changes to the object are reflected in both names since they still both refer to that same object. On the other hand, if two names refer to the same immutable object and one of the values is "changed," then one name will refer to the original object, and the other will refer to a new object in memory.

#### ACHTUNG!

Failing to correctly copy mutable objects can cause subtle problems. For example, consider a dictionary that maps items to their base prices. To make a similar dictionary that accounts for a small sales tax, we might try to make a copy by assigning a new name to the first dictionary.

```
>>> holy = {"moly": 1.99, "hand_grenade": 3, "grail": 1975.41}
>>> tax_prices = holy  # Try to make a copy for processing.
>>> for item, price in tax_prices.items():
...  # Add a 7 percent tax, rounded to the nearest cent.
...  tax_prices[item] = round(1.07 * price, 2)
...
# Now the base prices have been updated to the total price.
>>> print(tax_prices)
{'moly': 2.13, 'hand_grenade': 3.21, 'grail': 2113.69}

# However, dictionaries are mutable, so 'holy' and 'tax_prices' actually
# refer to the same object. The original base prices have been lost.
>>> print(holy)
{'moly': 2.13, 'hand_grenade': 3.21, 'grail': 2113.69}
```

To avoid this problem, explicitly create a copy of the object by casting it as a new structure. Changes made to the copy will not change the original object, since they are distinct objects in memory. To fix the above code, replace the second line with the following:

```
>>> tax_prices = dict(holy)
```

Then, after running the same procedure, the two dictionaries will be different.

**Problem 2.** Determine which Python object types are mutable and which are immutable by repeating the following experiment for an int, str, list, tuple, and set.

- 1. Create an object of the given type and assign a name to it.
- 2. Assign a new name to the first name.
- 3. Alter the object via only one of the names (for tuples, use my\_tuple += (1,)).
- 4. Check to see if the two names are equal. If they are, then changing one name also changes the other. Thus, both names refer to the same object and the object type is mutable. Otherwise, the names refer to different objects—meaning a new object was created in step 2—and therefore the object type is immutable.

For example, the following experiment shows that dict is a mutable type.

```
>>> dict_1 = {1: 'x', 2: 'b'}  # Create a dictionary.
>>> dict_2 = dict_1  # Assign it a new name.
>>> dict_2[1] = 'a'  # Change the 'new' dictionary.
>>> dict_1 == dict_2  # Compare the two names.
True  # Both names changed!
```

Print a statement of your conclusions that clearly indicates which object types are mutable and which are immutable.

#### ACHTUNG!

Mutable objects cannot be put into Python sets or used as keys in Python dictionaries. However, the values of a dictionary may be mutable or immutable.

```
>>> a_dict = {"key": "value"}  # Dictionaries are mutable.
>>> broken = {1, 2, 3, a_dict, a_dict}  # Try putting a dict in a set.
Traceback (most recent call last):
   File "<stdin>", line 1, in <module>
TypeError: unhashable type: 'dict'
>>> okay = {1: 2, "3": a_dict}  # Try using a dict as a value.
```

#### Modules

A module is a Python file containing code that is meant to be used in some other setting, and not necessarily run directly. The import statement loads code from a specified Python file. Importing a module containing some functions, classes, or other objects makes those functions, classes, or objects available for use by adding their names to the current namespace.

<sup>&</sup>lt;sup>1</sup>Python files that are primarily meant to be executed, not imported, are often called *scripts*.

All import statements should occur at the top of the file, below the header but before any other code. There are several ways to use import:

1. import <module > makes the specified module available under the alias of its own name.

2. import <module> as <name> creates an alias for an imported module. The alias is added to the current namespace, but the module name itself is not.

```
>>> import numpy as np  # The name 'np' gives access to the numpy
>>> np.sqrt(2)  # module, but the name 'numpy' does not.
1.4142135623730951
>>> numpy.sqrt(2)
Traceback (most recent call last):
   File "<stdin>", line 1, in <module>
NameError: name 'numpy' is not defined
```

3. from <module> import <object> loads the specified object into the namespace without loading anything else in the module or the module name itself. This is used most often to access specific functions from a module. The as statement can also be tacked on to create an alias.

```
>>> from random import randint # The name 'randint' gives access to the
>>> r = randint(0, 10000) # randint() function, but the rest of
>>> random.seed(r) # the random module is unavailable.
Traceback (most recent call last):
   File "<stdin>", line 1, in <module>
NameError: name 'random' is not defined
```

In each case, the final word of the import statement is the name that is added to the namespace.

#### Running and Importing

Consider the following simple Python module, saved as example1.py.

```
# example1.py

data = list(range(4))
def display():
    print("Data:", data)

if __name__ == "__main__":
    display()
    print("This file was executed from the command line or an interpreter.")
else:
    print("This file was imported.")
```

Executing the file from the command line executes the file line by line, including the code under the if \_\_name\_\_ == "\_\_main\_\_" clause.

```
$ python example1.py
Data: [0, 1, 2, 3]
This file was executed from the command line or an interpreter.
```

Executing the file with IPython's special %run command executes each line of the file and also adds the module's names to the current namespace. This is the quickest way to test individual functions via IPython.

```
In [1]: %run example1.py
Data: [0, 1, 2, 3]
This file was executed from the command line or an interpreter.
In [2]: display()
Data: [0, 1, 2, 3]
```

Importing the file also executes each line, but only adds the indicated alias to the namespace. Also, code under the if \_\_name\_\_ == "\_\_main\_\_" clause is **not** executed when a file is imported.

**Problem 3.** Create a module called calculator.py. Write a function that returns the sum of two arguments and a function that returns the product of two arguments. Also use import to add the sqrt() function from the math module to the namespace. When this file is either run or imported, nothing should be executed.

In your solutions file, import your new custom module. Write a function that accepts two numbers representing the lengths of the sides of a right triangle. Using only the functions from calculator.py, calculate and return the length of the hypotenuse of the triangle.

<sup>&</sup>lt;sup>2</sup>Try importing the this or antigravity modules. Importing these modules actually executes some code.

#### ACHTUNG!

If a module has been imported in IPython and the source code then changes, using import again does not refresh the name in the IPython namespace. Use run instead to correctly refresh the namespace. Consider this example where we test the function sum\_of\_squares(), saved in the file example2.py.

```
# example2.py

def sum_of_squares(x):
    """Return the sum of the squares of all positive integers
    less than or equal to x.
    """
    return sum([i**2 for i in range(1,x)])
```

In IPython, run the file and test sum\_of\_squares().

```
# Run the file, adding the function sum_of_squares() to the namespace.
In [1]: %run example2
In [2]: sum_of_squares(3)
Out[2]: 5  # Should be 14!
```

Since  $1^2+2^2+3^2=14$ , not 5, something has gone wrong. Modify the source file to correct the mistake, then run the file again in IPython.

```
# example2.py

def sum_of_squares(x):
    """Return the sum of the squares of all positive integers
    less than or equal to x.
    """
    return sum([i**2 for i in range(1,x+1)]) # Include the final term.
```

```
# Run the file again to refresh the namespace.
In [3]: %run example2

# Now sum_of_squares() is updated to the new, corrected version.
In [4]: sum_of_squares(3)
Out[4]: 14  # It works!
```

Remember that running or importing a file executes any freestanding code snippets, but any code under an if \_\_name\_\_ == "\_\_main\_\_" clause will **only** be executed when the file is run (not when it is imported).

#### The Python Standard Library

All Python distributions include a collection of modules for accomplishing a variety of common tasks, collectively called the *Python standard library*. Some commonly standard library modules are listed below, and the complete list is at https://docs.python.org/3/library/.

| Module    | Description   |
|-----------|---|
| cmath     | Mathematical functions for complex numbers.           |
| itertools | Tools for iterating through sequences in useful ways. |
| math      | Standard mathematical functions and constants.        |
| random    | Random variable generators.                           |
| string    | Common string literals.                               |
| sys       | Tools for interacting with the interpreter.           |
| time      | Time value generation and manipulation.               |

Use IPython's object introspection to quickly learn about how to use the various modules and functions in the standard library. Use? or help() for information on the module or one of its names. To see the entire module's namespace, use the tab key.

```
In [1]: import math
In [2]: math?
             module
String form: <module 'math' from '~/anaconda/lib/python3.6/ # ...
File:
             ~/anaconda/lib/python3.6/lib-dynload/ # ...
Docstring:
This module is always available. It provides access to the
mathematical functions defined by the C standard.
# Type the module name, a period, then press tab to see the module's namespace.
In [3]: math.
                # Press 'tab'.
    acos()
                cos()
                             factorial() isclose()
                                                      log2()
                                                                  tan()
    acosh()
                cosh()
                                         isfinite()
                                                     modf()
                                                                  tanh()
                            floor()
    asin()
                degrees()
                            fmod()
                                         isinf()
                                                     nan
                                                                  tau
                             frexp()
    asinh()
                                         isnan()
                                                      рi
                                                                  trunc()
                                         ldexp()
                                                     pow()
    atan()
                erf()
                             fsum()
                erfc()
                             gamma()
                                         lgamma()
                                                     radians()
    atan2()
    atanh()
                exp()
                             gcd()
                                         log()
                                                      sin()
    ceil()
                                         log10()
                                                      sinh()
                expm1()
                            hypot()
    copysign()
                fabs()
                             inf
                                         log1p()
                                                      sqrt()
In [3]: math.sqrt?
Docstring:
sqrt(x)
Return the square root of x.
Type:
           builtin_function_or_method
```

#### The Itertools Module

The itertools module makes it easy to iterate over one or more collections in specialized ways.

| Function                  | Description  |
|---------------------------|--|
| chain()                   | Iterate over several iterables in sequence.                |
| cycle()                   | Iterate over an iterable repeatedly.                       |
| <pre>combinations()</pre> | Return successive combinations of elements in an iterable. |
| <pre>permutations()</pre> | Return successive permutations of elements in an iterable. |
| <pre>product()</pre>      | Iterate over the Cartesian product of several iterables.   |

```
>>> from itertools import chain, cycle  # Import multiple names.

>>> list(chain("abc", ['d', 'e'], ('f', 'g')))  # Join several
['a', 'b', 'c', 'd', 'e', 'f', 'g']  # sequences together.

>>> for i,number in enumerate(cycle(range(4))):  # Iterate over a single
... if i > 10:  # sequence over and over.
... break
... print(number, end=' ')
...
0 1 2 3 0 1 2 3 0 1 2
```

A k-combination is a set of k elements from a collection where the ordering is unimportant. Thus the combination (a,b) and (b,a) are equivalent because they contain the same elements. One the other hand, a k-permutation is a sequence of k elements from a collection where the ordering matters. Even though (a,b) and (b,a) contain the same elements, they are counted as different permutations.

```
>>> from itertools import combinations, permutations

# Get all combinations of length 2 from the iterable "ABC".
>>> list(combinations("ABC", 2))
[('A', 'B'), ('A', 'C'), ('B', 'C')]

# Get all permutations of length 2 from "ABC". Note that order matters here.
>>> list(permutations("ABC", 2))
[('A', 'B'), ('A', 'C'), ('B', 'A'), ('B', 'C'), ('C', 'A'), ('C', 'B')]
```

**Problem 4.** The *power set* of a set A, denoted  $\mathcal{P}(A)$  or  $2^A$ , is the set of all subsets of A, including the empty set  $\emptyset$  and A itself. For example, the power set of the set  $A = \{a, b, c\}$  is  $2^A = \{\emptyset, \{a\}, \{b\}, \{c\}, \{a, b\}, \{a, c\}, \{b, c\}, \{a, b, c\}\}$ .

Write a function that accepts an iterable A. Use an itertools function to compute the power set of A as a list of sets (why couldn't it be a set of sets in Python?).

#### The Random Module

Many real-life events can be simulated by taking random samples from a probability distribution. For example, a coin flip can be simulated by randomly choosing between the integers 1 (for heads) and 0 (for tails). The random module includes functions for sampling from probability distributions and generating random data.

| Function             | Description  |
|----------------------|--|
| choice()             | Choose a random element from a non-empty sequence, such as a list. |
| randint()            | Choose a random integer integer over a closed interval.            |
| random()             | Pick a float from the interval $[0, 1)$ .                          |
| <pre>sample()</pre>  | Choose several unique random elements from a non-empty sequence.   |
| seed()               | Seed the random number generator.                                  |
| <pre>shuffle()</pre> | Randomize the ordering of the elements in a list.                  |

Some of the most common random utilities involve picking random elements from iterables.

```
>>> import random
>>> numbers = list(range(1,11))
                                   # Get the integers from 1 to 10.
>>> print(numbers)
[1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
>>> random.shuffle(numbers)
                                    # Mix up the ordering of the list.
>>> print(numbers)
                                    # Note that shuffle() returns nothing.
[5, 9, 1, 3, 8, 4, 10, 6, 2, 7]
>>> random.choice(numbers)
                                    # Pick a single element from the list.
>>> random.sample(numbers, 4)
                                    # Pick 4 unique elements from the list.
[5, 8, 3, 2]
>>> random.randint(1,10)
                                    # Pick a random number between 1 and 10.
10
```

#### The Time Module

The time module in the standard library include functions for dealing with time. In particular, the time() function measures the number of seconds from a fixed starting point, called "the Epoch" (January 1, 1970 for Unix machines).

```
>>> import time
>>> time.time()
1495243696.645818
```

The time() function is useful for measuring how long it takes for code to run: record the time just before and just after the code in question, then subtract the first measurement from the second to get the number of seconds that have passed.

#### The Sys Module

The sys (system) module includes methods for interacting with the Python interpreter. For example, sys.argv is a list of arguments passed to the interpreter when it runs a Python file.

```
# example3.py
"""Read a single command line argument and print it in all caps."""
import sys

if len(sys.argv) == 2:
   print(sys.argv[1].upper())
else:
   print("Exactly one extra command line argument is required")
   print("System Arguments:", sys.argv)
```

Now provide command line arguments for the program to process.

```
$ python example3.py  # No extra command line arguments.
Exactly one extra command line argument is required
System Arguments: ['example3.py']

$ python example3.py hello  # One extra command line argument.
HELLO

$ python example3.py with 2 many arguments
Exactly one extra command line argument is required
System Arguments: ['example3.py', 'with', '2', 'many', 'arguments']
```

Note that the first command line argument is always the filename, and that sys.argv is always a list of strings, even if a number is provided on the command line. In IPython, command line arguments are specified after the %run command.

```
In [1]: %run example3.py hello
HELLO
```

Another way to get input from the program user is to prompt the user for text. The built-in function input() pauses the program and waits for the user to type something. Like command line arguments, the user's input is parsed as a string.

```
>>> x = input("Enter a value for x: ")
Enter a value for x: 20  # Type '20' and press 'enter.'
>>> x
'20'  # Note that x contains a string.

>> y = int(input("Enter an integer for y: "))
Enter an integer for y: 16  # Type '16' and press 'enter.'
>>> y
16  # Note that y contains an integer.
```

**Problem 5.** Shut the box is a popular British pub game that is used to help children learn arithmetic. The player starts with the numbers 1 through 9, and the goal of the game is to eliminate as many of these numbers as possible. At each turn the player rolls two dice, then chooses a set of integers from the remaining numbers that sum up to the sum of the dice roll. These numbers are removed, and the dice are then rolled again. The game ends when none of the remaining integers can be combined to the sum of the dice roll, and the player's final score is the sum of the numbers that could not be eliminated. For a demonstration, see https://www.youtube.com/watch?v=mwURQC7mjDI.

Modify your solutions file so that when the file is run with the correct command line arguments (but **not** when it is imported), the user plays a game of shut the box. The provided module box.py contains some functions that will be useful in your implementation of the game. You do not need to understand exactly how the functions work, but you do need to be able to import and use them correctly. Your game should match the following specifications:

- Require three total command line arguments: the file name (included by default), the player's name, and a time limit in seconds. If there are not exactly three command line arguments, do not start the game.
- Track the player's remaining numbers, starting with 1 through 9.
- Use the random module to simulate rolling two six-sided dice. However, if the sum of the player's remaining numbers is 6 or less, role only one die.
- The player wins if they have no numbers left, and they lose if they are out of time or if they cannot choose numbers to match the dice roll.
- If the game is not over, print the player's remaining numbers, the sum of the dice roll, and the number of seconds remaining. Prompt the user for numbers to eliminate. The input should be one or more of the remaining integers, separated by spaces. If the user's input is invalid, prompt them for input again before rolling the dice again.

  (Hint: use round() to format the number of seconds remaining nicely.)

• When the game is over, display the player's name, their score, and the total number of seconds since the beginning of the game. Congratulate or mock the player appropriately.

(Hint: **Before you start coding**, write an outline for the entire program, adding one feature at a time. Only start implementing the game after you are completely finished designing it.)

Your game should look similar to the following examples. The characters in red are typed inputs from the user.

```
$ python standard_library.py LuckyDuke 60
Numbers left: [1, 2, 3, 4, 5, 6, 7, 8, 9]
Roll: 12
Seconds left: 60.0
Numbers to eliminate: 3 9
Numbers left: [1, 2, 4, 5, 6, 7, 8]
Roll: 9
Seconds left: 53.51
Numbers to eliminate: 8 1
Numbers left: [2, 4, 5, 6, 7]
Roll: 7
Seconds left: 51.39
Numbers to eliminate: 7
Numbers left: [2, 4, 5, 6]
Roll: 2
Seconds left: 48.24
Numbers to eliminate: 2
Numbers left: [4, 5, 6]
Roll: 11
Seconds left: 45.16
Numbers to eliminate: 5 6
Numbers left: [4]
Roll: 4
Seconds left: 42.76
Numbers to eliminate: 4
Score for player LuckyDuke: 0 points
Time played: 15.82 seconds
Congratulations!! You shut the box!
```

The next two examples show different ways that a player could lose (which they usually do), as well as examples of invalid user input. Use the box module's parse\_input() to detect invalid input.

```
$ python standard_library.py ShakySteve 10
Numbers left: [1, 2, 3, 4, 5, 6, 7, 8, 9]
Roll: 7
Seconds left: 10.0
                                     # Must enter a number.
Numbers to eliminate: Seven
Invalid input
Seconds left: 7.64
Numbers to eliminate: 1, 2, 4 # Do not use commas.
Invalid input
Seconds left: 4.55
Numbers to eliminate: 1 2 3 # Numbers don't sum to the roll.
Invalid input
Seconds left: 2.4
Numbers to eliminate: 1 2 4
Numbers left: [3, 5, 6, 7, 8, 9]
Roll: 8
Seconds left: 0.31
Numbers to eliminate: 8
Game over!
                                       # Time is up!
Score for player ShakySteve: 30 points
Time played: 11.77 seconds
Better luck next time >:)
$ python standard_library.py SnakeEyesTom 10000
Numbers left: [1, 2, 3, 4, 5, 6, 7, 8, 9]
Seconds left: 10000.0
Numbers to eliminate: 2
Numbers left: [1, 3, 4, 5, 6, 7, 8, 9]
Roll: 2
Game over!
                                      # Numbers cannot match roll.
Score for player SnakeEyesTom: 43 points
Time played: 1.53 seconds
Better luck next time >:)
```

#### **Additional Material**

#### More Built-in Functions

The following built-in functions are worth knowing, especially for working with iterables and writing very readable conditional statements.

| Function         | Description   |  |
|------------------|---|--|
| all()            | Return True if bool(entry) evaluates to True for every entry in   |  |
|                  | the input iterable.   |  |
| <pre>any()</pre> | Return True if bool(entry) evaluates to True for any entry in the |  |
|                  | input iterable.   |  |
| bool()           | Evaluate a single input object as True or False.                  |  |
| eval()           | Execute a string as Python code and return the output.            |  |
| <pre>map()</pre> | Apply a function to every item of the input iterable and return   |  |
|                  | an iterable of the results.                                       |  |

```
>>> from random import randint
# Get 5 random numbers between 1 and 10, inclusive.
>>> numbers = [randint(1,10) for _ in range(5)]

# If all of the numbers are less than 8, print the list.
>>> if all([num < 8 for num in numbers]):
...    print(numbers)
...
[1, 5, 6, 3, 3]

# If none of the numbers are divisible by 3, print the list.
>>> if not any([num % 3 == 0 for num in numbers]):
...    print(numbers)
...
```

#### Two-Player Shut the Box

Consider modifying your shut the box program so that it pits two players against each other (one player tries to shut the box while the other tries to keep it open). The first player plays a regular round as described in Problem 5. Suppose he or she eliminates every number but 2, 3, and 6. The second player then begins a round with the numbers 1, 4, 5, 7, 8, and 9, the numbers that the first player had eliminated. If the second player loses, the first player gets another round to try to shut the box with the numbers that the second player had eliminated. Play continues until one of the players eliminates their entire list. In addition, each player should have their own time limit that only ticks down during their turn. If time runs out on your turn, you lose no matter what.

#### **Python Packages**

Large programming projects often have code spread throughout several folders and files. In order to get related files in different folders to communicate properly, the associated directories must be organized into a Python *packages*. This is a common procedure when creating smart phone applications and other programs that have graphical user interfaces (GUIs).

A package is simply a folder that contains a file called \_\_init\_\_.py. This file is always executed first whenever the package is used. A package must also have a file called \_\_main\_\_.py in order to be executable. Executing the package will run \_\_init\_\_.py and then \_\_main\_\_.py, but importing the package will only run \_\_init\_\_.py.

Use the regular syntax to import a module or subpackage that is in the current package, and use from <subpackage.module> import <object> to load a module within a subpackage. Once a name has been loaded into a package's \_\_init\_\_.py, other files in the same package can load the same name with from . import <object>. To access code in the directory one level above the current directory, use the syntax from .. import <object> This tells the interpreter to go up one level and import the object from there. This is called an explicit relative import and cannot be done in files that are executed directly (like \_\_main\_\_.py).

Finally, to execute a package, run Python from the shell with the flag -m (for "module-name") and exclude the extension .py.

```
$ python -m package_name
```

See https://docs.python.org/3/tutorial/modules.html#packages for examples and more details.

# 3

### Introduction to NumPy

Lab Objective: NumPy is a powerful Python package for manipulating data with multi-dimensional vectors. Its versatility and speed makes Python an ideal language for applied and computational mathematics. In this lab we introduce basic NumPy data structures and operations as a first step to numerical computing in Python.

#### Arrays

In many algorithms, data can be represented mathematically as a *vector* or a *matrix*. Conceptually, a vector is just a list of numbers and a matrix is a two-dimensional list of numbers (a list of lists). However, even basic linear algebra operations like matrix multiplication are cumbersome to implement and slow to execute when data is stored this way. The NumPy module<sup>1</sup> [Oli06, ADH<sup>+</sup>01, Oli07] offers a much better solution.

The basic object in NumPy is the *array*, which is conceptually similar to a matrix. The NumPy array class is called **ndarray** (for "n-dimensional array"). The simplest way to explicitly create a 1-D **ndarray** is to define a list, then cast that list as an **ndarray** with NumPy's **array()** function.

```
>>> import numpy as np

# Create a 1-D array by passing a list into NumPy's array() function.
>>> np.array([8, 4, 6, 0, 2])
array([8, 4, 6, 0, 2])

# The string representation has no commas or an array() label.
>>> print(np.array([1, 3, 5, 7, 9]))
[1 3 5 7 9]
```

The alias "np" for numpy is standard in the Python community.

An ndarray can have arbitrarily many dimensions. A 2-D array is a 1-D array of 1-D arrays (like a list of lists), a 3-D array is a 1-D array of 2-D arrays (a list of lists of lists), and, more generally, an n-dimensional array is a 1-D array of (n-1)-dimensional arrays (a list of lists of lists of lists...). Each dimension is called an axis. For a 2-D array, the 0-axis indexes the rows and the 1-axis indexes the columns. Elements are accessed using brackets and indices, with the axes separated by commas.

<sup>&</sup>lt;sup>1</sup>NumPy is *not* part of the standard library, but it is included in most Python distributions.

```
# Create a 2-D array by passing a list of lists into array().
>>> A = np.array( [ [1, 2, 3], [4, 5, 6] ] )
>>> print(A)
[[1 2 3]
   [4 5 6]]

# Access elements of the array with brackets.
>>> print(A[0, 1], A[1, 2])
2 6

# The elements of a 2-D array are 1-D arrays.
>>> A[0]
array([1, 2, 3])
```

**Problem 1.** There are two main ways to perform matrix multiplication in NumPy: with NumPy's dot() function (np.dot(A, B)), or with the @ operator (A @ B). Write a function that defines the following matrices as NumPy arrays.

$$A = \begin{bmatrix} 3 & -1 & 4 \\ 1 & 5 & -9 \end{bmatrix} \qquad B = \begin{bmatrix} 2 & 6 & -5 & 3 \\ 5 & -8 & 9 & 7 \\ 9 & -3 & -2 & -3 \end{bmatrix}$$

Return the matrix product AB.

For examples of array initialization and matrix multiplication, use object introspection in IPython to look up the documentation for np.ndarray, np.array() and np.dot().

```
In [1]: import numpy as np
In [2]: np.array? # press 'enter'
```

#### ACHTUNG!

The @ operator was not introduced until Python 3.5. It triggers the \_\_matmul\_\_() magic method, which for the ndarray is essentially a wrapper around np.dot(). If you are using a previous version of Python, always use np.dot() to perform basic matrix multiplication.

#### **Basic Array Operations**

NumPy arrays behave differently with respect to the binary arithmetic operators + and \* than Python lists do. For lists, + concatenates two lists and \* replicates a list by a scalar amount (strings also behave this way).

<sup>&</sup>lt;sup>a</sup>See the lab on Object Oriented Programming for an overview of magic methods.

```
# Addition concatenates lists together.
>>> [1, 2, 3] + [4, 5, 6]
[1, 2, 3, 4, 5, 6]

# Mutliplication concatenates a list with itself a given number of times.
>>> [1, 2, 3] * 4
[1, 2, 3, 1, 2, 3, 1, 2, 3, 1, 2, 3]
```

NumPy arrays act like mathematical vectors and matrices: + and \* perform component-wise addition or multiplication.

**Problem 2.** Write a function that defines the following matrix as a NumPy array.

$$A = \left[ \begin{array}{rrr} 3 & 1 & 4 \\ 1 & 5 & 9 \\ -5 & 3 & 1 \end{array} \right]$$

Return the matrix  $-A^3 + 9A^2 - 15A$ .

In this context,  $A^2 = AA$  (the matrix product, not the component-wise square). The somewhat surprising result is a demonstration of the Cayley-Hamilton theorem.

#### **Array Attributes**

An ndarray object has several attributes, some of which are listed below.

| ${ m Attribute}$ | Description  |
|------------------|--|
| dtype            | The type of the elements in the array.                     |
| ndim             | The number of axes (dimensions) of the array.              |
| shape            | A tuple of integers indicating the size in each dimension. |
| size             | The total number of elements in the array.                 |

```
>>> A = np.array([[1, 2, 3],[4, 5, 6]])
# 'A' is a 2-D array with 2 rows, 3 columns, and 6 entries.
>>> print(A.ndim, A.shape, A.size)
2 (2, 3) 6
```

Note that ndim is the number of entries in shape, and that the size of the array is the product of the entries of shape.

#### **Array Creation Routines**

In addition to casting other structures as arrays via np.array(), NumPy provides efficient ways to create certain commonly-used arrays.

| Function     | Returns   |  |
|--------------|---|--|
| arange()     | Array of sequential integers (like list(range())).            |  |
| eye()        | 2-D array with ones on the diagonal and zeros elsewhere.      |  |
| ones()       | Array of given shape and type, filled with ones.              |  |
| ones_like()  | Array of ones with the same shape and type as a given array.  |  |
| zeros()      | os() Array of given shape and type, filled with zeros.        |  |
| zeros_like() | Array of zeros with the same shape and type as a given array. |  |
| full()       | Array of given shape and type, filled with a specified value. |  |
| full_like()  | Full array with the same shape and type as a given array.     |  |

Each of these functions accepts the keyword argument dtype to specify the data type. Common types include np.bool\_, np.int64, np.float64, and np.complex128.

```
# A 1-D array of 5 zeros.
>>> np.zeros(5)
array([ 0., 0., 0., 0., 0.])
# A 2x5 matrix (2-D array) of integer ones.
>>> np.ones((2,5), dtype=np.int) # The shape is specified as a tuple.
array([[1, 1, 1, 1, 1],
       [1, 1, 1, 1, 1]])
# The 2x2 identity matrix.
>>> I = np.eye(2)
>>> print(I)
[[ 1. 0.]
 [ 0. 1.]]
# Array of 3s the same size as 'I'.
>>> np.full_like(I, 3)
                                    # Equivalent to np.full(I.shape, 3).
array([[ 3., 3.],
       [3., 3.]])
```

Unlike native Python data structures, all elements of a NumPy array must be of the same data type. To change an existing array's data type, use the array's astype() method.

```
# A list of integers becomes an array of integers.
>>> x = np.array([0, 1, 2, 3, 4])
>>> print(x)
[0 1 2 3 4]
>>> x.dtype
dtype('int64')

# Change the data type to one of NumPy's float types.
>>> x = x.astype(np.float64)  # Equivalent to x = np.float64(x).
>>> print(x)
[ 0. 1. 2. 3. 4.]  # Floats are displayed with periods.
>>> x.dtype
dtype('float64')
```

The following functions are for dealing with the diagonal, upper, or lower portion of an array.

| Function | Description   |  |
|----------|---|--|
| diag()   | Extract a diagonal or construct a diagonal array.                       |  |
| tril()   | Get the lower-triangular portion of an array by replacing entries above |  |
|          | the diagonal with zeros.  |  |
| triu()   | Get the upper-triangular portion of an array by replacing entries below |  |
|          | the diagonal with zeros.  |  |

See http://docs.scipy.org/doc/numpy/reference/routines.array-creation.html for the official documentation on NumPy's array creation routines.

**Problem 3.** Write a function that defines the following matrices as NumPy arrays using the functions presented in this section (not np.array()). Calculate the matrix product ABA. Change the data type of the resulting matrix to np.int64, then return it.

$$A = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \qquad B = \begin{bmatrix} -1 & 5 & 5 & 5 & 5 & 5 & 5 \\ -1 & -1 & 5 & 5 & 5 & 5 & 5 \\ -1 & -1 & -1 & 5 & 5 & 5 & 5 \\ -1 & -1 & -1 & -1 & 5 & 5 & 5 \\ -1 & -1 & -1 & -1 & -1 & -1 & 5 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 \end{bmatrix}$$

#### **Data Access**

#### **Array Slicing**

Indexing for a 1-D NumPy array uses the slicing syntax x[start:stop:step]. If there is no colon, a single entry of that dimension is accessed. With a colon, a range of values is accessed. For multi-dimensional arrays, use a comma to separate slicing syntax for each axis.

```
# Make an array of the integers from 0 to 10 (exclusive).
>>> x = np.arange(10)
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
# Access elements of the array with slicing syntax.
>>> x[3]
                                     # The element at index 3.
3
>>> x[:3]
                                     # Everything before index 3.
array([0, 1, 2])
>>> x[3:]
                                     # Everything from index 3 on.
array([3, 4, 5, 6, 7, 8, 9])
>>> x[3:8]
                                     # Everything between index 3 and index 8 (\leftarrow
    exclusive).
array([3, 4, 5, 6, 7])
>>> A = np.array([[0,1,2,3,4],[5,6,7,8,9]])
>>> A
array([[0, 1, 2, 3, 4],
       [5, 6, 7, 8, 9]])
# Use a comma to separate the dimensions for multi-dimensional arrays.
>>> A[1, 2]
                                     # The element at row 1, column 2.
7
>>> A[:, 2:]
                                     # All of the rows, from column 2 on.
array([[2, 3, 4],
       [7, 8, 9]])
```

#### Note

Indexing and slicing operations return a *view* of the array. Changing a view of an array also changes the original array. In other words, **arrays are mutable**. To create a copy of an array, use np.copy() or the array's copy() method. Changes to a copy of an array does not affect the original array, but copying an array uses more time and memory than getting a view.

#### **Fancy Indexing**

So-called  $fancy\ indexing$  is a second way to access or change the elements of an array. Instead of using slicing syntax, provide either an array of indices or an array of boolean values (called a mask) to extract specific elements.

```
>>> x = np.arange(0, 50, 10)  # The integers from 0 to 50 by tens.
>>> x
array([ 0, 10, 20, 30, 40])

# An array of integers extracts the entries of 'x' at the given indices.
>>> index = np.array([3, 1, 4])  # Get the 3rd, 1st, and 4th elements.
>>> x[index]  # Same as np.array([x[i] for i in index]).
array([30, 10, 40])

# A boolean array extracts the elements of 'x' at the same places as 'True'.
>>> mask = np.array([True, False, False, True, False])
>>> x[mask]  # Get the Oth and 3rd entries.
array([ 0, 30])
```

Fancy indexing is especially useful for extracting or changing the values of an array that meet some sort of criterion. Use comparison operators like < and == to create masks.

```
>>> y = np.arange(10, 20, 2)
                                   # Every other integers from 10 to 20.
>>> y
array([10, 12, 14, 16, 18])
# Extract the values of 'y' larger than 15.
>>> mask = y > 15
                                     # Same as np.array([i > 15 \text{ for i in y}]).
>>> mask
array([False, False, False, True, True], dtype=bool)
>>> y[mask]
                                     # Same as y[y > 15]
array([16, 18])
# Change the values of 'y' that are larger than 15 to 100.
>>> y[mask] = 100
>>> print(y)
[10 12 14 100 100]
```

While indexing and slicing always return a view, fancy indexing always returns a copy.

**Problem 4.** Write a function that accepts a single array as input. Make a copy of the array, then use fancy indexing to set all negative entries of the copy to 0. Return the copy.

#### **Array Manipulation**

#### Shaping

An array's shape attribute describes its dimensions. Use np.reshape() or the array's reshape() method to give an array a new shape. The total number of entries in the old array and the new array must be the same in order for the shaping to work correctly. Using a -1 in the new shape tuple makes the specified dimension as long as necessary.

Use np.ravel() to flatten a multi-dimensional array into a 1-D array and np.transpose() or the T attribute to transpose a 2-D array in the matrix sense.

```
[ 1, 5, 9],
[ 2, 6, 10],
[ 3, 7, 11]])
```

#### Note

By default, all NumPy arrays that can be represented by a single dimension, including column slices, are automatically reshaped into "flat" 1-D arrays. For example, by default an array will have 10 elements instead of 10 arrays with one element each. Though we usually represent vectors vertically in mathematical notation, NumPy methods such as dot() are implemented to purposefully work well with 1-D "row arrays".

However, it is occasionally necessary to change a 1-D array into a "column array". Use np.reshape(), np.vstack(), or slice the array and put np.newaxis on the second axis. Note that np.transpose() does not alter 1-D arrays.

Do not force a 1-D vector to be a column vector unless necessary.

#### Stacking

NumPy has functions for *stacking* two or more arrays with similar dimensions into a single block matrix. Each of these methods takes in a single tuple of arrays to be stacked in sequence.

| Function                  | Description  |
|---------------------------|--|
| concatenate()             | Join a sequence of arrays along an existing axis     |
| hstack()                  | Stack arrays in sequence horizontally (column wise). |
| ${\tt vstack}()$          | Stack arrays in sequence vertically (row wise).      |
| <pre>column_stack()</pre> | Stack 1-D arrays as columns into a 2-D array.        |

```
>>> A = np.arange(6).reshape((2,3))
>>> B = np.zeros((4,3))
# vstack() stacks arrays vertically (row-wise).
>>> np.vstack((A,B,A))
array([[ 0., 1., 2.],
                                 # A
      [3., 4., 5.],
      [ 0., 0., 0.],
                                 # B
      [0., 0., 0.],
      [ 0., 0., 0.],
      [ 0., 0., 0.],
      [0., 1., 2.],
                                 # A
      [3., 4., 5.]])
>>> A = A.T
>>> B = np.ones((3,4))
# hstack() stacks arrays horizontally (column-wise).
>>> np.hstack((A,B,A))
array([[ 0., 3., 1., 1., 1., 1., 0., 3.],
      [1., 4., 1., 1., 1., 1., 4.],
      [2., 5., 1., 1., 1., 2., 5.]
# column_stack() stacks arrays horizontally, including 1-D arrays.
>>> np.column_stack((A, np.zeros(3), np.ones(3), np.full(3, 2)))
array([[ 0., 3., 0., 1., 2.],
      [1., 4., 0., 1., 2.],
      [ 2., 5., 0., 1., 2.]])
```

See http://docs.scipy.org/doc/numpy-1.10.1/reference/routines.array-manipulation.html for more array manipulation routines and documentation.

**Problem 5.** Write a function that defines the following matrices as NumPy arrays.

$$A = \begin{bmatrix} 0 & 2 & 4 \\ 1 & 3 & 5 \end{bmatrix} \qquad B = \begin{bmatrix} 3 & 0 & 0 \\ 3 & 3 & 0 \\ 3 & 3 & 3 \end{bmatrix} \qquad C = \begin{bmatrix} -2 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & -2 \end{bmatrix}$$

Use NumPy's stacking functions to create and return the block matrix:

$$\left[\begin{array}{ccc} \mathbf{0} & A^\mathsf{T} & I \\ A & \mathbf{0} & \mathbf{0} \\ B & \mathbf{0} & C \end{array}\right],$$

where I is the  $3 \times 3$  identity matrix and each  $\mathbf{0}$  is a matrix of all zeros of appropriate size. A block matrix of this form is used in the interior point method for linear optimization.

#### Array Broadcasting

Many matrix operations make sense only when the two operands have the same shape, such as element-wise addition. *Array broadcasting* extends such operations to accept some (but not all) operands with different shapes, and occurs automatically whenever possible.

Suppose, for example, that we would like to add different values to the columns of an  $m \times n$  matrix A. Adding a 1-D array x with the n entries to A will automatically do this correctly. To add different values to the different rows of A, first reshape a 1-D array of m values into a column array. Broadcasting then correctly takes care of the operation.

Broadcasting can also occur between two 1-D arrays, once they are reshaped appropriately.

```
>>> A = np.arange(12).reshape((4,3))
>>> x = np.arange(3)
>>> A
array([[ 0, 1, 2],
       [3, 4, 5],
       [6, 7, 8],
       [ 9, 10, 11]])
>>> x
array([0, 1, 2])
# Add the entries of 'x' to the corresponding columns of 'A'.
>>> A + x
array([[ 0, 2, 4],
       [3, 5, 7],
       [6, 8, 10],
       [ 9, 11, 13]])
>>> y = np.arange(0, 40, 10).reshape((4,1))
>>> y
array([[ 0],
       [10],
       [20],
       [30]])
# Add the entries of 'y' to the corresponding rows of 'A'.
>>> A + y
array([[ 0, 1, 2],
       [13, 14, 15],
       [26, 27, 28],
```

#### Numerical Computing with NumPy

#### **Universal Functions**

A universal function is one that operates on an entire array element-wise. Universal functions are significantly more efficient than using a loop to operate individually on each element of an array.

| Function                                | Description                                     |
|---|---|
| abs() or absolute()                     | Calculate the absolute value element-wise.      |
| exp() / log()                           | Exponential $(e^x)$ / natural log element-wise. |
| $	exttt{maximum()} / 	exttt{minimum()}$ | Element-wise maximum / minimum of two arrays.   |
| sqrt()                                  | The positive square-root, element-wise.         |
| sin(), cos(), tan(), etc.               | Element-wise trigonometric operations.          |

```
>>> x = np.arange(-2,3)
>>> print(x, np.abs(x))  # Like np.array([abs(i) for i in x]).

[-2 -1 0 1 2] [2 1 0 1 2]

>>> np.sin(x)  # Like np.array([math.sin(i) for i in x]).

array([-0.90929743, -0.84147098, 0. , 0.84147098, 0.90929743])
```

See http://docs.scipy.org/doc/numpy/reference/ufuncs.html#available-ufuncs for a more comprehensive list of universal functions.

#### ACHTUNG!

The math module has many useful functions for numerical computations. However, most of these functions can only act on single numbers, not on arrays. NumPy functions can act on either scalars or entire arrays, but math functions tend to be a little faster for acting on scalars.

```
>>> import math

# Math and NumPy functions can both operate on scalars.
>>> print(math.exp(3), np.exp(3))
20.085536923187668 20.0855369232

# However, math functions cannot operate on arrays.
```

#### Other Array Methods

The np.ndarray class itself has many useful methods for numerical computations.

| Method           | Returns   |  |
|------------------|---|--|
| all()            | True if all elements evaluate to True.                  |  |
| any()            | True if any elements evaluate to True.                  |  |
| argmax()         | Index of the maximum value.                             |  |
| argmin()         | Index of the minimum value.                             |  |
| argsort()        | Indices that would sort the array.                      |  |
| clip()           | restrict values in an array to fit within a given range |  |
| max()            | The maximum element of the array.                       |  |
| mean()           | The average value of the array.                         |  |
| min()            | The minimum element of the array.                       |  |
| sort()           | Return nothing; sort the array in-place.                |  |
| std()            | The standard deviation of the array.                    |  |
| sum()            | The sum of the elements of the array.                   |  |
| <pre>var()</pre> | The variance of the array.                              |  |

Each of these np.ndarray methods has an equivalent NumPy function. For example, A.max() and np.max(A) operate the same way. The one exception is the sort() function: np.sort() returns a sorted copy of the array, while A.sort() sorts the array in-place and returns nothing.

Every method listed can operate along an axis via the keyword argument axis. If axis is specified for a method on an n-D array, the return value is an (n-1)-D array, the specified axis having been collapsed in the evaluation process. If axis is not specified, the return value is usually a scalar. Refer to the NumPy Visual Guide in the appendix for more visual examples.

See http://docs.scipy.org/doc/numpy/reference/generated/numpy.ndarray.html for a more comprehensive list of array methods.

**Problem 6.** A matrix is called *row-stochastic*<sup>a</sup> if its rows each sum to 1. Stochastic matrices are fundamentally important for finite discrete random processes and some machine learning algorithms.

Write a function than accepts a matrix (as a 2-D array). Divide each row of the matrix by the row sum and return the new row-stochastic matrix. Use array broadcasting and the axis argument instead of a loop.

#### Problem 7. This problem comes from https://projecteuler.net.

In the  $20 \times 20$  grid below, four numbers along a diagonal line have been marked in red.

```
08 02 22 97 38 15 00 40 00 75 04 05 07 78 52 12 50 77 91 08
49 49 99 40 17 81 18 57 60 87 17 40 98 43 69 48 04 56 62 00
81 49 31 73 55 79 14 29 93 71 40 67 53 88 30 03 49 13 36 65
52 70 95 23 04 60 11 42 69 24 68 56 01 32 56 71 37 02 36 91
22 31 16 71 51 67 63 89 41 92 36 54 22 40 40 28 66 33 13 80
24 47 32 60 99 03 45 02 44 75 33 53 78 36 84 20 35 17 12 50
32 98 81 28 64 23 67 10 26 38 40 67 59 54 70 66 18 38 64 70
67 26 20 68 02 62 12 20 95 63 94 39 63 08 40 91 66 49 94 21
24 55 58 05 66 73 99 26 97 17 78 78 96 83 14 88 34 89 63 72
21 36 23 09 75 00 76 44 20 45 35 14 00 61 33 97 34 31 33 95
78\ 17\ 53\ 28\ 22\ 75\ 31\ 67\ 15\ 94\ 03\ 80\ 04\ 62\ 16\ 14\ 09\ 53\ 56\ 92
16 39 05 42 96 35 31 47 55 58 88 24 00 17 54 24 36 29 85 57
86 56 00 48 35 71 89 07 05 44 44 37 44 60 21 58 51 54 17 58
19\ 80\ 81\ 68\ 05\ 94\ 47\ 69\ 28\ 73\ 92\ 13\ 86\ 52\ 17\ 77\ 04\ 89\ 55\ 40
04\ 52\ 08\ 83\ 97\ 35\ 99\ 16\ 07\ 97\ 57\ 32\ 16\ 26\ 26\ 79\ 33\ 27\ 98\ 66
88 36 68 87 57 62 20 72 03 46 33 67 46 55 12 32 63 93 53 69
04 42 16 73 38 25 39 11 24 94 72 18 08 46 29 32 40 62 76 36
20 69 36 41 72 30 23 88 34 62 99 69 82 67 59 85 74 04 36 16
20 73 35 29 78 31 90 01 74 31 49 71 48 86 81 16 23 57 05 54
01 70 54 71 83 51 54 69 16 92 33 48 61 43 52 01 89 19 67 48
```

The product of these numbers is  $26 \times 63 \times 78 \times 14 = 1788696$ . Write a function that returns the greatest product of four adjacent numbers in the same direction (up, down, left, right, or diagonally) in the grid.

<sup>&</sup>lt;sup>a</sup>Similarly, a matrix is called *column-stochastic* if its columns each sum to 1.

For convenience, this array has been saved in the file grid.npy. Use the following syntax to extract the array:

```
>>> grid = np.load("grid.npy")
```

One way to approach this problem is to iterate through the rows and columns of the array, checking small slices of the array at each iteration and updating the current largest product. Array slicing, however, provides a much more efficient solution.

The naïve method for computing the greatest product of four adjacent numbers in a horizontal row might be as follows:

Instead, use array slicing to construct a single array where the (i, j)th entry is the product of the four numbers to the right of the (i, j)th entry in the original grid. Then find the largest element in the new array.

```
>>> np.max(grid[:,:-3] * grid[:,1:-2] * grid[:,2:-1] * grid[:,3:])
48477312
```

Use slicing to similarly find the greatest products of four vertical, right diagonal, and left diagonal adjacent numbers.

(Hint: Consider drawing the portions of the grid that each slice in the above code covers, like the examples in the visual guide. Then draw the slices that produce vertical, right diagonal, or left diagonal sequences, and translate the pictures into slicing syntax.)

#### ACHTUNG!

All of the examples in this lab use NumPy arrays, objects of type np.ndarray. NumPy also has a "matrix" data structure called np.matrix that was built specifically for MATLAB users who are transitioning to Python and NumPy. It behaves slightly differently than the regular array class, and can cause some unexpected and subtle problems.

For consistency (and your sanity), **never** use a NumPy matrix; **always** use NumPy arrays. If necessary, cast a matrix object as an array with np.array().

#### Additional Material

#### Random Sampling

The submodule np.random holds many functions for creating arrays of random values chosen from probability distributions such as the uniform, normal, and multinomial distributions. It also contains some utility functions for getting non-distributional random samples, such as random integers or random samples from a given array.

| Function                         | Description   |
|----------------------------------|---|
| choice()                         | Take random samples from a 1-D array.                     |
| random()                         | Uniformly distributed floats over $[0, 1)$ .              |
| randint()                        | Random integers over a half-open interval.                |
| random_integers()                | Random integers over a closed interval.                   |
| randn()                          | Sample from the standard normal distribution.             |
| permutation()                    | Randomly permute a sequence / generate a random sequence. |
|                                  |   |
| Function                         | Distribution  |
| beta()                           | Beta distribution over [0, 1].                            |
| binomial()                       | Binomial distribution.                                    |
| exponential()                    | Exponential distribution.                                 |
| gamma()                          | Gamma distribution.                                       |
| <pre>geometric()</pre>           | Geometric distribution.                                   |
| <pre>multinomial()</pre>         | Multivariate generalization of the binomial distribution. |
| <pre>multivariate_normal()</pre> | Multivariate generalization of the normal distribution.   |
| normal()                         | Normal / Gaussian distribution.                           |
| poisson()                        | Poisson distribution.                                     |
| uniform()                        | Uniform distribution.                                     |

Note that many of these functions have counterparts in the standard library's random module. These NumPy functions, however, are much better suited for working with large collections of random samples.

#### Saving and Loading Arrays

It is often useful to save an array as a file for later use. NumPy provides several easy methods for saving and loading array data.

| Function             | Description  |  |
|----------------------|--|--|
| save()               | Save a single array to a .npy file.                          |  |
| savez()              | Save multiple arrays to a .npz file.                         |  |
| <pre>savetxt()</pre> | Save a single array to a .txt file.                          |  |
| load()               | Load and return an array or arrays from a .npy or .npz file. |  |
| loadtxt()            | Load and return an array from a text file.                   |  |

```
# Save a 100x100 matrix of uniformly distributed random values.
>>> x = np.random.random((100,100))
>>> np.save("uniform.npy", x)  # Or np.savetxt("uniform.txt", x).

# Read the array from the file and check that it matches the original.
>>> y = np.load("uniform.npy")  # Or np.loadtxt("uniform.txt").
>>> np.allclose(x, y)  # Check that x and y are close entry-wise.
True
```

To save several arrays to a single file, specify a keyword argument for each array in np.savez(). Then np.load() will return a dictionary-like object with the keyword parameter names from the save command as the keys.

```
# Save two 100x100 matrices of normally distributed random values.
>>> x = np.random.randn(100,100)
>>> y = np.random.randn(100,100)
>>> np.savez("normal.npz", first=x, second=y)

# Read the arrays from the file and check that they match the original.
>>> arrays = np.load("normal.npz")
>>> np.allclose(x, arrays["first"])
True
>>> np.allclose(y, arrays["second"])
True
```

## 4

## Object-oriented Programming

Lab Objective: Python is a class-based language. A class is a blueprint for an object that binds together specified variables and routines. Creating and using custom classes is often a good way to write clean, efficient, well-designed programs. In this lab we learn how to define and use Python classes. In subsequent labs we will often create customized classes for use in algorithms.

#### Classes

A Python *class* is a code block that defines a custom object and determines its behavior. The **class** key word defines and names a new class. Other statements follow, indented below the class name, to determine the behavior of objects instantiated by the class.

A class needs a method called a *constructor* that is called whenever the class instantiates a new object. The constructor specifies the initial state of the object. In Python, a class's constructor is always named <code>\_\_init\_\_()</code>. For example, the following code defines a class for storing information about backpacks.

```
class Backpack:
    """A Backpack object class. Has a name and a list of contents.

Attributes:
    name (str): the name of the backpack's owner.
    contents (list): the contents of the backpack.

"""

def __init__(self, name):  # This function is the constructor.
    """Set the name and initialize an empty list of contents.

Parameters:
    name (str): the name of the backpack's owner.

"""
    self.name = name  # Initialize some attributes.
    self.contents = []
```

An attribute is a variable stored within an object. The Backpack class has two attributes: name and contents. In the body of the class definition, attributes are assigned and accessed via the name self. This name refers to the object internally once it has been created.

#### Instantiation

The class code block above only defines a blueprint for backpack objects. To create an actual backpack object, call the class name like a function. This triggers the constructor and returns a new *instance* of the class, an object whose type is the class.

```
# Import the Backpack class and instantiate an object called 'my_backpack'.
>>> from object_oriented import Backpack
>>> my_backpack = Backpack("Fred")
>>> type(my_backpack)
<class 'object_oriented.Backpack'>

# Access the object's attributes with a period and the attribute name.
>>> print(my_backpack.name, my_backpack.contents)
Fred []

# The object's attributes can be modified after instantiation.
>>> my_backpack.name = "George"
>>> print(my_backpack.name, my_backpack.contents)
George []
```

#### NOTE

Every object in Python has some built-in attributes. For example, modules have a <code>\_\_name\_\_</code> attribute that identifies the scope in which it is being executed. If the module is being run directly, and not imported, then <code>\_\_name\_\_</code> is set to "<code>\_\_main\_\_</code>". Therefore, any commands under an <code>if \_\_name\_\_</code> == "<code>\_\_main\_\_</code>": clause are ignored when the module is imported.

#### Methods

In addition to storing variables as attributes, classes can have functions attached to them. A function that belongs to a specific class is called a *method*.

```
class Backpack:
    # ...
    def put(self, item):
        """Add an item to the backpack's list of contents."""
        self.contents.append(item) # Use 'self.contents', not just 'contents'.

def take(self, item):
        """Remove an item from the backpack's list of contents."""
        self.contents.remove(item)
```

The first argument of each method must be **self**, to give the method access to the attributes and other methods of the class. The **self** argument is only included in the declaration of the class methods, **not** when calling the methods on an instantiation of the class.

```
# Add some items to the backpack object.
>>> my_backpack.put("notebook")  # my_backpack is passed implicitly to
>>> my_backpack.put("pencils")  # Backpack.put() as the first argument.
>>> my_backpack.contents
['notebook', 'pencils']

# Remove an item from the backpack.  # This is equivalent to
>>> my_backpack.take("pencils")  # Backpack.take(my_backpack, "pencils")
>>> my_backpack.contents
['notebook']
```

#### **Problem 1.** Expand the Backpack class to match the following specifications.

- 1. Modify the constructor so that it accepts three total arguments: name, color, and max\_size (in that order). Make max\_size a keyword argument that defaults to 5. Store each input as an attribute.
- 2. Modify the put() method to check that the backpack does not go over capacity. If there are already max\_size items or more, print "No Room!" and do not add the item to the contents list.
- 3. Write a new method called dump() that resets the contents of the backpack to an empty list. This method should not receive any arguments (except self).
- 4. Documentation is especially important in classes so that the user knows what an object's attributes represent and how to use methods appropriately. Update (or write) the docstrings for the \_\_init\_\_(), put(), and dump() methods, as well as the actual class docstring (under class but before \_\_init\_\_()) to reflect the changes from parts 1-3 of this problem.

To ensure that your class works properly, write a test function outside of the Backpack class that instantiates and analyzes a Backpack object.

```
def test_backpack():
    testpack = Backpack("Barry", "black")  # Instantiate the object.
    if testpack.name != "Barry":  # Test an attribute.
        print("Backpack.name assigned incorrectly")
    for item in ["pencil", "pen", "paper", "computer"]:
        testpack.put(item)  # Test a method.
    print("Contents:", testpack.contents)
    # ...
```

#### Inheritance

To create a new class that is similar to one that already exists, it is often better to *inherit* the methods and attributes from an existing class rather than create a new class from scratch. This creates a class hierarchy: a class that inherits from another class is called a subclass, and the class that a subclass inherits from is called a superclass. To define a subclass, add the name of the superclass as an argument at the end of the class declaration.

For example, since a knapsack is a kind of backpack (but not all backpacks are knapsacks), we create a special Knapsack subclass that inherits the structure and behaviors of the Backpack class and adds some extra functionality.

```
# Inherit from the Backpack class in the class definition.
class Knapsack(Backpack):
    """A Knapsack object class. Inherits from the Backpack class.
    A knapsack is smaller than a backpack and can be tied closed.
    Attributes:
        name (str): the name of the knapsack's owner.
        color (str): the color of the knapsack.
        max_size (int): the maximum number of items that can fit inside.
        contents (list): the contents of the backpack.
        closed (bool): whether or not the knapsack is tied shut.
    def __init__(self, name, color, max_size=3):
        """Use the Backpack constructor to initialize the name, color,
        and max_size attributes. A knapsack only holds 3 item by default.
        Parameters:
            name (str): the name of the knapsack's owner.
            color (str): the color of the knapsack.
            max_size (int): the maximum number of items that can fit inside.
        Backpack.__init__(self, name, color, max_size)
        self.closed = True
```

A subclass may have new attributes and methods that are unavailable to the superclass, such as the closed attribute in the Knapsack class. If methods from the superclass need to be changed for the subclass, they can be overridden by defining them again in the subclass. New methods can be included normally.

```
def take(self, item):  # Override the take() method.
   """If the knapsack is untied, use the Backpack.take() method."""
   if self.closed:
        print("I'm closed!")
   else:
        Backpack.take(self, item)

def weight(self):  # Define a new method just for knapsacks.
   """Calculate the weight of the knapsack by counting the length of the string representations of each item in the contents list.
   """
   return sum(len(str(item)) for item in self.contents)
```

Since Knapsack inherits from Backpack, a knapsack object is a backpack object. All methods defined in the Backpack class are available as instances of the Knapsack class. For example, the dump() method is available even though it is not defined explicitly in the Knapsack class.

The built-in function <code>issubclass()</code> shows whether or not one class is derived from another. Similarly, <code>isinstance()</code> indicates whether or not an object belongs to a specified class hierarchy. Finally, <code>hasattr()</code> shows whether or not a class or object <code>has</code> a specified attribute or method.

```
>>> from object_oriented import Knapsack
>>> my_knapsack = Knapsack("Brady", "brown")
# A Knapsack is a Backpack, but a Backpack is not a Knapsack.
>>> print(issubclass(Knapsack, Backpack), issubclass(Backpack, Knapsack))
True False
>>> isinstance(my_knapsack, Knapsack) and isinstance(my_knapsack, Backpack)
True
# The put() and take() method now require the knapsack to be open.
>>> my_knapsack.put('compass')
I'm closed!
# Open the knapsack and put in some items.
>>> my_knapsack.closed = False
>>> my_knapsack.put("compass")
>>> my_knapsack.put("pocket knife")
>>> my_knapsack.contents
['compass', 'pocket knife']
# The Knapsack class has a weight() method, but the Backpack class does not.
>>> print(hasattr(my_knapsack, 'weight'), hasattr(my_backpack, 'weight'))
True False
# The dump method is inherited from the Backpack class.
>>> my_knapsack.dump()
>>> my_knapsack.contents
Г٦
```

**Problem 2.** Write a Jetpack class that inherits from the Backpack class.

- 1. Override the constructor so that in addition to a name, color, and maximum size, it also accepts an amount of fuel. Change the default value of max\_size to 2, and set the default value of fuel to 10. Store the fuel as an attribute.
- 2. Add a fly() method that accepts an amount of fuel to be burned and decrements the fuel attribute by that amount. If the user tries to burn more fuel than remains, print "Not enough fuel!" and do not decrement the fuel.
- 3. Override the dump() method so that both the contents and the fuel tank are emptied.
- 4. Write clear, detailed docstrings for the class and each of its methods.

#### NOTE

All classes are subclasses of the built-in object class, even if no parent class is specified in the class definition. In fact, the syntax "class ClassName(object):" is not uncommon (or incorrect) for the class declaration, and is equivalent to the simpler "class ClassName:".

#### Magic Methods

A magic method is a special method used to make an object behave like a built-in data type. Magic methods begin and end with two underscores, like the constructor \_\_init\_\_(). Every Python object is automatically endowed with several magic methods, which can be revealed through IPython.

```
In [1]: %run object_oriented.py
In [2]: b = Backpack("Oscar", "green")
                    # Press 'tab' to see standard methods and attributes.
In [3]: b.
                   max_size take()
          color
          contents name
          dump()
                   put()
In [3]: b.__
                    # Press 'tab' to see magic methods and hidden attributes.
          __add__()
                              __getattribute__ __new__()
                                                  __reduce__()
          __class__
                              __gt__
                                                  __reduce_ex__()
          __delattr__
                              __hash__
          __dict__
                              __init__()
                                                   __repr__
                               __init_subclass__() __setattr__
          __dir__()
                                                   __sizeof__()
          __doc__
                              __le__
                              __lt__()
                                                   __str__
          __eq__
                                                   __subclasshook__()
          __format__()
                               __module__
                                                   __weakref__
          __ge__
                               __ne__
```

# Note

Many programming languages distinguish between *public* and *private* variables. In Python, all attributes are public, period. However, attributes that start with an underscore are hidden from the user, which is why magic methods do not show up at first in the preceding code box.

The more common magic methods define how an object behaves with respect to addition and other binary operations. For example, how should addition be defined for backpacks? A simple option is to add the number of contents. Then if backpack A has 3 items and backpack B has 5 items, A + B should return 8. To incorporate this idea, we implement the \_\_add\_\_() magic method.

```
class Backpack:
    # ...
    def __add__(self, other):
        """Add the number of contents of each Backpack."""
        return len(self.contents) + len(other.contents)
```

Using the + binary operator on two Backpack objects calls the class's \_\_add\_\_() method. The object on the left side of the + is passed in to \_\_add\_\_() as self and the object on the right side of the + is passed in as other.

```
>>> pack1 = Backpack("Rose", "red")
>>> pack2 = Backpack("Carly", "cyan")

# Put some items in the backpacks.
>>> pack1.put("textbook")
>>> pack2.put("water bottle")
>>> pack2.put("snacks")

# Add the backpacks together.
>>> pack1 + pack2  # Equivalent to pack1.__add__(pack2).
3
```

# Comparisons

Magic methods also facilitate object comparisons. For example, the \_\_lt\_\_() method corresponds to the < operator. Suppose one backpack is considered "less" than another if it has fewer items in its list of contents.

```
class Backpack(object)
    # ...
    def __lt__(self, other):
        """If 'self' has fewer contents than 'other', return True.
        Otherwise, return False.
        """"
        return len(self.contents) < len(other.contents)</pre>
```

Using the < binary operator on two Backpack objects calls \_\_lt\_\_(). As with addition, the object on the left side of the < operator is passed to \_\_lt\_\_() as self, and the object on the right is passed in as other.

```
>>> pack1, pack2 = Backpack("Maggy", "magenta"), Backpack("Yolanda", "yellow")
>>> pack1 < pack2  # Equivalent to pack1.__lt__(pack2).
False

>>> pack2.put('pencils')
>>> pack1 < pack2
True</pre>
```

Comparison methods should return either True or False, while methods like \_\_add\_\_() might return a numerical value or another kind of object.

| $\operatorname{Method}$ | Arithmetic Operator | Method | Comparison Operator |
|-------------------------|---------------------|--------|---------------------|
| add()                   | +                   | lt()   | <                   |
| sub()                   | -                   | le()   | <=                  |
| mul()                   | *                   | gt()   | >                   |
| pow()                   | **                  | ge()   | >=                  |
| truediv()               | /                   | eq()   | ==                  |
| floordiv()              | //                  | ne()   | !=                  |

Table 4.1: Common magic methods for arithmetic and comparisons. What each of these operations do is up to the programmer and should be carefully documented. For more methods and details, see https://docs.python.org/3/reference/datamodel.html#special-method-names.

# Problem 3. Endow the Backpack class with two additional magic methods:

- The \_\_eq\_\_() magic method is used to determine if two objects are equal, and is invoked by the == operator. Implement the \_\_eq\_\_() magic method for the Backpack class so that two Backpack objects are equal if and only if they have the same name, color, and number of contents.
- 2. The \_\_str\_\_() magic method returns the string representation of an object. This method is invoked by str() and used by print(). Implement the \_\_str\_\_() method in the Backpack class so that printing a Backpack object yields the following output (that is, construct and return the following string).

```
Owner: <name>
Color: <color>
Size: <number of items in contents>
Max Size: <max_size>
Contents: [<item1>, <item2>, ...]
```

(Hint: Use the tab and newline characters '\t' and '\n' to align output nicely.)

# ACHTUNG!

Magic methods for comparison are **not** automatically related. For example, even though the Backpack class implements the magic methods for < and ==, two Backpack objects cannot respond to the <= operator unless \_\_le\_\_() is explicitly defined. The exception to this rule is the != operator: as long as \_\_eq\_\_() is defined, A!=B is False if and only if A==B is True.

# **Problem 4.** Write a ComplexNumber class from scratch.

- 1. Complex numbers are denoted a+bi where  $a,b \in \mathbb{R}$  and  $i=\sqrt{-1}$ . Write the constructor so it accepts two numbers. Store the first as self.real and the second as self.imag.
- 2. The *complex conjugate* of a+bi is defined as  $\overline{a+bi}=a-bi$ . Write a conjugate() method that returns the object's complex conjugate as a new ComplexNumber object.
- 3. Add the following magic methods:
  - (a) Implement \_\_str\_\_() so that a+bi is printed out as (a+bj) for  $b \ge 0$  and (a-bj) for b < 0.
  - (b) The magnitude of a + bi is  $|a + bi| = \sqrt{a^2 + b^2}$ . The \_\_abs\_\_() magic method determines the output of the built-in abs() function (absolute value). Implement \_\_abs\_\_() so that it returns the magnitude of the complex number.
  - (c) Implement \_\_eq\_\_() so that two ComplexNumber objects are equal if and only if they have the same real and imaginary parts.
  - (d) Implement \_\_add\_\_(), \_\_sub\_\_(), \_\_mul\_\_(), and \_\_truediv\_\_() appropriately. Each of these should return a new ComplexNumber object.

Write a function to test your class by comparing it to Python's built-in complex type.

```
def test_ComplexNumber(a, b):
    py_cnum, my_cnum = complex(a, b), ComplexNumber(a, b)

# Validate the constructor.
if my_cnum.real != a or my_cnum.imag != b:
    print("__init__() set self.real and self.imag incorrectly")

# Validate conjugate() by checking the new number's imag attribute.
if py_cnum.conjugate().imag != my_cnum.conjugate().imag:
    print("conjugate() failed for", py_cnum)

# Validate __str__().
if str(py_cnum) != str(my_cnum):
    print("__str__() failed for", py_cnum)
# ...
```

# **Additional Material**

# Static Attributes

Attributes that are accessed through self are called *instance* attributes because they are bound to a particular instance of the class. In contrast, a *static* attribute is one that is shared between all instances of the class. To make an attribute static, declare it inside of the class block but outside of any of the class's methods, and do not use self. Since the attribute is not tied to a specific instance of the class, it may be accessed or changed via the class name without even instantiating the class at all.

```
>>> pack1, pack2 = Backpack("Bill", "blue"), Backpack("William", "white")
>>> print(pack1.brand, pack2.brand, Backpack.brand)
Adidas Adidas Adidas

# Change the brand name for the class to change it for all class instances.
>>> Backpack.brand = "Nike"
>>> print(pack1.brand, pack2.brand, Backpack.brand)
Nike Nike Nike
```

# Static Methods

Individual class methods can also be static. A static method cannot be dependent on the attributes of individual instances of the class, so there can be no references to self inside the body of the method and self is not listed as an argument in the function definition. Thus static methods only have access to static attributes and other static methods. Include the tag @staticmethod above the function definition to designate a method as static.

```
# Static methods can be called without instantiating the class.
>>> Backpack.origin()
Manufactured by Nike, inc.

# The method can also be accessed by individual class instances.
>>> pack = Backpack("Larry", "lime")
>>> pack.origin()
Manufactured by Nike, inc.
```

To practice these principles, consider adding a static attribute to the Backpack class to serve as a counter for a unique ID. In the constructor for the Backpack class, add an instance variable called self.ID. Set this ID based on the static ID variable, then increment the static ID so that the next Backpack object will have a different ID.

# More Magic Methods

Consider how the following methods might be implemented for the Backpack class. These methods are particularly important for custom data structure classes.

| $\operatorname{Method}$ | Operation                         | Trigger Function           |
|-------------------------|-----------------------------------|----------------------------|
| bool()                  | Truth value                       | bool()                     |
| len()                   | Object length or size             | len()                      |
| repr()                  | Object representation             | repr()                     |
| getitem()               | Indexing and slicing              | self[index]                |
| setitem()               | Assignment via indexing           | <pre>self[index] = x</pre> |
| iter()                  | Iteration over the object         | iter()                     |
| reversed()              | Reverse iteration over the object | reversed()                 |
| contains()              | Membership testing                | in                         |

See https://docs.python.org/3/reference/datamodel.html#special-method-names for more details and documentation on all magic methods.

# Hashing

A hash value is an integer that uniquely identifies an object. The built-in hash() function calculates an object's hash value by calling its \_\_hash\_\_() magic method.

In Python, the built-in set and dict structures use hash values to store and retrieve objects in memory quickly. If an object is *unhashable*, it cannot be put in a set or be used as a key in a dictionary. See https://docs.python.org/3/glossary.html#term-hashable for details.

If the \_\_hash\_\_() method is not defined, the default hash value is the object's memory address (accessible via the built-in function id()) divided by 16, rounded down to the nearest integer. However, two objects that compare as equal via the \_\_eq\_\_() magic method must have the same hash value. The following simple \_\_hash\_\_() method for the Backpack class conforms to this rule and returns an integer.

```
class Backpack:
    # ...
    def __hash__(self):
        return hash(self.name) ^ hash(self.color) ^ hash(len(self.contents))
```

The caret operator ^ is a bitwise XOR (exclusive or). The bitwise AND operator & and the bitwise OR operator | are also good choices to use.

 $See \, https://docs.python.org/3/reference/datamodel.html \verb|#object.__hash\__for more on hashing.$ 

# Introduction to Matplotlib

Lab Objective: Matplotlib is the most commonly used data visualization library in Python. Being able to visualize data helps to determine patterns and communicate results, and is a key component of applied and computational mathematics. In this lab we introduce techniques for visualizing data in 1, 2, and 3 dimensions. The plotting techniques presented here will be used in the remainder of the labs in the manual.

# Line Plots

Raw numerical data is rarely helpful unless it can be visualized. The quickest way to visualize a simple 1-dimensional array is with a *line plot*. The following code creates an array of outputs of the function  $f(x) = x^2$ , then visualizes the array using the matplotlib module<sup>1</sup> [Hun07].

```
>>> import numpy as np
>>> from matplotlib import pyplot as plt

>>> y = np.arange(-5,6)**2
>>> y
array([25, 16, 9, 4, 1, 0, 1, 4, 9, 16, 25])

# Visualize the plot.
>>> plt.plot(y) # Draw the line plot.
[<matplotlib.lines.Line2D object at 0x1084762d0>]
>>> plt.show() # Reveal the resulting plot.
```

The result is shown in Figure 5.1a. Just as np is a standard alias for NumPy, plt is a standard alias for matplotlib.pyplot in the Python community.

The call plt.plot(y) creates a figure and draws straight lines connecting the entries of y relative to the y-axis. The x-axis is (by default) the index of the array, which in this case is the integers from 0 to 10. Calling plt.show() then displays the figure.

<sup>&</sup>lt;sup>1</sup>Like NumPy, Matplotlib is *not* part of the Python standard library, but it is included in most Python distributions. See https://matplotlib.org/ for the complete Matplotlib documentation.

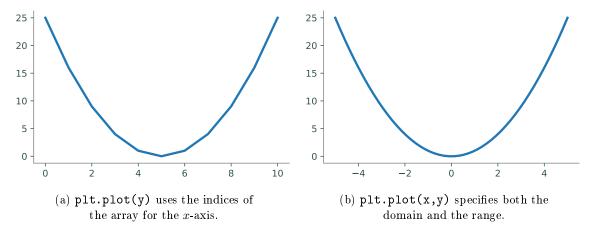


Figure 5.1: Plots of  $f(x) = x^2$  over the interval [-5, 5].

**Problem 1.** NumPy's random module has tools for sampling from probability distributions. For instance, np.random.normal() draws samples from the normal (Gaussian) distribution. The size parameter specifies the shape of the resulting array.

Write a function that accepts an integer n as input.

- 1. Use np.random.normal() to create an  $n \times n$  array of values randomly sampled from the standard normal distribution.
- 2. Compute the mean of each row of the array.

  (Hint: Use np.mean() and specify the axis keyword argument.)
- 3. Return the variance of these means.

  (Hint: Use np.var() to calculate the variance).

Define another function that creates an array of the results of the first function with inputs  $n = 100, 200, \ldots, 1000$ . Plot (and show) the resulting array.

# Specifying a Domain

An obvious problem with Figure 5.1a is that the x-axis does not correspond correctly to the y-axis for the function  $f(x) = x^2$  that is being drawn. To correct this, define an array x for the domain, then use it to calculate the image y = f(x). The command plt.plot(x,y) plots x against y by drawing a line between the consecutive points (x[i], y[i]).

Another problem with Figure 5.1a is its poor resolution: the curve is visibly bumpy, especially near the bottom of the curve. NumPy's linspace() function makes it easy to get a higher-resolution domain. Recall that np.arange() returns an array of evenly-spaced values in a given interval, where

the **spacing** between the entries is specified. In contrast, **np.linspace()** creates an array of evenly-spaced values in a given interval where the **number of elements** is specified.

The resulting plot is shown in Figure 5.1b. This time, the x-axis correctly matches up with the y-axis. The resolution is also much better because x and y have 50 entries each instead of only 10.

Subsequent calls to plt.plot() modify the same figure until plt.show() is executed, which displays the current figure and resets the system. This behavior can be altered by specifying separate figures or axes, which we will discuss shortly.

# NOTE

Plotting can seem a little mystical because the actual plot doesn't appear until plt.show() is executed. Matplotlib's *interactive mode* allows the user to see the plot be constructed one piece at a time. Use plt.ion() to turn interactive mode on and plt.ioff() to turn it off. This is very useful for quick experimentation. Try executing the following commands in IPython:

```
In [1]: import numpy as np
In [2]: from matplotlib import pyplot as plt

# Turn interactive mode on and make some plots.
In [3]: plt.ion()
In [4]: x = np.linspace(1, 4, 100)
In [5]: plt.plot(x, np.log(x))
In [6]: plt.plot(x, np.exp(x))

# Clear the figure, then turn interactive mode off.
In [7]: plt.clf()
In [8]: plt.ioff()
```

Use interactive mode **only** with IPython. Using interactive mode in a non-interactive setting may freeze the window or cause other problems.

**Problem 2.** Write a function that plots the functions  $\sin(x)$ ,  $\cos(x)$ , and  $\arctan(x)$  on the domain  $[-2\pi, 2\pi]$  (use np.pi for  $\pi$ ). Make sure the domain is refined enough to produce a figure with good resolution.

# Plot Customization

plt.plot() receives several keyword arguments for customizing the drawing. For example, the color and style of the line are specified by the following string arguments.

| $\mathbf{Key}$ | Color       | Key         | Style         |
|----------------|-------------|-------------|---------------|
| 'b'            | blue        | 1 = 1       | solid line    |
| 'g'            | green       | 1 == 1      | dashed line   |
| 'r'            | $_{ m red}$ | $^{-1} = 1$ | dash-dot line |
| 'c'            | cyan        | 1:1         | dotted line   |
| 'k'            | black       | 101         | circle marker |

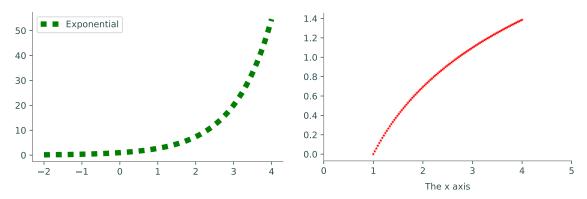
Specify one or both of these string codes as the third argument to plt.plot() to change from the default color and style. Other plt functions further customize a figure.

| Function                       | Description                              |
|--------------------------------|--|
| legend()                       | Place a legend in the plot               |
| title()                        | Add a title to the plot                  |
| <pre>xlim() / ylim()</pre>     | Set the limits of the $x$ - or $y$ -axis |
| <pre>xlabel() / ylabel()</pre> | Add a label to the $x$ - or $y$ -axis    |

```
>>> x1 = np.linspace(-2, 4, 100)
>>> plt.plot(x1, np.exp(x1), 'g:', linewidth=6, label="Exponential")
>>> plt.title("This is the title.", fontsize=18)
>>> plt.legend(loc="upper left")  # plt.legend() uses the 'label' argument of
>>> plt.show()  # plt.plot() to create a legend.

>>> x2 = np.linspace(1, 4, 100)
>>> plt.plot(x2, np.log(x2), 'r*', markersize=4)
>>> plt.xlim(0, 5)  # Set the visible limits of the x axis.
>>> plt.xlabel("The x axis")  # Give the x axis a label.
>>> plt.show()
```

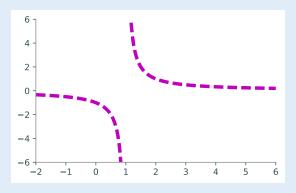
# This is the title.



**Problem 3.** Write a function to plot the curve  $f(x) = \frac{1}{x-1}$  on the domain [-2, 6].

- 1. Although f(x) has a discontinuity at x = 1, a single call to plt.plot() in the usual way will make the curve look continuous. Split up the domain into [-2, 1) and (1, 6]. Plot the two sides of the curve separately so that the graph looks discontinuous at x = 1.
- 2. Plot both curves with a dashed magenta line. Set the keyword argument linewidth (or lw) of plt.plot() to 4 to make the line a little thicker than the default setting.
- 3. Use plt.xlim() and plt.ylim() to change the range of the x-axis to [-2, 6] and the range of the y-axis to [-6, 6].

The plot should resemble the figure below.



# Figures, Axes, and Subplots

The window that plt.show() reveals is called a *figure*, stored in Python as a plt.Figure object. A space on a figure where a plot is drawn is called an *axes*, a plt.Axes object. A figure can have multiple axes, and a single program may create several figures. There are several ways to create or grab figures and axes with plt functions.

| Function             | Description                                    |  |
|----------------------|--|--|
| axes()               | Add an axes to the current figure              |  |
| figure()             | Create a new figure or grab an existing figure |  |
| gca()                | Get the current axes                           |  |
|                      | Get the current figure                         |  |
| <pre>subplot()</pre> | Add a single subplot to the current figure     |  |
| subplots()           | Create a figure and add several subplots to it |  |

Usually when a figure has multiple axes, they are organized into non-overlapping *subplots*. The command plt.subplot(nrows, ncols, plot\_number) creates an axes in a subplot grid where nrows is the number of rows of subplots in the figure, ncols is the number of columns, and plot\_number specifies which subplot to modify. If the inputs for plt.subplot() are all integers, the commas between the entries can be omitted. For example, plt.subplot(3,2,2) can be shortened to plt.subplot(322).

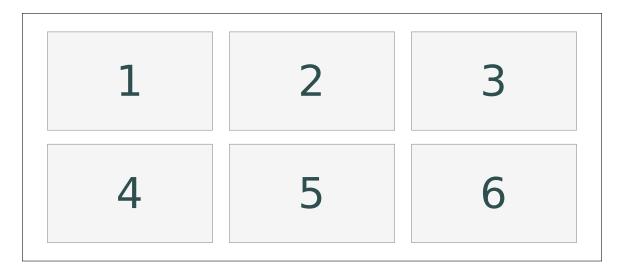
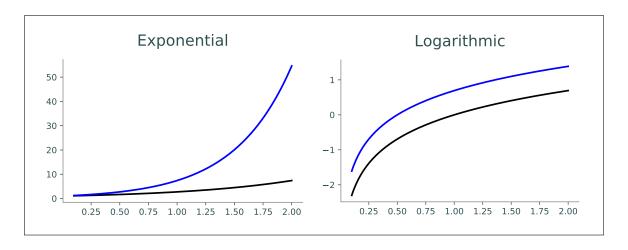


Figure 5.3: The layout of subplots with plt.subplot(2,3,i) (2 rows, 3 columns), where i is the index pictured above. The outer border is the figure that the axes belong to.

```
>>> x = np.linspace(.1, 2, 200)
# Create a subplot to cover the left half of the figure.
>>> ax1 = plt.subplot(121)
>>> ax1.plot(x, np.exp(x), 'k', lw=2)
>>> ax1.plot(x, np.exp(2*x), 'b', lw=2)
>>> plt.title("Exponential", fontsize=18)

# Create another subplot to cover the right half of the figure.
>>> ax2 = plt.subplot(122)
>>> ax2.plot(x, np.log(x), 'k', lw=2)
>>> ax2.plot(x, np.log(2*x), 'b', lw=2)
>>> ax2.set_title("Logarithmic", fontsize=18)
>>> plt.show()
```



# Note

Plotting functions such as plt.plot() are shortcuts for accessing the current axes on the current figure and calling a method on that Axes object. Calling plt.subplot() changes the current axis, and calling plt.figure() changes the current figure. Use plt.gca() to get the current axes and plt.gcf() to get the current figure. Compare the following equivalent strategies for producing a figure with two subplots.

```
>>> x = np.linspace(-5, 5, 100)

# 1. Use plt.subplot() to switch the current.
>>> plt.subplot(121)
>>> plt.plot(x, 2*x)
>>> plt.subplot(122)
>>> plt.plot(x, x**2)

# 2. Use plt.subplot() to explicitly grab the two subplot axes.
>>> ax1 = plt.subplot(121)
>>> ax1.plot(x, 2*x)
>>> ax2 = plt.subplot(122)
>>> ax2.plot(x, x**2)

# 3. Use plt.subplots() to get the figure and all subplots simultaneously.
>>> fig, axes = plt.subplots(1, 2)
>>> axes[0].plot(x, 2*x)
>>> axes[1].plot(x, x**2)
```

**Problem 4.** Write a function that plots the functions  $\sin(x)$ ,  $\sin(2x)$ ,  $2\sin(x)$ , and  $2\sin(2x)$  on the domain  $[0, 2\pi]$ , each in a separate subplot of a single figure.

- 1. Arrange the plots in a  $2 \times 2$  grid of subplots.
- 2. Set the limits of each subplot to  $[0, 2\pi] \times [-2, 2]$ . (Hint: Consider using plt.axis([xmin, xmax, ymin, ymax]) instead of plt.xlim() and plt.ylim() to set all boundaries simultaneously.)
- 3. Use plt.title() or ax.set\_title() to give each subplot an appropriate title.
- 4. Use plt.suptitle() or fig.suptitle() to give the overall figure a title.
- 5. Use the following colors and line styles.

```
\sin(x): green solid line. \sin(2x): red dashed line.
```

 $2\sin(x)$ : blue dashed line.  $2\sin(2x)$ : magenta dotted line.

# ACHTUNG!

Be careful not to mix up the following functions.

- 1. plt.axes() creates a new place to draw on the figure, while plt.axis() (or ax.axis()) sets properties of the x- and y-axis in the current axes, such as the x and y limits.
- 2. plt.subplot() (singular) returns a single subplot belonging to the current figure, while plt.subplots() (plural) creates a new figure and adds a collection of subplots to it.

# Other Kinds of Plots

Line plots are not always the most illuminating choice of graph to describe a set of data. Matplotlib provides several other easy ways to visualize data.

• A scatter plot plots two 1-dimensional arrays against each other without drawing lines between the points. Scatter plots are particularly useful for data that is not correlated or ordered.

To create a scatter plot, use plt.plot() and specify a point marker (such as 'o' or '\*') for the line style, or use plt.scatter() (or ax.scatter()). Beware that plt.scatter() has slightly different arguments and syntax than plt.plot().

• A histogram groups entries of a 1-dimensional data set into a given number of intervals, called bins. Each bin has a bar whose height indicates the number of values that fall in the range of the bin. Histograms are best for displaying distributions, relating data values to frequency.

To create a histogram, use plt.hist() (or ax.hist()). Use the argument bins to specify the edges of the bins or to choose a number of bins. The range argument specifies the outer limits of the first and last bins.

```
# Get 500 random samples from two normal distributions.
>>> x = np.random.normal(scale=1.5, size=500)
>>> y = np.random.normal(scale=0.5, size=500)

# Draw a scatter plot of x against y, using transparent circle markers.
>>> ax1 = plt.subplot(121)
>>> ax1.plot(x, y, 'o', markersize=5, alpha=.5)

# Draw a histogram to display the distribution of the data in x.
>>> ax2 = plt.subplot(122)
>>> ax2.hist(x, bins=np.arange(-4.5, 5.5))  # Or, equivalently,
# ax2.hist(x, bins=9, range=[-4.5, 4.5])
>>> plt.show()
```



**Problem 5.** The Fatality Analysis Reporting System (FARS) is a nationwide census that provides yearly data regarding fatal injuries suffered in motor vehicle traffic crashes.<sup>a</sup> The array contained in FARS.npy is a small subset of the FARS database from 2010–2014. Each of the 148,206 rows in the array represents a different car crash; the columns represent the hour (in military time, as an integer), the longitude, and the latitude, in that order.

Write a function to visualize the data in FARS.npy. Use np.load() to load the data, then create a single figure with two subplots:

- 1. A scatter plot of longitudes against latitudes. Because of the large number of data points, use black pixel markers (use "k," as the third argument to plt.plot()). Label both axes using plt.xlabel() and plt.ylabel() (or ax.set\_xlabel() and ax.set\_ylabel()). (Hint: Use plt.axis("equal") or ax.set\_aspect("equal") so that the x- and y-axis are scaled the same way.
- 2. A histogram of the hours of the day, with one bin per hour. Set the limits of the x-axis appropriately. Label the x-axis. You should be able to clearly see which hours of the day experience more traffic.

Matplotlib also has tools for creating other kinds of plots for visualizing 1-dimensional data, including bar plots and box plots. See the Matplotlib Appendix for examples and syntax.

# Visualizing 3-D Surfaces

Line plots, histograms, and scatter plots are good for visualizing 1- and 2-dimensional data, including the domain and range of a function  $f: \mathbb{R} \to \mathbb{R}$ . However, visualizing 3-dimensional data or a function  $g: \mathbb{R}^2 \to \mathbb{R}$  (two inputs, one output) requires a different kind of plot. The process is similar to creating a line plot but requires slightly more setup: first construct an appropriate domain, then calculate the image of the function on that domain.

NumPy's np.meshgrid() function is the standard tool for creating a 2-dimensional domain in the Cartesian plane. Given two 1-dimensional coordinate arrays, np.meshgrid() creates two corresponding coordinate matrices. See Figure 5.6.

<sup>&</sup>lt;sup>a</sup>See http://www.nhtsa.gov/FARS.

Figure 5.6: np.meshgrid(x, y), returns the arrays X and Y. The returned arrays give the x- and y-coordinates of the points in the grid formed by x and y. Specifically, the arrays X and Y satisfy (X[i,j], Y[i,j]) = (x[i],y[j]).

```
>>> x, y = [0, 1, 2], [3, 4, 5]  # A rough domain over [0,2]x[3,5].
>>> X, Y = np.meshgrid(x, y)  # Combine the 1-D data into 2-D data.
>>> for xrow, yrow in zip(X,Y):
... print(xrow, yrow, sep='\t')
...
[0 1 2] [3 3 3]
[0 1 2] [4 4 4]
[0 1 2] [5 5 5]
```

With a 2-dimensional domain, g(x,y) is usually visualized with two kinds of plots.

• A heat map assigns a color to each point in the domain, producing a 2-dimensional colored picture describing a 3-dimensional shape. Darker colors typically correspond to lower values while lighter colors typically correspond to higher values.

Use plt.pcolormesh() to create a heat map.

• A contour map draws several level curves of g on the 2-dimensional domain. A level curve corresponding to the constant c is the collection of points  $\{(x,y) \mid c=g(x,y)\}$ . Coloring the space between the level curves produces a discretized version of a heat map. Including more and more level curves makes a filled contour plot look more and more like the complete, blended heat map.

Use plt.contour() to create a contour plot and plt.contourf() to create a filled contour plot. Specify either the number of level curves to draw, or a list of constants corresponding to specific level curves.

These functions each receive the keyword argument cmap to specify a color scheme (some of the better schemes are "viridis", "magma", and "coolwarm"). For the list of all Matplotlib color schemes, see http://matplotlib.org/examples/color/colormaps\_reference.html.

Finally, plt.colorbar() draws the color scale beside the plot to indicate how the colors relate to the values of the function.

```
# Create a 2-D domain with np.meshgrid().
>>> x = np.linspace(-np.pi, np.pi, 100)
>>> y = x.copy()
>>> X, Y = np.meshgrid(x, y)
>>> Z = np.sin(X) * np.sin(Y)
                                  # Calculate g(x,y) = \sin(x)\sin(y).
# Plot the heat map of f over the 2-D domain.
>>> plt.subplot(131)
>>> plt.pcolormesh(X, Y, Z, cmap="viridis")
>>> plt.colorbar()
>>> plt.xlim(-np.pi, np.pi)
>>> plt.ylim(-np.pi, np.pi)
# Plot a contour map of f with 10 level curves.
>>> plt.subplot(132)
>>> plt.contour(X, Y, Z, 10, cmap="coolwarm")
>>> plt.colorbar()
# Plot a filled contour map, specifying the level curves.
>>> plt.subplot(133)
>>> plt.contourf(X, Y, Z, [-1, -.8, -.5, 0, .5, .8, 1], cmap="magma")
>>> plt.colorbar()
>>> plt.show()
```



**Problem 6.** Write a function to plot  $g(x,y) = \frac{\sin(x)\sin(y)}{xy}$  on the domain  $[-2\pi, 2\pi] \times [-2\pi, 2\pi]$ .

- 1. Create 2 subplots: one with a heat map of g, and one with a contour map of g. Choose an appropriate number of level curves, or specify the curves yourself.
- 2. Set the limits of each subplot to  $[-2\pi, 2\pi] \times [-2\pi, 2\pi]$ .
- 3. Choose a non-default color scheme.
- 4. Include the color scale bar for each subplot.

# **Additional Material**

# Further Reading and Tutorials

Plotting takes some getting used to. See the following materials for more examples.

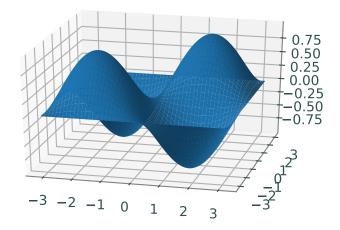
- https://www.labri.fr/perso/nrougier/teaching/matplotlib/.
- https://matplotlib.org/users/pyplot\_tutorial.html.
- http://scipy-lectures.org/intro/matplotlib/.
- The Matplotlib Appendix in this manual.

# 3-D Plotting

Matplotlib can also be used to plot 3-dimensional surfaces. The following code produces the surface corresponding to  $g(x, y) = \sin(x)\sin(y)$ .

```
# Create the domain and calculate the range like usual.
>>> x = np.linspace(-np.pi, np.pi, 200)
>>> y = np.copy(x)
>>> X, Y = np.meshgrid(x, y)
>>> Z = np.sin(X) * np.sin(Y)

# Draw the corresponding 3-D plot using some extra tools.
>>> from mpl_toolkits.mplot3d import Axes3D
>>> fig = plt.figure()
>>> ax = fig.add_subplot(1,1,1, projection='3d')
>>> ax.plot_surface(X, Y, Z)
>>> plt.show()
```



# **Animations**

Lines and other graphs can be altered dynamically to produce animations. Follow these steps to create a Matplotlib animation:

- 1. Calculate all data that is needed for the animation.
- 2. Define a figure explicitly with plt.figure() and set its window boundaries.
- 3. Draw empty objects that can be altered dynamically.
- 4. Define a function to update the drawing objects.
- 5. Use matplotlib.animation.FuncAnimation().

The submodule matplotlib.animation contains the tools for putting together and managing animations. The function matplotlib.animation.FuncAnimation() accepts the figure to animate, the function that updates the figure, the number of frames to show before repeating, and how fast to run the animation (lower numbers mean faster animations).

```
from matplotlib.animation import FuncAnimation
def sine animation():
    # Calculate the data to be animated.
    x = np.linspace(0, 2*np.pi, 200)[:-1]
    y = np.sin(x)
    # Create a figure and set the window boundaries of the axes.
    fig = plt.figure()
   plt.xlim(0, 2*np.pi)
   plt.ylim(-1.2, 1.2)
    # Draw an empty line. The comma after 'drawing' is crucial.
    drawing, = plt.plot([],[])
    # Define a function that updates the line data.
    def update(index):
        drawing.set_data(x[:index], y[:index])
        return drawing,
                                             # Note the comma!
    a = FuncAnimation(fig, update, frames=len(x), interval=10)
    plt.show()
```

Try using the following function in place of update(). Can you explain why this animation is different from the original?

```
def wave(index):
    drawing.set_data(x, np.roll(y, index))
    return drawing,
```

To animate multiple objects at once, define the objects separately and make sure the update function returns both objects.

```
def sine_cosine_animation():
    x = np.linspace(0, 2*np.pi, 200)[:-1]
    y1, y2 = np.sin(x), np.cos(x)

    fig = plt.figure()
    plt.xlim(0, 2*np.pi)
    plt.ylim(-1.2, 1.2)

    sin_drawing, = plt.plot([],[])
    cos_drawing, = plt.plot([],[])

    def update(index):
        sin_drawing.set_data(x[:index], y1[:index])
        cos_drawing.set_data(x[:index], y2[:index])
        return sin_drawing, cos_drawing,

a = FuncAnimation(fig, update, frames=len(x), interval=10)
    plt.show()
```

Animations can also be 3-dimensional. The only major difference is an extra operation to set the 3-dimensional component of the drawn object. The code below animates the space curve parametrized by the following equations:

```
x(\theta) = \cos(\theta)\cos(6\theta), \quad y(\theta) = \sin(\theta)\cos(6\theta), \quad z(\theta) = \frac{\theta}{10}
```

```
def rose_animation_3D():
   theta = np.linspace(0, 2*np.pi, 200)
    x = np.cos(theta) * np.cos(6*theta)
    y = np.sin(theta) * np.cos(6*theta)
    z = theta / 10
   fig = plt.figure()
   ax = fig.gca(projection='3d')  # Make the figure 3-D.
ax.set_xlim3d(-1.2, 1.2)  # Use ax instead of plt.
    ax.set_ylim3d(-1.2, 1.2)
    ax.set_aspect("equal")
    drawing, = ax.plot([],[],[]) # Provide 3 empty lists.
    # Update the first 2 dimensions like usual, then update the 3-D component.
    def update(index):
        drawing.set_data(x[:index], y[:index])
        drawing.set_3d_properties(z[:index])
        return drawing,
    a = FuncAnimation(fig, update, frames=len(x), interval=10, repeat=False)
    plt.show()
```

# 6

# Exceptions and File Input/Ouput

Lab Objective: In Python, an exception is an error detected during execution. Exceptions are important for regulating program usage and for correctly reporting problems to the programmer and end user. An understanding of exceptions is essential to safely read data from and write data to external files. Being able to interact with external files is important for analyzing data and communicating results. In this lab we learn exception syntax and file interaction protocols.

# **Exceptions**

An exception formally indicates an error and terminates the program early. Some of the more common exception types are listed below, along with the kinds of problems they typically indicate.

| Exception         | Indication  |
|-------------------|---|
| AttributeError    | An attribute reference or assignment failed.                    |
| ImportError       | An import statement failed.                                     |
| IndexError        | A sequence subscript was out of range.                          |
| NameError         | A local or global name was not found.                           |
| TypeError         | An operation or function was applied to an object of            |
|                   | inappropriate type.   |
| ValueError        | An operation or function received an argument that had          |
|                   | the right type but an inappropriate value.                      |
| ZeroDivisionError | The second argument of a division or modulo operation was zero. |

```
>>> print(x)
Traceback (most recent call last):
   File "<stdin>", line 1, in <module>
NameError: name 'x' is not defined

>>> [1, 2, 3].fly()
Traceback (most recent call last):
   File "<stdin>", line 1, in <module>
AttributeError: 'list' object has no attribute 'fly'
```

# Raising Exceptions

Most exceptions are due to coding mistakes and typos. However, exceptions can also be used intentionally to indicate a problem to the user or programmer. To create an exception, use the keyword raise, followed by the name of the exception class. As soon as an exception is raised, the program stops running unless the exception is handled properly.

```
>>> if 7 is not 7.0:
                                     # Raise an exception with an error message.
        raise Exception("ints and floats are different!")
Traceback (most recent call last):
  File "<stdin>", line 2, in <module>
Exception: ints and floats are different!
>>> for x in range(10):
       if x > 5:
                                     # Raise a specific kind of exception.
           raise ValueError("'x' should not exceed 5.")
        print(x, end=' ')
. . .
0 1 2 3 4 5
Traceback (most recent call last):
 File "<stdin>", line 3, in <module>
ValueError: 'x' should not exceed 5.
```

# **Problem 1.** Consider the following arithmetic "magic" trick.

- 1. Choose a 3-digit number where the first and last digits differ by 2 or more (say, 123).
- 2. Reverse this number by reading it backwards (321).
- 3. Calculate the positive difference of these numbers (321 123 = 198).
- 4. Add the reverse of the result to itself (198 + 891 = 1089).

The result of the last step will always be 1089, regardless of the original number chosen in step 1 (can you explain why?).

The following function prompts the user for input at each step of the magic trick, but does not check that the user's inputs are correct.

Modify arithmagic() so that it verifies the user's input at each step. Raise a ValueError with an informative error message if any of the following occur:

- The first number (step\_1) is not a 3-digit number.
- The first number's first and last digits differ by less than 2.
- The second number (step\_2) is not the reverse of the first number.
- The third number (step\_3) is not the positive difference of the first two numbers.
- The fourth number (step\_4) is not the reverse of the third number.

(Hint: input() always returns a string, so each variable is a string initially. Use int() to cast the variables as integers when necessary. The built-in function abs() may also be useful.)

# Handling Exceptions

To prevent an exception from halting the program, it must be handled by placing the problematic lines of code in a try block. An except block then follows with instructions for what to do in the event of an exception.

In this example, the name e represents the exception within the except block. Printing e displays its error message. If desired, e can be raised again with raise e or just raise.

The try-except control flow can be expanded with two other blocks, forming a code structure similar to a sequence of if-elif-else blocks.

- 1. The try block is executed until an exception is raised (if at all).
- 2. An except statement specifying the same kind of exception that was raised in the try block "catches" the exception, and the block is then executed. There may be multiple except blocks following a single try block (similiar to having several elif statements following a single if statement), and a single except statement may specify multiple kinds of exceptions to catch.
- 3. The else block is executed if an exception was **not** raised in the try block.
- 4. The **finally** block is always executed if it is included.

```
>>> try:
... print("Entering try block...", end='')
       house_on_fire = False
. . .
       raise ValueError("The house is on fire!")
... # Check for multiple kinds of exceptions using parentheses.
... except (ValueError, TypeError) as e:
       print("caught an exception.")
       house_on_fire = True
                                   # Skipped due to the exception.
...else:
       print("no exceptions raised.")
finally:
       print("The house is on fire:", house_on_fire)
Entering try block...caught an exception.
The house is on fire: True
>>> try:
       print("Entering try block...", end='')
      house_on_fire = False
... except ValueError as e:
                                 # Skipped because there was no exception.
... print("caught a ValueError.")
      house_on_fire = True
... except TypeError as e:
                                 # Also skipped.
      print("caught a TypeError.")
       house_on_fire = True
else:
       print("no exceptions raised.")
finally:
      print("The house is on fire:", house_on_fire)
Entering try block...no exceptions raised.
The house is on fire: False
```

The code in the finally block is always executed, even if a return statement or an uncaught exception occurs in any block following the try statement.

See https://docs.python.org/3/tutorial/errors.html for more examples.

# ACHTUNG!

An except statement with no specified exception type catches **any** exception raised in the corresponding try block. This approach can mistakenly mask unexpected errors. Always be specific about the kinds of exceptions you expect to encounter.

```
>>> def divider(x, y):
       try:
            return x / yy
                                   # The mispelled yy raises a NameError.
                                   # Catch ANY exception.
        except:
           print("y must not equal zero!")
>>> divider(2, 3)
y must not equal zero!
>>> def divider(x, y):
       try:
           return x / yy
       except ZeroDivisionError: # Specify an exception type.
           print("y must not equal zero!")
>>> divider(2, 3)
Traceback (most recent call last):
 File "<stdin>", line 1, in <module>
 File "<stdin>", line 3, in divider
NameError: name 'yy' is not defined
                                        # Now the mistake is obvious.
```

**Problem 2.** A random walk is a path created by a sequence of random steps. The following function simulates a random walk by repeatedly adding or subtracting 1 to a running total.

```
from random import choice

def random_walk(max_iters=1e12):
    walk = 0
    directions = [1, -1]
    for i in range(int(max_iters)):
        walk += choice(directions)
    return walk
```

A KeyboardInterrupt is a special exception that can be triggered at any time by entering ctrl+c (on most systems) in the keyboard. Modify random\_walk() so that if the user raises a KeyboardInterrupt by pressing ctrl+c while the program is running, the function catches the exception and prints "Process interrupted at iteration i". If no KeyboardInterrupt is raised, print "Process completed". In both cases, return walk as before.

#### NOTE

The built-in exceptions are organized into a class hierarchy. For example, the ValueError class inherits from the generic Exception class. Thus, a ValueError is an Exception, but an Exception is not a ValueError.

```
>>> try:
... raise ValueError("caught!")
... except Exception as e:  # A ValueError is an Exception.
... print(e)
...
caught!  # The exception was caught.

>>> try:
... raise Exception("not caught!")
... except ValueError as e:  # A Exception is not a ValueError.
... print(e)
...
Traceback (most recent call last):
   File "<stdin>", line 2, in <module>
Exception: not caught!  # The exception wasn't caught!
```

See https://docs.python.org/3/library/exceptions.html for the complete list of built-in exceptions and the exception class hierarchy.

# File Input and Output

A file object acts as an interface to a file stream, meaning, it allows a program to read from or write to external files. The built-in function open() creates a file object. It accepts the name of the file to open and an editing mode. The mode determines the kind of access that the user has to the file. There are four common modes:

- 'r': read. Open an existing file for reading. The file must already exist, or open() raises a FileNotFoundError. This is the default mode.
- 'w': write. Create a new file or overwrite an existing file (careful!) and open it for writing.
- 'x': write new. Create a new file and open it for writing. If the file already exists, open() raises a FileExistsError. This is a safer form of 'w' because it never overwrites existing files.
- 'a': append. Open a file for writing and append new data to the end of the file if it already exists.

```
>>> myfile = open("hello_world.txt", 'r')  # Open a file for reading.
>>> print(myfile.read())  # Print the contents of the file.
Hello,  # (it's a really small file.)
World!
>>> myfile.close()  # Close the file connection.
```

# The With Statement

An IOError indicates that some input or output operation has failed. A simple try-finally control flow can ensure that a file stream is closed safely.

The with statement provides an alternative method for safely opening and closing files. Use with open(<filename>, <mode>) as <alias>: to create an indented block in which the file is open and available under the specified alias. At the end of the block, the file is automatically and safely closed, even in the event of an exception. This is the preferred file-reading method when a file only needs to be accessed briefly.

In both cases, if the file hello\_world.txt does not exist in the current directory, open() raises a FileNotFoundError. However, errors in the try or with blocks do not prevent the file from being safely closed.

# Reading and Writing

Open file objects have an implicit *cursor* that determines the location in the file to read from or write to. After the entire file has been read once, either the file must be closed and reopened, or the cursor must be reset to the beginning of the file with seek(0) before it can be read again.

Some of the more important file object attributes and methods are listed below.

| Attribute               | Description  |
|-------------------------|--|
| closed                  | True if the object is closed.  |
| mode                    | The access mode used to open the file object.                                  |
| name                    | The name of the file.  |
|                         |  |
| $\operatorname{Method}$ | Description  |
| close()                 | Close the connection to the file.  |
| read()                  | Read a given number of bytes; with no input, read the entire file.             |
| readline()              | Read a line of the file, including the newline character at the end.           |
| readlines()             | Call readline() repeatedly and return a list of the resulting lines.           |
| seek()                  | Move the cursor to a new position.   |
| tell()                  | Report the current position of the cursor.                                     |
| write()                 | Write a single string to the file (spaces are <b>not</b> added).               |
| writelines()            | Write a list of strings to the file (newline characters are <b>not</b> added). |

Only strings can be written to files; to write a non-string type, first cast it as a string with str(). Be mindful of spaces and newlines to separate the data.

```
>>> with open("out.txt", 'w') as outfile:  # Open 'out.txt' for writing.
... for i in range(10):
... outfile.write(str(i**2)+' ')  # Write some strings (and spaces).
...
>>> outfile.closed  # The file is closed automatically.
True
```

**Problem 3.** Define a class called ContentFilter. Implement the constructor so that it accepts the name of a file to be read.

1. If the file name is invalid in any way, prompt the user for another filename using input(). Continue prompting the user until they provide a valid filename.

```
>>> cf1 = ContentFilter("hello_world.txt")  # File exists.
>>> cf2 = ContentFilter("not-a-file.txt")  # File doesn't exist.
Please enter a valid file name: still-not-a-file.txt
Please enter a valid file name: hello_world.txt
>>> cf3 = ContentFilter([1, 2, 3])  # Not even a string.
Please enter a valid file name: hello_world.txt
```

(Hint: open() might raise a FileNotFoundError, a TypeError, or an OSError.)

2. Read the file and store its name and contents as attributes (store the contents as a single string). Make sure the file is securely closed.

# **String Formatting**

The str class has several useful methods for parsing and formatting strings. They are particularly useful for processing data from a source file and for preparing data to be written to an external file.

| Method         | Returns   |
|----------------|---|
| count()        | The number of times a given substring occurs within the string.           |
| find()         | The lowest index where a given substring is found.                        |
| isalpha()      | True if all characters in the string are alphabetic $(a, b, c, \ldots)$ . |
| isdigit()      | True if all characters in the string are digits $(0, 1, 2,)$ .            |
| isspace()      | True if all characters in the string are whitespace (" ", '\t', '\n').    |
| join()         | The concatenation of the strings in a given iterable with a               |
|                | specified separator between entries.                                      |
| lower()        | A copy of the string converted to lowercase.                              |
| upper()        | A copy of the string converted to uppercase.                              |
| replace()      | A copy of the string with occurrences of a given substring                |
|                | replaced by a different specified substring.                              |
| ${	t split}()$ | A list of segments of the string, using a given character or string       |
|                | as a delimiter.   |
| strip()        | A copy of the string with leading and trailing whitespace removed.        |

The join() method translates a list of strings into a single string by concatenating the entries of the list and placing the principal string between the entries. Conversely, split() translates the principal string into a list of substrings, with the separation determined by a single input.

```
# str.join() puts the string between the entries of a list.
>>> words = ["state", "of", "the", "art"]
>>> "-".join(words)
'state-of-the-art'

# str.split() creates a list out of a string, given a delimiter.
>>> "One fish\nTwo fish\nRed fish\nBlue fish\n".split('\n')
['One fish', 'Two fish', 'Red fish', 'Blue fish', '']

# If no delimiter is provided, the string is split by whitespace characters.
>>> "One fish\nTwo fish\nRed fish\nBlue fish\n".split()
['One', 'fish', 'Two', 'fish', 'Red', 'fish', 'Blue', 'fish']
```

Can you tell the difference between the following routines?

```
>>> with open("hello_world.txt", 'r') as myfile:
...     contents = myfile.readlines()
...
>>> with open("hello_world.txt", 'r') as myfile:
...     contents = myfile.read().split('\n')
```

**Problem 4.** Add the following methods to the ContentFilter class for writing the contents of the original file to new files. Each method should accept the name of a file to write to and a keyword argument mode that specifies the file access mode, defaulting to 'w'. If mode is not 'w', 'x', or 'a', raise a ValueError with an informative message.

- 1. uniform(): write the data to the outfile with uniform case. Include an additional keyword argument case that defaults to "upper".
  - If case="upper", write the data in upper case. If case="lower", write the data in lower case. If case is not one of these two values, raise a ValueError.
- 2. reverse(): write the data to the outfile in reverse order. Include an additional keyword argument unit that defaults to "line".
  - If unit="word", reverse the ordering of the words in each line, but write the lines in the same order as the original file. If unit="line", reverse the ordering of the lines, but do not change the ordering of the words on each individual line. If unit is not one of these two values, raise a ValueError.
- 3. transpose(): write a "transposed" version of the data to the outfile. That is, write the first word of each line of the data to the first line of the new file, the second word of each line of the data to the second line of the new file, and so on. Viewed as a matrix of words, the rows of the input file then become the columns of the output file, and vice versa. You may assume that there are an equal number of words on each line of the input file.

Also implement the \_\_str\_\_() magic method so that printing a ContentFilter object yields the following output. You may want to calculate these statistics in the constructor.

```
Source file: <filename>
Total characters: <The total number of characters in the file>
Alphabetic characters: <The number of letters>
Numerical characters: <The number of digits>
Whitespace characters: <The number of spaces, tabs, and newlines>
Number of lines: <The number of lines>
```

(Hint: list comprehensions are **very** useful for some of these functions. For example, what does [line[::-1] for line in lines] do? What about sum([s.isspace() for s in data])?) Compare your class to the following example.

```
# cf_example1.txt
A b C
d E f
```

```
>>> cf = ContentFilter("cf_example1.txt")
>>> cf.uniform("uniform.txt", mode='w', case="upper")
>>> cf.uniform("uniform.txt", mode='a', case="lower")
>>> cf.reverse("reverse.txt", mode='w', unit="word")
>>> cf.reverse("reverse.txt", mode='a', unit="line")
>>> cf.transpose("transpose.txt", mode='w')
```

```
# uniform.txt
A B C
D E F
a b c
d e f
```

```
# reverse.txt
C b A
f E d
d E f
A b C
```

```
# transpose.txt
A d
b E
C f
```

# **Additional Material**

# **Custom Exception Classes**

Custom exceptions can be defined by writing a class that inherits from some existing exception class. The generic Exception class is typically the parent class of choice.

```
>>> class TooHardError(Exception):
...    pass
...
>>> raise TooHardError("This lab is impossible!")
Traceback (most recent call last):
    File "<stdin>", line 1, in <module>
__main__.TooHardError: This lab is impossible!
```

This may seem like a trivial extension of the Exception class, but it is useful to do because the interpreter never automatically raises a TooHardError. Any TooHardError must have originated from a hand-written raise command, making it easier to identify the exact source of the problem.

# Chaining Exceptions

Sometimes, especially in large programs, it is useful to raise one kind of exception just after catching another. The two exceptions can be linked together using the **from** statement. This syntax makes it possible to see where the error originated from and to "pass it up" to another part of the program.

```
>>> try:
... raise TooHardError("This lab is impossible!")
... except TooHardError as e:
... raise NotImplementedError("Lab is incomplete") from e
...
Traceback (most recent call last):
   File "<stdin>", line 2, in <module>
   __main__.TooHardError: This lab is impossible!

The above exception was the direct cause of the following exception:

Traceback (most recent call last):
   File "<stdin>", line 4, in <module>
NotImplementedError: Lab is incomplete
```

# More String Formatting Tools

Concatenating string values with non-string values can be cumbersome and tedious. The str class's format() method makes it easier to insert non-string values into the middle of a string. Write the desired output in its entirety, replacing non-string values with curly braces {}. Then use the format() method, entering each replaced value in order.

```
# Join the data using string concatenation.
>>> day, month, year = 10, "June", 2017
```

```
>>> print("Is today", day, str(month) + ',', str(year) + "?")
Is today 10 June, 2017?

# Join the data using str.format().
>>> print("Is today {} {}, {}?".format(day, month, year))
Is today 10 June, 2017?
```

This method is extremely flexible and provides many convenient ways to format string output nicely. Consider the following code for printing out a simple progress bar from within a loop.

```
>>> iters = int(1e7)
>>> chunk = iters // 20
>>> for i in range(iters):
... print("\r[{:<20}] i = {}".format('='*((i//chunk)+1), i),
... end='', flush=True)
...
```

Here the string "\r[{:<20}]" used in conjunction with the format() method tells the cursor to go back to the beginning of the line, print an opening bracket, then print the first argument of format() left-aligned with at least 20 total spaces before printing the closing bracket. The comma after the print command suppresses the automatic newline character, keeping the output of each individual print statement on the same line.

Printing at each iteration dramatically slows down the progression through the loop. How does the following code solve that problem?

```
>>> for i in range(iters):
... if not i % chunk:
... print("\r[{:<20}] i = {}".format('='*((i//chunk)+1),i),
... end='', flush=True)
...
```

See https://docs.python.org/3/library/string.html#format-string-syntax for more examples and specific syntax for using str.format(). For a more robust progress bar printer, research the tqdm module.

# Standard Library Modules for I/O

The standard library has other tools for input and output operations. For details on each module, see https://docs.python.org/3/library.

| $\operatorname{Module}$ | Description   |
|-------------------------|---|
| csv                     | CSV (comma separated value) file writing and parsing.         |
| io                      | Support for file objects and open().                          |
| os                      | Communication with the operating system.                      |
| ${\tt os.path}$         | Common path operations such as checking for file existence.   |
| pickle                  | Create portable serialized representations of Python objects. |

# **Unit Testing**

Lab Objective: Finding and fixing programming errors can be difficult and time consuming, especially in large or complex programs. Unit testing is a formal strategy for finding and eliminating errors quickly as a program is constructed and for ensuring that the program still works whenever it is modified. A single unit test checks a small piece code (usually a function or class method) for correctness, independent of the rest of the program. A well-written collection of unit tests can ensure that every unit of code functions as intended, thereby certifying that the program is correct. In this lab we learn to write unit tests in Python and practice test-driven development. Applying these principles will greatly speed up the coding process and improve your code quality.

# **Unit Tests**

A unit test verifies a piece of code by running a series of test cases and comparing actual outputs with expected outputs. Each test case is usually checked with an assert statement, a shortcut for raising an AssertionError with an optional error message if a boolean statement is false.

```
# Store the result of a boolean expression in a variable.
>>> result = str(5)=='5'

# Check the result, raising an error if it is false.
>>> if result is False:
... raise AssertionError("incorrect result")

# Do the same check in one line with an assert statement.
>>> assert result, "incorrect result"

# Asserting a false statement raises an AssertionError.
>>> assert 5=='5', "5 is not a string"
Traceback (most recent call last):
   File "<stdin>", line 4, in <module>
AssertionError: 5 is not a string
```

Now suppose we wanted to test a simple add() function, located in the file specs.py.

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```
# specs.py

def add(a, b):
    """Add two numbers."""
    return a + b
```

In a corresponding file called test\_specs.py, which should contain all of the unit tests for the code in specs.py, we write a unit test called test\_add() to verify the add() function.

```
# test_specs.py
import specs

def test_add():
    assert specs.add(1, 3) == 4, "failed on positive integers"
    assert specs.add(-5, -7) == -12, "failed on negative integers"
    assert specs.add(-6, 14) == 8
```

In this case, running test\_add() raises no errors since all three test cases pass. Unit test functions don't need to return anything, but they should raise an exception if a test case fails.

# NOTE

This style of external testing—checking that certain inputs result in certain outputs—is called black box testing. The actual structure of the code is not considered, but what it produces is thoroughly examined. In fact, the author of a black box test doesn't even need to be the person who eventually writes the program: having one person write tests and another write the code helps detect problems that one developer or the other may not have caught individually.

# **PyTest**

Python's pytest module<sup>1</sup> provides tools for building tests, running tests, and providing detailed information about the results. To begin, run pytest in the current directory. Without any test files, the output should be similar to the following.

Given some test files, say test\_calendar.py and test\_google.py, the output of pytest identifies failed tests and provides details on why they failed.

¹Pytest is not part of the standard libray, but it is included in Anaconda's Python distribution. Install pytest with [basicstyle=]conda install pytest if needed. The standard library's [basicstyle=]unittest module also provides a testing framework, but is less popular and straightforward than PyTest.

```
$ pytest
------ test session starts ------
platform darwin -- Python 3.6.0, pytest-3.0.5, py-1.4.32, pluggy-0.4.0
rootdir: /Users/Student/example_tests, inifile:
collected 12 items
test_calendar.py .....
test_google.py .F..
_____ test_subtract _____
  def test_subtract():
     assert google.subtract(42, 17)==25, "subtract() failed for a > b > 0"
     AssertionError: subtract() failed for a > b > 0
     assert 35 == 25
Ε
      + where 35 = \langle function subtract at 0x102d4eb90 \rangle (42, 17)
         where <function subtract at 0x102d4eb90> = google.subtract
test_google.py:11: AssertionError
```

Each dot represents a passed test and each F represents a failed test. They show up in order, so in the example above, only the second of four tests in test\_google.py failed.

# ACHTUNG!

PyTest will not find or run tests if they are not contained in files named test\_\*.py or \*\_test.py, where \* represents any number of characters. In addition, the unit tests themselves must be named test\_\*() or \*\_test(). If you need to change this behavior, consult the documentation at http://pytest.org/latest/example/pythoncollection.html.

# **Problem 1.** The following function contains a subtle but important error.

```
def smallest_factor(n):
    """Return the smallest prime factor of the positive integer n."""
    if n == 1: return 1
    for i in range(2, int(n**.5)):
        if n % i == 0: return i
    return n
```

Write a unit test for this function, including test cases that you suspect might uncover the error (what are the edge cases for this function?). Use pytest to run your unit test and discover a test case that fails, then use this information to correct the function.

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# Coverage

Successful unit tests include enough test cases to test the entire program. Coverage refers to the number of lines of code that are executed by at least one test case. One tool for measuring coverage is called pytest-cov, an extension of pytest. This tool must be installed separately, as it does not come bundled with Anaconda. To install, run the following code in a terminal.

```
$ conda install pytest-cov
```

Add the flag --cov to the pytest command to print out code coverage information. Running pytest --cov in the same directory as specs.py and test\_specs.py yields the following output.

```
$ pytest --cov
platform darwin -- Python 3.6.0, pytest-3.0.5, py-1.4.32, pluggy-0.4.0
rootdir: /Users/Student/Testing, inifile:
plugins: cov-2.3.1
collected 7 items
test_specs.py ......
----- coverage: platform darwin, python 3.6.6-final-0 ------
          Stmts Miss Cover
_____
specs.py 73 34
                      53%
test_specs.py
            46
                 0 100%
TOTAL
           119 34
                      71%
======== 7 passed in 0.03 seconds ===========================
```

Here, Stmts refers to the number of lines of code covered by a unit test, while Miss is the number of lines that are not currently covered. Notice that the file test\_specs.py has 100% coverage while specs.py does not. Test files generally have 100% coverage, since pytest is designed to run these files in their entirety. However, specs.py does not have full coverage and requires additional unit tests. To find out which lines are not yet covered, pytest-cov has a useful feature called cov-report that creates an HTML file for visualizing the current line coverage.

Instead of printing coverage statistics, this command creates various files with coverage details in a new directory called htmlcov/. The file htmlcov/specs\_py.html, which can be viewed in an internet browser, highlights in red the lines of specs.py that are not yet covered by any unit tests.

#### Note

Statement coverage is categorized as white box testing because it requires an understanding of the code's structure. While most black box tests can be written before a program is actually implemented, white box tests should be added to the collection of unit tests after the program is completed. By designing unit tests so that they cover every statement in a program, you may discover that some lines of code are unreachable, find that a conditional statement isn't functioning as intended, or uncover problems that accompany edge cases.

**Problem 2.** With pytest-cov installed, check your coverage of smallest\_factor() from Problem 1. Write additional test cases if necessary to get complete coverage. Then, write a comprehensive unit test for the following (correctly written) function.

## **Testing Exceptions**

Many programs are designed to raise exceptions in response to bad input or an unexpected error. A good unit test makes sure that the program raises the exceptions that it is expected to raise, but also that it doesn't raise any unexpected exceptions. The raises() method in pytest is a clean, formal way of asserting that a program raises a desired exception.

```
# specs.py

def divide(a, b):
    """Divide two numbers, raising an error if the second number is zero."""
    if b == 0:
        raise ZeroDivisionError("second input cannot be zero")
    return a / b
```

The corresponding unit tests checks that the function raises the ZeroDivisionError correctly.

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```
# test_specs.py
import pytest

def test_divide():
    assert specs.divide(4,2) == 2, "integer division"
    assert specs.divide(5,4) == 1.25, "float division"
    pytest.raises(ZeroDivisionError, specs.divide, a=4, b=0)
```

If calling divide(a=4, b=0) results in a ZeroDivisionError, pytest.raises() catches the exception and the test case passes. On the other hand, if divide(a=4, b=0) does not raise a ZeroDivisionError, or if it raises a different kind of exception, the test fails.

To ensure that the ZeroDivisionError is coming from the written raise statement, combine pytest.raises() and the with statement to check the exception's error message.

```
def test_divide():
    assert specs.divide(4,2) == 2, "integer division"
    assert specs.divide(5,4) == 1.25, "float division"
    with pytest.raises(ZeroDivisionError) as excinfo:
        specs.divide(4, 0)
    assert excinfo.value.args[0] == "second input cannot be zero"
```

Here excinfo is an object containing information about the exception; the actual exception object is stored in excinfo.value, and hence excinfo.value.args[0] is the error message.

**Problem 3.** Write a comprehensive unit test for the following function. Make sure that each exception is raised properly by explicitly checking the exception message. Use pytest-cov and its cov-report tool to confirm that you have full coverage for this function.

```
def operate(a, b, oper):
    """Apply an arithmetic operation to a and b."""
    if type(oper) is not str:
        raise TypeError("oper must be a string")
    elif oper == '+':
        return a + b
    elif oper == '-':
        return a - b
    elif oper == '*':
        return a * b
    elif oper == '/':
        if b == 0:
            raise ZeroDivisionError("division by zero is undefined")
        return a / b
    raise ValueError("oper must be one of '+', '/', '-', or '*'")
```

#### **Fixtures**

Consider the following class for representing rational numbers as reduced fractions.

```
class Fraction(object):
    """Reduced fraction class with integer numerator and denominator."""
    def __init__(self, numerator, denominator):
        if denominator == 0:
            raise ZeroDivisionError("denominator cannot be zero")
        elif type(numerator) is not int or type(denominator) is not int:
            raise TypeError("numerator and denominator must be integers")
        def gcd(a,b):
            while b != 0:
                a, b = b, a \% b
            return a
        common_factor = gcd(numerator, denominator)
        self.numer = numerator // common_factor
        self.denom = denominator // common_factor
   def __str__(self):
        if self.denom != 1:
           return "{} / {}".format(self.numer, self.denom)
        else:
           return str(self.numer)
    def __float__(self):
        return self.numer / self.denom
   def __eq__(self, other):
        if type(other) is Fraction:
            return self.numer==other.numer and self.denom==other.denom
        else:
            return float(self) == other
   def __add__(self, other):
        return Fraction(self.numer*other.numer + self.denom*other.denom,
                                                        self.denom*other.denom)
   def __sub__(self, other):
        return Fraction(self.numer*other.numer - self.denom*other.denom,
                                                        self.denom*other.denom)
   def __mul__(self, other):
        return Fraction(self.numer*other.numer, self.denom*other.denom)
   def __truediv__(self, other):
        if self.denom*other.numer == 0:
           raise ZeroDivisionError("cannot divide by zero")
        return Fraction(self.numer*other.denom, self.denom*other.numer)
```

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To test this class, it would be nice to have some ready-made Fraction objects to use in each unit test. A fixture, a function marked with the @pytest.fixture decorator, sets up variables that can be used as mock data for multiple unit tests. The individual unit tests take the fixture function in as input and unpack the constructed tests. Below, we define a fixture that instantiates three Fraction objects. The unit tests for the Fraction class use these objects as test cases.

```
@pytest.fixture
def set_up_fractions():
   frac_1_3 = specs.Fraction(1, 3)
   frac_1_2 = specs.Fraction(1, 2)
   frac_n2_3 = specs.Fraction(-2, 3)
    return frac_1_3, frac_1_2, frac_n2_3
def test_fraction_init(set_up_fractions):
   frac_1_3, frac_1_2, frac_n2_3 = set_up_fractions
   assert frac_1_3.numer == 1
   assert frac_1_2.denom == 2
   assert frac_n2_3.numer == -2
   frac = specs.Fraction(30, 42)
                                                   # 30/42 reduces to 5/7.
    assert frac.numer == 5
    assert frac.denom == 7
def test_fraction_str(set_up_fractions):
   frac_1_3, frac_1_2, frac_n2_3 = set_up_fractions
    assert str(frac_1_3) == "1/3"
   assert str(frac_1_2) == "1/2"
    assert str(frac_n2_3) == "-2/3"
def test_fraction_float(set_up_fractions):
    frac_1_3, frac_1_2, frac_n2_3 = set_up_fractions
    assert float(frac_1_3) == 1 / 3.
   assert float(frac_1_2) == .5
    assert float(frac_n2_3) == -2 / 3.
def test_fraction_eq(set_up_fractions):
   frac_1_3, frac_1_2, frac_n2_3 = set_up_fractions
   assert frac_1_2 == specs.Fraction(1, 2)
    assert frac_1_3 == specs.Fraction(2, 6)
    assert frac_n2_3 == specs.Fraction(8, -12)
```

Problem 4. Add test cases to the unit tests provided above to get full coverage for the \_\_init\_\_(), \_\_str\_\_(), \_\_float\_\_(), and \_\_eq\_\_() methods. You may modify the fixture function if it helps. Also add unit tests for the magic methods \_\_add\_\_(), \_\_sub\_\_(), \_\_mul\_\_(), and \_\_truediv\_\_(). Verify that you have full coverage with pytest-cov.

Additionally, **two** of the Fraction class's methods are implemented incorrectly. Use your tests to find the issues, then correct the methods so that your tests pass.

See http://doc.pytest.org/en/latest/index.html for complete documentation on pytest.

# **Test-driven Development**

Test-driven development (TDD) is the programming style of writing tests **before** implementing the actual code. It may sound tedious at first, but TDD incentivizes simple design and implementation, speeds up the actual coding, and gives quantifiable checkpoints for the development process. TDD can be summarized in the following steps:

- 1. Define with great detail the program specifications. Write function declarations, class definitions, and especially docstrings, determining exactly what each function or class method should accept and return.
- 2. Write a unit test for each unit of the program, usually black box tests.
- 3. Implement the program code, making changes until all tests pass.

For adding new features or cleaning existing code, the process is similar.

- 1. Redefine program specifications to account for planned modifications.
- 2. Add or modify tests to match the new specifications.
- 3. Change the code until all tests pass.



If the test cases are sufficiently thorough, then when the tests all pass, the program can be considered complete. Remember, however, that it is not sufficient to just have tests, but to have tests that accurately and rigorously test the code. To check that the test cases are sufficient, examine the test coverage and add additional tests if necessary.

See https://en.wikipedia.org/wiki/Test-driven\_development for more discussion on TDD and https://en.wikipedia.org/wiki/Behavior-driven\_development for an overview of Behavior-driven development (BDD), a close relative of TDD.

**Problem 5.** Set is a card game about finding patterns. Each card contains a design with 4 different properties: color (red, green or purple), shape (diamond, oval or squiggly), quantity (one, two, or three) and pattern (solid, striped or outlined). A set is a group of three cards which are either all the same or all different for each property. You can try playing Set online at http://smart-games.org/en/set/start.

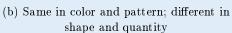
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This collection of cards contains six unique sets:



(a) Same in quantity and shape; different in pattern and color

Here is a group of twelve Set cards.





(c) Same in pattern; different in shape, quantity and color (d) Same in shape; different in quantity, pattern and color



(e) Different in all aspects

(f) Different in all aspects

Each Set card can be uniquely represented by a 4-bit integer in base 3, a where each digit represents a different property and each property has three possible values. A full hand in Set is a group of twelve unique cards, so a hand can be represented by a list of twelve 4-digit integers in base 3. For example, the hand shown above could be represented by the following list.

The following function definitions provide a framework for partially implementing Set by calculating the number of sets in a given hand.

```
def count sets(cards):
    """Return the number of sets in the provided Set hand.
        cards (list(str)) a list of twelve cards as 4-bit integers in
        base 3 as strings, such as ["1022", "1122", ..., "1020"].
        (int) The number of sets in the hand.
    Raises:
        ValueError: if the list does not contain a valid Set hand, meaning
            - there are not exactly 12 cards,
            - the cards are not all unique,
            - one or more cards does not have exactly 4 digits, or
            - one or more cards has a character other than 0, 1, or 2.
    0.00
    pass
def is_set(a, b, c):
    """Determine if the cards a, b, and c constitute a set.
    Parameters:
        a, b, c (str): string representations of 4-bit integers in base 3.
            For example, "1022", "1122", and "1020" (which is not a set).
    Returns:
        True if a, b, and c form a set, meaning the ith digit of a, b,
            and c are either the same or all different for i=1,2,3,4.
        False if a, b, and c do not form a set.
    0.00
    pass
```

Write unit tests for these functions, but **do not** implement them yet. Focus on what the functions should do rather than on how they will be implemented.

(Hint: if three cards form a set, then the first digits of the cards are either all the same or all different. Then the sums of these digits can only be 0, 3, or 6. Thus, a group of cards forms a set only if for each set of digits—first digits, second digits, etc.—the sum is a multiple of 3.)

**Problem 6.** After you have written unit tests for the functions in Problem 5, implement the actual functions. If needed, add additional test cases to get full coverage.

(Hint: The combinations() function from the standard library module itertools may be useful in implementing count\_sets().)

<sup>&</sup>lt;sup>a</sup>A 4-bit integer in base 3 contains four digits that are either 0, 1 or 2. For example, 0000 and 1201 are 4-bit integers in base 3, whereas 000 is not because it has only three digits, and 0123 is not because it contains the number 3.

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# **Additional Material**

# The Python Debugger

Python has a built in debugger called pdb to aid in finding mistakes in code during execution. The debugger can be run either in a terminal or in a Jupyter Notebook.

A *break point*, set with pdb.set\_trace(), is a spot where the program pauses execution. Once the program is paused, use the following commands to tell the program what to do next.

| Command         | Description   |
|-----------------|---|
| n               | next: executes the next line                                      |
| p <var></var>   | <b>p</b> rint: display the value of the specified variable.       |
| С               | continue: stop debugging and run the program normally to the end. |
| q               | quit: terminate the program.                                      |
| 1               | list: show several lines of code around the current line.         |
| r               | return: return to the end of a subroutine.                        |
| <enter></enter> | Execute the most recent command again.                            |

For example, suppose we have a long loop where the value of a variable changes unpredictably.

```
# pdb_example.py
import pdb
from random import randint

i = 0
pdb.set_trace()  # Set a break point.
while i < 1000000000:
    i += randint(1, 10)
print("DONE")</pre>
```

Run the file in the terminal to begin a debugging session.

```
$ python pdb_example.py
> /Users/Student/pdb_example.py(7)<module>()
-> while i < 100000000:
(Pdb) 1
                                                     # Show where we are.
 2
        import pdb
  3
        from random import randint
  4
 5
        i = 0
        pdb.set_trace()
 7
    -> while i < 1000000000:
            i += randint(1, 10)
 9
        print("DONE")
[EOF]
```

We can check the value of the variable i at any step with p i, and we can even change the value of i mid-program.

```
(Pdb) n
                                                   # Execute a few lines.
> /Users/Student/pdb_example.py(8)<module>()
-> i += randint(1, 10)
(Pdb) n
> /Users/Student/pdb_example.py(7)<module>()
-> while i < 100000000:
(Pdb) n
> /Users/Student/pdb_example.py(8)<module>()
-> i += randint(1, 10)
(Pdb) p i
                                                   # Check the value of i.
(Pdb) n
                                                   # Execute another line.
> /Users/Student/pdb_example.py(7)<module>()
-> while i < 1000000000:
(Pdb) p i
                                                   # Check i again.
14
# Change the value of i.
(Pdb) c
                                                   # Continue the program.
DONE
```

See https://docs.python.org/3/library/pdb.html for documentation and examples for the Python debugger.

# Other Testing Suites

There are several frameworks other than pytest for writing unit tests. Each shares the same basic structure, but the setup, syntax, and particular features vary. For more unit testing practice, try out the standard library's unittest (https://docs.python.org/3/library/unittest.html) or doctest (https://docs.python.org/3/library/doctest.html), or the third-party nose module (https://nose.readthedocs.io/en/latest/). For a much larger list of unit testing tools, see https://wiki.python.org/moin/PythonTestingToolsTaxonomy.

#### The Fractions Module

The standard library's fractions module (https://docs.python.org/3/library/fractions.html) has a Fraction class that is similar to the Fraction class presented in this lab. Its structure and syntax is a little different from this lab's class, but it is a little more robust in that it can take in floats, decimals, integers, and strings to its constructor. See also the decimals module (https://docs.python.org/3/library/decimal.html) for tools relating to decimal arithmetic.

# 8

# Data Visualization

Lab Objective: This lab demonstrates how to communicate information through clean, concise, and honest data visualization. We recommend completing the exercises in a Jupyter Notebook.

# The Importance of Visualizations

Visualizations of data can reveal insights that are not immediately obvious from simple statistics. The data set in the following exercise is known as *Anscombe's quartet*. It is famous for demonstrating the importance of data visualization.

**Problem 1.** The file anscombe.npy contains the quartet of data points shown in the table below. For each section of the quartet,

- Plot the data as a scatter plot on the box  $[0, 20] \times [0, 13]$ .
- Use scipy.stats.linregress() to calculate the slope and intercept of the least squares regression line for the data and its correlation coefficient (the first three return values).
- Plot the least squares regression line over the scatter plot on the domain  $x \in [0, 20]$ .
- Report the mean and variance in x and y, the slope and intercept of the regression line, and the correlation coefficient. Compare these statistics to those of the other sections.
- Describe how the section is similar to the others and how it is different.

| I                |       | II   |      | III  |       | IV   |       |
|------------------|-------|------|------|------|-------|------|-------|
| $\boldsymbol{x}$ | y     | x    | y    | x    | y     | x    | y     |
| 10.0             | 8.04  | 10.0 | 9.14 | 10.0 | 7.46  | 8.0  | 6.58  |
| 8.0              | 6.95  | 8.0  | 8.14 | 8.0  | 6.77  | 8.0  | 5.76  |
| 13.0             | 7.58  | 13.0 | 8.74 | 13.0 | 12.74 | 8.0  | 7.71  |
| 9.0              | 8.81  | 9.0  | 8.77 | 9.0  | 7.11  | 8.0  | 8.84  |
| 11.0             | 8.33  | 11.0 | 9.26 | 11.0 | 7.81  | 8.0  | 8.47  |
| 14.0             | 9.96  | 14.0 | 8.10 | 14.0 | 8.84  | 8.0  | 7.04  |
| 6.0              | 7.24  | 6.0  | 6.13 | 6.0  | 6.08  | 8.0  | 5.25  |
| 4.0              | 4.26  | 4.0  | 3.10 | 4.0  | 5.39  | 19.0 | 12.50 |
| 12.0             | 10.84 | 12.0 | 9.13 | 12.0 | 8.15  | 8.0  | 5.56  |
| 7.0              | 4.82  | 7.0  | 7.26 | 7.0  | 6.42  | 8.0  | 7.91  |
| 5.0              | 5.68  | 5.0  | 4.74 | 5.0  | 5.73  | 8.0  | 6.89  |

# Improving Specific Types of Visualizations

Effective data visualizations show specific comparisons and relationships in the data. Before designing a visualization, decide what to look for or what needs to be communicated. Then choose the visual scheme that makes sense for the data. The following sections demonstrate how to improve commonly used plots to communicate information visually.

#### Line Plots

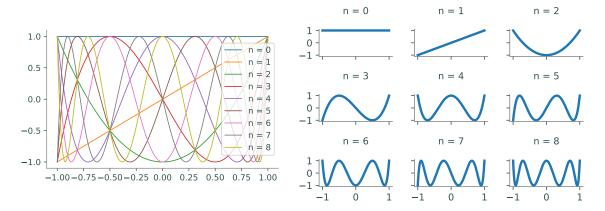


Figure 8.1: Line plots can be used to visualize and compare mathematical functions. For example, this figure shows the first nine Chebyshev polynomials in one plot (left) and small multiples (right). Using small multiples makes comparison easy and shows how each polynomial changes as n increases.

```
>>> import numpy as np
>>> from matplotlib import pyplot as plt

# Plot the first 9 Chebyshev polynomials in the same plot.
>>> T = np.polynomial.Chebyshev.basis
>>> x = np.linspace(-1, 1, 200)
>>> for n in range(9):
... plt.plot(x, T(n)(x), label="n = "+str(n))
...
>>> plt.axis([-1.1, 1.1, -1.1, 1.1])  # Set the window limits.
>>> plt.legend(loc="right")
```

A line plot connects ordered (x, y) points with straight lines, and is best for visualizing one or two ordered arrays, such as functional outputs over an ordered domain or a sequence of values over time. Sometimes, plotting multiple lines on the same plot helps the viewer compare two different data sets. However, plotting several lines on top of each other makes the visualization difficult to read, even with a legend. For example, Figure 8.1 shows the first nine *Chebyshev polynomials*, a family of orthogonal polynomials that satisfies the recursive relation

$$T_0(x) = 1,$$
  $T_1(x) = x,$   $T_{n+1} = 2xT_n(x) - T_{n-1}(x).$ 

The plot on the right makes comparison easier by using *small multiples*. Instead of using a legend, the figure makes a separate subplot with a title for each polynomial. Adjusting the figure size and the line thickness also makes the information easier to read.

#### NOTE

Matplotlib titles and annotations can be formatted with LATEX, a system for creating technical documents.<sup>a</sup> To do so, use an **r** before the string quotation mark and surround the text with dollar signs. For example, add the following line of code to the loop from the previous example.

... 
$$plt.title(r"$T_{{}}(x)$".format(n))$$

The format() method inserts the input n at the curly braces. The title of the sixth subplot, instead of being "n = 5," will then be " $T_5(x)$ ."

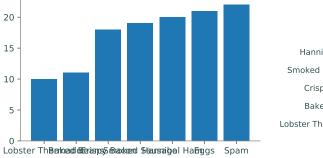
**Problem 2.** The n+1 Bernstein basis polynomials of degree n are defined as follows:

$$b_{v,n}(x) = \binom{n}{v} x^v (1-x)^{n-v}, \qquad v = 0, 1, \dots, n$$

Plot the first 10 Bernstein basis polynomials  $(n=0,\ 1,\ 2,\ 3)$  as small multiples on the domain  $[0,1]\times[0,1]$ . Label the subplots for clarity, adjust tick marks and labels for simplicity, and set the window limits of each plot to be the same. Consider arranging the subplots so that the rows correspond with n and the columns with v.

Hint: The constant  $\binom{n}{v} = \frac{n!}{v!(n-v)!}$  is called the *binomial coefficient* and can be efficiently computed with scipy.special.comb().

#### **Bar Charts**



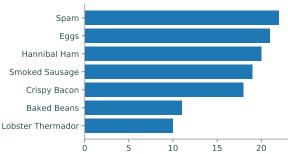


Figure 8.2: Bar charts are used to compare quantities between categorical variables. The labels on the vertical bar chart (left) are more difficult to read than the labels on the horizontal bar chart (right). Although the labels can be rotated, horizontal text is much easier to read than vertical text.

<sup>&</sup>lt;sup>a</sup>See http://www.latex-project.org/ for more information.

A bar chart plots categorical data in a sequence of bars. They are best for small, discrete, one-dimensional data sets. In Matplotlib, plt.bar() creates a vertical bar chart or plt.barh() creates a horizontal bar chart. These functions receive the locations of each bar followed by the height of each bar (as lists or arrays). In most situations, horizontal bar charts are preferable to vertical bar charts because horizontal labels are easier to read than vertical labels. Data in a bar chart should also be sorted in a logical way, such as alphabetically, by size, or by importance.

## Histograms

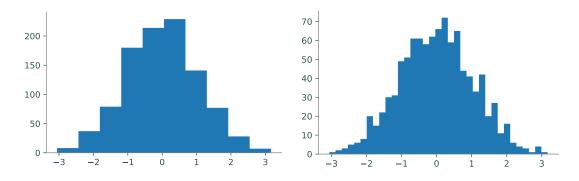


Figure 8.3: Histograms are used to show the distribution of one-dimensional data. Experimenting with different values for the bin size is important when plotting a histogram. Using only 10 bins (left) doesn't give a good sense for how the randomly generated data is distributed. However, using 35 bins (right) reveals the shape of a normal distribution.

```
>>> data = np.random.normal(size=10000)
>>> fig, ax = plt.subplots(1, 2)
>>> ax[0].hist(data, bins=10)
>>> ax[1].hist(data, bins=35)
```

A histogram partitions an interval into a number of bins and counts the number of values that fall into each bin. Histograms are ideal for visualizing how unordered data in a single array is distributed over an interval. For example, if data are drawn from a probability distribution, a histogram approximates the distribution's probability density function. Use plt.hist() to create a histogram. The arguments bins and range specify the number of bins to draw and over what domain. A histogram with too few or too many bins will not give a clear view of the distribution.

## **Scatter Plots**

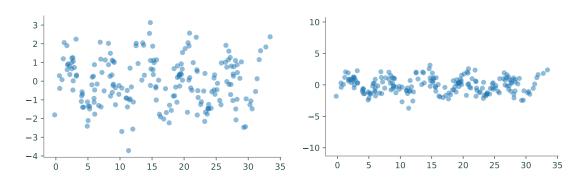


Figure 8.4: Scatter plots show correlations between variables by plotting markers at coordinate points. The figure above displays randomly perturbed data that is visualized using two scatter plots with alpha=.5 and edgecolor='none'. The default (left) makes it harder to see correlation and pattern whereas making the axes equal better reveals the oscillatory behavior in the perturbed sine wave.

```
>>> np.random.seed(0)
>>> x = np.linspace(0,10*np.pi,200) + np.random.normal(size=200)
>>> y = np.sin(x) + np.random.normal(size=200)

>>> plt.scatter(x, y, alpha=.5, edgecolor='none')
>>> plt.show()

>>> plt.scatter(x, y, alpha=.5, edgecolor='none')
>>> plt.axis('equal')
>>> plt.show()
```

A scatter plot draws (x, y) points without connecting them. Scatter plots are best for displaying data sets without a natural order, or where each point is a distinct, individual instance. They are frequently used to show correlation between variables in a data set. Use plt.scatter() to create a scatter plot.<sup>1</sup>

<sup>&</sup>lt;sup>1</sup>Scatter plots can also be drawn with plt.plot() by specifying a point marker such as '.', ',', 'o', or '+'. The keywords s and c can be used to change the marker size and marker color, respectively.

Similar data points in a scatter plot may overlap, as in Figure 8.4. Specifying an *alpha value* reveals overlapping data by making the markers transparent (see Figure 8.5 for an example). The keyword alpha accepts values between 0 (completely transparent) and 1 (completely opaque). When plotting lots of overlapping points, the outlines on the markers can make the visualization look cluttered. Setting the edgecolor keyword to zero removes the outline and improves the visualization.

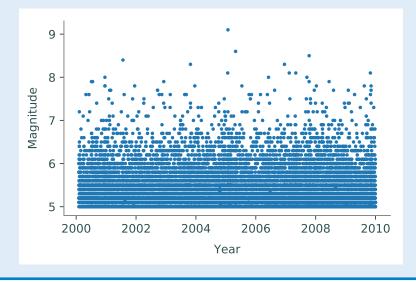
**Problem 3.** The file MLB.npy contains measurements from over 1,000 recent Major League Baseball players, compiled by UCLA.<sup>a</sup> Each row in the array represents a player; the columns are the player's height (in inches), weight (in pounds), and age (in years), in that order.

Create several visualizations to show the correlations between height, weight, and age in the MLB data set. Use at least one scatter plot. Adjust the marker size, plot a regression line, change the window limits, and use small multiples where appropriate.

**Problem 4.** The file earthquakes.npy contains data from over 17,000 earthquakes between 2000 and 2010 that were at least a 5 on the Richter scale.<sup>a</sup> Each row in the array represents an earthquake; the columns are the earthquake's date (as a fraction of the year), magnitude (on the Richter scale), longitude, and latitude, in that order.

Because each earthquake is a distinct event, a good way to start visualizing this data might be a scatter plot of the years versus the magnitudes of each earthquake.

```
>>> year, magnitude, longitude, latitude = np.load("earthquakes.npy").T
>>> plt.plot(year, magnitude, '.')
>>> plt.xlabel("Year")
>>> plt.ylabel("Magnitude")
```



 $<sup>^</sup>a\mathrm{See}\ \mathrm{http://wiki.stat.ucla.edu/socr/index.php/SOCR\_Data\_MLB\_HeightsWeights.}$ 

Unfortunately, this plot communicates very little information because the data is so cluttered. Describe the data with at least two better visualizations. Include line plots, scatter plots, and histograms as appropriate. Your plots should answer the following questions:

- 1. How many earthquakes happened every year?
- 2. How often do stronger earthquakes happen compared to weaker ones?
- 3. Where do earthquakes happen? Where do the strongest earthquakes happen? (Hint: Use plt.axis("equal") or ax.set\_aspect("equal") to fix the aspect ratio, which may improve comparisons between longitude and latitude.)

#### Hexbins

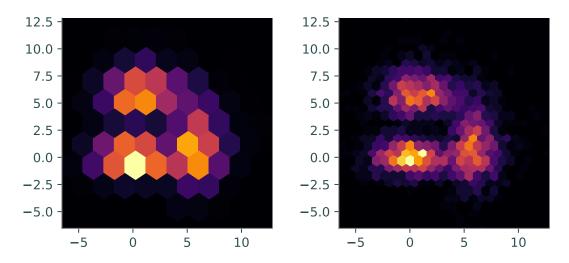


Figure 8.5: Hexbins can be used instead of using a three-dimensional histogram to show the distribution of two-dimensional data. Choosing the right gridsize will give a better picture of the distribution. The figure above shows random data plotted as hexbins with a gridsize of 10 (left) and 25 (right). Hexbins use color to show height via a colormap and both histograms above use the 'inferno' colormap.

```
# Add random draws from various distributions in two dimensions.
>>> a = np.random.exponential(size=1000) + np.random.normal(size=1000) + 5
>>> b = np.random.exponential(size=1000) + 2*np.random.normal(size=1000)
>>> x = np.hstack((a, b, 2*np.random.normal(size=1000)))
>>> y = np.hstack((b, a, np.random.normal(size=1000)))

# Plot the samples with hexbins of gridsize 10 and 25.
>>> fig, axes = plt.subplots(1, 2)
>>> window = [x.min(), x.max(), y.min(), y.max()]
>>> for ax, size in zip(axes, [10, 25]):
```

 $<sup>{}^</sup>a\mathrm{See}$  http://earthquake.usgs.gov/earthquakes/search/.

```
... ax.hexbin(x, y, gridsize=size, cmap='inferno')
... ax.axis(window)
... ax.set_aspect("equal")
...
>>> plt.show()
```

A hexbin is a way of representing the frequency of ocurrances in a two-dimensional plane. Similar to a histogram, which sorts one-dimensional data into bins, a hexbin sorts two-dimensional data into hexagonal bins arranged in a grid and uses color instead of height to show frequency. Creating an effective hexbin relies on choosing an appropriate gridsize and colormap. The colormap is a function that assigns data points to an ordering of colors. Use plt.hexbin() to create a hexbin and use the cmap keyword to specify the colormap.

## **Heat Maps and Contour Plots**

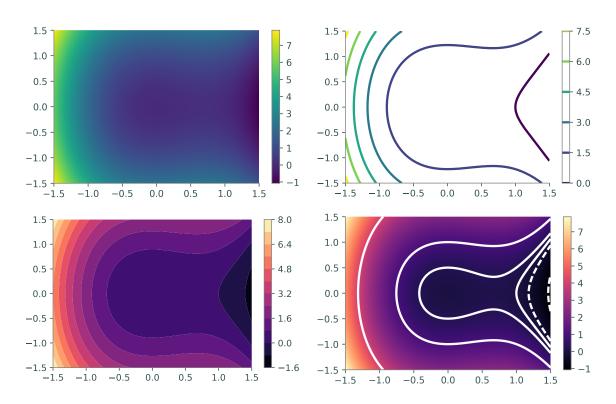


Figure 8.6: Heat maps visualize three-dimensional functions or surfaces by using color to represent the value in one dimension. With continuous data, it can be hard to identify regions of interest. Contour plots solve this problem by visualizing the level curves of the surface. Top left: heat map. Top right: contour plot. Bottom left: heat map. Bottom right: contours plotted on a heat map.

```
# Construct a 2-D domain with np.meshgrid() and calculate f on the domain.
>>> x = np.linspace(-1.5, 1.5, 200)
>>> X, Y = np.meshgrid(x, x)
>>> Z = Y**2 - X**3 + X**2
```

```
# Plot f using a heat map, a contour map, and a filled contour map.
>>> fig, ax = plt.subplots(2,2)
>>> ax[0,0].pcolormesh(X, Y, Z, cmap="viridis")  # Heat map.
>>> ax[0,1].contour(X, Y, Z, 6, cmap="viridis")  # Contour map.
>>> ax[1,0].contourf(X, Y, Z, 12, cmap="magma")  # Filled contour map.

# Plot specific level curves and a heat map with a colorbar.
>>> ax[1,1].contour(X, Y, Z, [-1, -.25, 0, .25, 1, 4], colors="white")
>>> cax = ax[1,1].pcolormesh(X, Y, Z, cmap="magma")
>>> fig.colorbar(cax, ax=ax[1,1])
>>> plt.show()
```

Let  $f: \mathbb{R}^2 \to \mathbb{R}$  be a scalar-valued function on a 2-dimensional domain. A heat map of f assigns a color to each (x,y) point in the domain based on the value of f(x,y), while a contour plot is a drawing of the level curves of f. The level curve corresponding to the constant c is the set  $\{(x,y) \mid c=f(x,y)\}$ . A filled contour plot colors in the sections between the level curves and is a discretized version of a heat map. The values of c corresponding to the level curves are automatically chosen to be evenly spaced over the range of values of f on the domain. However, it is sometimes better to strategically specify the curves by providing a list of c constants.

Consider the function  $f(x,y)=y^2-x^3+x^2$  on the domain  $[-\frac{3}{2},\frac{3}{2}]\times[-\frac{3}{2},\frac{3}{2}]$ . A heat map of f reveals that it has a large basin around the origin. Since f(0,0)=0, choosing several level curves close to 0 more closely describes the topography of the basin. The fourth subplot in 8.6 uses the curves with  $c=-1, -\frac{1}{4}, 0, \frac{1}{4}, 1$ , and 4.

When plotting hexbins, heat maps, and contour plots, be sure to choose a colormap that best represents the data. Avoid using spectral or rainbow colormaps like "jet" because they are not perceptually uniform, meaning that the rate of change in color is not constant. Because of this, data points may appear to be closer together or farther apart than they actually are. This creates visual false positives or false negatives in the visualization and can affect the interpretation of the data. As a default, we recommend using the sequential colormaps "viridis" or "inferno" because they are designed to be perceptually uniform and colorblind friendly. For the complete list of Matplotlib color maps, see http://matplotlib.org/examples/color/colormaps\_reference.html.

#### **Problem 5.** The Rosenbrock function is defined as

$$f(x,y) = (1-x)^2 + 100(y-x^2)^2.$$

The minimum value of f is 0, which occurs at the point (1,1) at the bottom of a steep, banana-shaped valley of the function.

Use a heat map and a contour plot to visualize the Rosenbrock function. Also plot the minimizer (1,1). Use a different sequential colormap for each visualization.

#### **Best Practices**

Good scientific visualizations make comparison easy and clear. The eye is very good at detecting variation in one dimension and poor in two or more dimensions. For example, consider Figure 8.7. Despite the difficulty, most people can probably guess which slice of a pie chart is the largest or smallest. However, it's almost impossible to confidently answer the question by how much? The bar charts may not be as aesthetically pleasing but they make it much easier to precisely compare the data. Avoid using pie charts as well as other visualizations that make accurate comparison difficult, such as radar charts, bubble charts, and stacked bar charts.

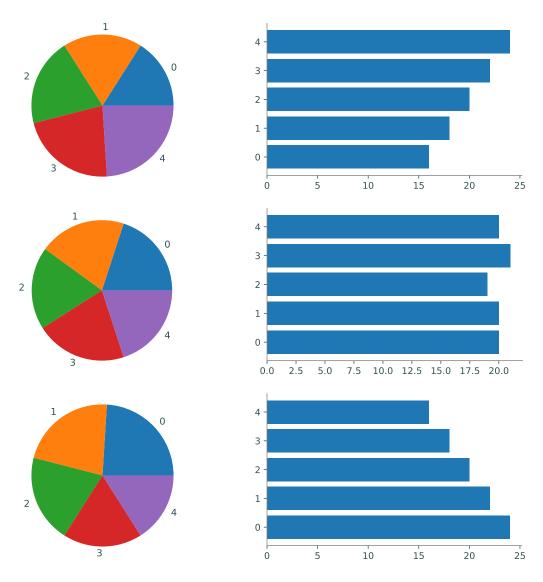


Figure 8.7: The pie charts on the left may be more colorful but it's extremely difficult to quantify the difference between each slice. Instead, the horizontal bar charts on the right make it very easy to see the difference between each variable.

No visualization perfectly represents data, but some are better than others. Finding the best visualization for a data set is an iterative process. Experiment with different visualizations by adjusting their parameters: color, scale, size, shape, position, and length. It may be necessary to use a data transformation or visualize various subsets of the data. As you iterate, keep in mind the saying attributed to George Box: "All models are wrong, but some are useful." Do whatever is needed to make the visualization useful and effective.

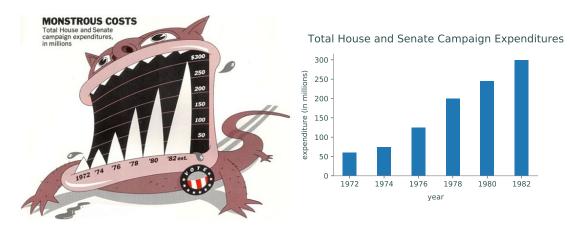
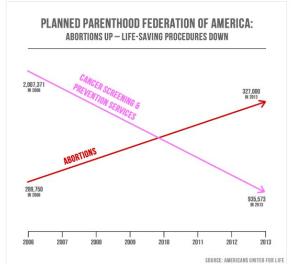


Figure 8.8: Chartjunk refers to anything that does not communicate data. In the image on the left, the cartoon monster distorts the bar chart and manipulates the feelings of the viewer to think negatively about the results. The image on the right shows the same data without chartjunk, making it simple and very easy to interpret the data objectively.

Good visualizations are as simple as possible and no simpler. Edward Tufte coined the term chartjunk to mean anything (pictures, icons, colors, and text) that does not represent data or is distracting. Though chartjunk might appear to make data graphics more memorable than plain visualizations, it is more important to be clear and precise in order to prevent misinterpretation. The physicist Richard Feynman said, "For a successful technology, reality must take precedence over public relations, for Nature cannot be fooled." Remove chartjunk and anything that prevents the viewer from objectively interpreting the data.



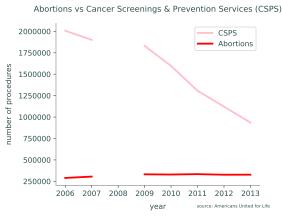


Figure 8.9: The chart on the left is an example of a dishonest graphic shown at a United States congressional hearing in 2015. The chart on the right shows a more accurate representation of the data by showing the y-axis and revealing the missing data from 2008. Source: PolitiFact.

Visualizations should be honest. Figure 8.9 shows how visualizations can be dishonest. The misleading graphic on the left was used as evidence in a United States congressional hearing in 2015. With the y-axis completely removed, it is easy to miss that each line is shown on a different y-axis even though they are measured in the same units. Furthermore, the chart fails to indicate that data is missing from the year 2008. The graphic on the right shows a more accurate representation of the data.<sup>2</sup>

Never use data visualizations to deceive or manipulate. Always present information on who created it, where the data came from, how it was collected, whether it was cleaned or transformed, and whether there are conflicts of interest or possible biases present. Use specific titles and axis labels, and include units of measure. Choose an appropriate window size and use a legend or other annotations where appropriate.

**Problem 6.** The file countries.npy contains information from 20 different countries. Each row in the array represents a different country; the columns are the 2015 population (in millions of people), the 2015 GDP (in billions of US dollars), the average male height (in centimeters), and the average female height (in centimeters), in that order.<sup>a</sup>

The countries corresponding are listed below in order.

<sup>&</sup>lt;sup>2</sup>For more information about this graphic, visit http://www.politifact.com/truth-o-meter/statements/2015/oct/01/jason-chaffetz/chart-shown-planned-parenthood-hearing-misleading-/.

Visualize this data set with at least four plots, using at least one scatter plot, one histogram, and one bar chart. List the major insights that your visualizations reveal. (Hint: consider using np.argsort() and fancy indexing to sort the data for the bar chart.)

 $^a See \ https://en.wikipedia.org/wiki/List_of_countries_by_GDP_(nominal), \\ https://en.wikipedia.org/wiki/List_of_countries_and_dependencies_by_population, and \\ http://www.averageheight.co/.$ 

For more about data visualization, we recommend the following books and websites.

- How to Lie with Statistics by Darrell Huff (1954).
- ullet The Visual Display of Quantitative Information by Edward Tufte (2nd edition).
- Visual Explanations by Edward Tufte.
- Envisioning Information by Edward Tufte.
- Beautiful Evidence by Edward Tufte.
- The Functional Art by Alberto Cairo.
- Visualization Analysis and Design by Tamara Munzner.
- Designing New Default Colormaps: https://bids.github.io/colormap/.

# 9

# Profiling

Lab Objective: Efficiency is essential to algorithmic programming. Profiling is the process of measuring the complexity and efficiency of a program, allowing the programmer to see what parts of the code need to be optimized. In this lab we present common techniques for speeding up Python code, including the built-in profiler and the Numba module.

# Magic Commands in IPython

IPython has tools for quickly timing and profiling code. These "magic commands" start with one or two % characters—one for testing a single line of code, and two for testing a block of code.

- %time: Execute some code and print out its execution time.
- %timeit: Execute some code several times and print out the average execution time.
- %prun: Run a statement through the Python code profiler, printing the number of function calls and the time each takes. We will demonstrate this tool a little later.

<sup>1 %</sup>prun is a shortcut for cProfile.run(); see https://docs.python.org/3/library/profile.html for details.

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# **Choosing Faster Algorithms**

The best way to speed up a program is to use an efficient algorithm. A bad algorithm, even when implemented well, is never an adequate substitute for a good algorithm.

**Problem 1.** This problem comes from https://projecteuler.net (problems 18 and 67).

By starting at the top of the triangle below and moving to adjacent numbers on the row below, the maximum total from top to bottom is 23.

That is, 3 + 7 + 4 + 9 = 23.

The following function finds the maximum path sum of the triangle in triangle.txt by recursively computing the sum of every possible path—the "brute force" approach.

```
def max_path(filename="triangle.txt"):
    """Find the maximum vertical path in a triangle of values."""
    with open(filename, 'r') as infile:
        data = [[int(n) for n in line.split()]
                        for line in infile.readlines()]
    def path_sum(r, c, total):
        """Recursively compute the max sum of the path starting in row r
        and column c, given the current total.
        total += data[r][c]
        if r == len(data) - 1:
                                    # Base case.
            return total
        else:
                                    # Recursive case.
            return max(path_sum(r+1, c, total), # Next row, same column.
                       path_sum(r+1, c+1, total)) # Next row, next column.
    return path_sum(0, 0, 0)
                                    # Start the recursion from the top.
```

The data in triangle.txt contains 15 rows and hence 16384 paths, so it is possible to solve this problem by trying every route. However, for a triangle with 100 rows, there are 2<sup>99</sup> paths to check, which would take billions of years to compute even for a program that could check one trillion routes per second. No amount of improvement to max\_path() can make it run in an acceptable amount of time on such a triangle—we need a different algorithm.

Write a function that accepts a filename containing a triangle of integers. Compute the largest path sum with the following strategy: starting from the next to last row of the triangle, replace each entry with the sum of the current entry and the greater of the two "child entries." Continue this replacement up through the entire triangle. The top entry in the triangle will be the maximum path sum. In other words, work from the bottom instead of from the top.

Use your function to find the maximum path sum of the 100-row triangle stored in triangle\_large.txt. Make sure that your new function still gets the correct answer for the smaller triangle.txt. Finally, use %time or %timeit to time both functions on triangle.txt. Your new function should be about 100 times faster than the original.

#### The Profiler

The profiling command %prun lists the functions that are called during the execution of a piece of code, along with the following information.

| $\operatorname{Heading}$ | Description  |
|--------------------------|--|
| primitive calls          | The number of calls that were not caused by recursion.                                     |
| ncalls                   | The number of calls to the function. If recursion occurs, the output                       |
|                          | is <total calls="" number="" of="">/<number calls="" of="" primitive="">.</number></total> |
| tottime                  | The amount of time spent in the function, not including calls to other functions.          |
| percall                  | The amount of time spent in each call of the function.                                     |
| cumtime                  | The amount of time spent in the function, including calls to other functions.              |

```
# Profile the original function from Problem 1.
In[3]: %prun max_path("triangle.txt")
```

 $81947\ function\ calls\ (49181\ primitive\ calls)$  in 0.036 seconds Ordered by: internal time

```
percall filename:lineno(function)
ncalls
         tottime
                  percall
                            cumtime
32767/1
           0.025
                    0.000
                              0.034
                                       0.034 profiling.py:18(path_sum)
  16383
           0.005
                    0.000
                              0.005
                                       0.000 {built-in method builtins.max}
  32767
           0.003
                    0.000
                              0.003
                                       0.000 {built-in method builtins.len}
      1
           0.002
                    0.002
                              0.002
                                       0.002 {method 'readlines' of '_io._IOBase' objects}
      1
           0.000
                    0.000
                              0.000
                                       0.000 {built-in method io.open}
      1
           0.000
                    0.000
                              0.036
                                       0.036 profiling.py:12(max_path)
      1
           0.000
                    0.000
                              0.000
                                       0.000 profiling.py:15(<listcomp>)
      1
           0.000
                    0.000
                              0.036
                                       0.036 {built-in method builtins.exec}
      2
           0.000
                    0.000
                              0.000
                                       0.000 codecs.py:318(decode)
      1
           0.000
                    0.000
                              0.036
                                       0.036 <string>:1(<module>)
     15
           0.000
                    0.000
                              0.000
                                       0.000 {method 'split' of 'str' objects}
           0.000
                    0.000
                              0.000
                                       0.000 _bootlocale.py:23(getpreferredencoding)
      1
      2
           0.000
                    0.000
                              0.000
                                       0.000 {built-in method _codecs.utf_8_decode}
                                       0.000 {built-in method _locale.nl_langinfo}
           0.000
                    0.000
                              0.000
      1
      1
           0.000
                    0.000
                              0.000
                                       0.000 codecs.py:259(__init__)
      1
           0.000
                    0.000
                              0.000
                                       0.000 codecs.py:308(__init__)
      1
           0.000
                    0.000
                              0.000
                                       0.000 {method 'disable' of '_lsprof.Profiler' objects}
```

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# **Optimizing Python Code**

A poor implementation of a good algorithm is better than a good implementation of a bad algorithm, but clumsy implementation can still cripple a program's efficiency. The following are a few important practices for speeding up a Python program. Remember, however, that such improvements are futile if the algorithm is poorly suited for the problem.

#### **Avoid Repetition**

A clean program does no more work than is necessary. The ncalls column of the profiler output is especially useful for identifying parts of a program that might be repetitive. For example, the profile of max\_path() indicates that len() was called 32,767 times—exactly as many times as path\_sum(). This is an easy fix: save len(data) as a variable somewhere outside of path\_sum().

```
In [4]: def max_path_clean(filename="triangle.txt"):
            with open(filename, 'r') as infile:
                data = [[int(n) for n in line.split()]
                                 for line in infile.readlines()]
            N = len(data)
                                 # Calculate len(data) outside of path_sum().
            def path_sum(r, c, total):
                total += data[r][c]
                if r == N - 1: # Use N instead of len(data).
                    return total
                else:
                    return max(path_sum(r+1, c,
                                path_sum(r+1, c+1, total))
            return path_sum(0, 0, 0)
   . . . :
In [5]: %prun max_path_clean("triangle.txt")
```

49181 function calls (16415 primitive calls) in 0.026 seconds Ordered by: internal time

```
ncalls tottime
                percall
                           cumtime percall filename:lineno(function)
32767/1
           0.020
                    0.000
                             0.025
                                      0.025 <ipython-input-5-9e8c48bb1aba>:6(path_sum)
 16383
           0.005
                    0.000
                             0.005
                                      0.000 {built-in method builtins.max}
           0.002
                    0.002
                             0.002
                                      0.002 {method 'readlines' of '_io._IOBase' objects}
      1
      1
           0.000
                    0.000
                             0.000
                                      0.000 {built-in method io.open}
      1
           0.000
                    0.000
                             0.026
                                      0.026 <ipython-input-5-9e8c48bb1aba>:1(max_path_clean)
           0.000
                    0.000
                             0.000
                                      0.000 <ipython-input-5-9e8c48bb1aba>:3(<listcomp>)
      1
      1
           0.000
                    0.000
                             0.027
                                      0.027 {built-in method builtins.exec}
     15
           0.000
                    0.000
                             0.000
                                      0.000 {method 'split' of 'str' objects}
      1
           0.000
                    0.000
                             0.027
                                      0.027 <string>:1(<module>)
      2
           0.000
                    0.000
                             0.000
                                      0.000 codecs.py:318(decode)
           0.000
                    0.000
                                       0.000 _bootlocale.py:23(getpreferredencoding)
      1
                             0.000
      2
           0.000
                    0.000
                                      0.000 {built-in method _codecs.utf_8_decode}
                             0.000
           0.000
                    0.000
                             0.000
                                      0.000 {built-in method _locale.nl_langinfo}
      1
           0.000
                    0.000
                             0.000
      1
                                      0.000 codecs.py:308(__init__)
      1
           0.000
                    0.000
                             0.000
                                      0.000 codecs.py:259(__init__)
      1
           0.000
                    0.000
                             0.000
                                       0.000 {built-in method builtins.len}
      1
           0.000
                    0.000
                             0.000
                                       0.000 {method 'disable' of '_lsprof.Profiler' objects}
```

Note that the total number of primitive function calls decreased from 49,181 to 16,415. Using %timeit also shows that the run time decreased by about 15%. Moving code outside of a loop or an often-used function usually results in a similar speedup.

Another important way of reducing repetition is carefully controlling loop conditions to avoid unnecessary iterations. Consider the problem of identifying Pythagorean triples, sets of three distinct integers a < b < c such that  $a^2 + b^2 = c^2$ . The following function identifies all such triples where each term is less than a parameter N by checking all possible triples.

Since a < b < c by definition, any computations where  $b \le a$  or  $c \le b$  are unnecessary. Additionally, once a and b are chosen, c can be no greater than  $\sqrt{a^2 + b^2}$ . The following function changes the loop conditions to avoid these cases and takes care to only compute  $a^2 + b^2$  once for each unique pairing (a, b).

These improvements have a drastic impact on run time, even though the main approach—checking by brute force—is the same.

```
In [6]: %time triples = pythagorean_triples_slow(500)
CPU times: user 1min 51s, sys: 389 ms, total: 1min 51s
Wall time: 1min 52s  # 112 seconds.

In [7]: %time triples = pythagorean_triples_fast(500)
CPU times: user 1.56 s, sys: 5.38 ms, total: 1.57 s
Wall time: 1.57 s  # 98.6% faster!
```

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**Problem 2.** The following function computes the first N prime numbers.

```
def primes(N):
    """Compute the first N primes."""
    primes_list = []
    current = 2
    while len(primes_list) < N:
        isprime = True
        for i in range(2, current):  # Check for nontrivial divisors.
            if current % i == 0:
                isprime = False
        if isprime:
            primes_list.append(current)
        current += 1
    return primes_list</pre>
```

This function takes about 6 minutes to find the first 10,000 primes on a fast computer.

Without significantly modifying the approach, rewrite primes() so that it can compute 10,000 primes in under 0.1 seconds. Use the following facts to reduce unnecessary iterations.

- A number is not prime if it has one or more divisors other than 1 and itself. (Hint: recall the break statement.)
- If  $p \nmid n$ , then  $ap \nmid n$  for any integer a. Also, if  $p \mid n$  and  $0 , then <math>p \leq \sqrt{n}$ .
- Except for 2, primes are always odd.

Your new function should be helpful for solving problem 7 on https://projecteuler.net.

## **Avoid Loops**

NumPy routines and built-in functions are often useful for eliminating loops altogether. Consider the simple problem of summing the rows of a matrix, implemented in three ways.

```
>>> def row_sum_awful(A):
        """Sum the rows of A by iterating through rows and columns."""
        m,n = A.shape
. . .
        row_totals = np.empty(m)
                                        # Allocate space for the output.
       for i in range(m):
                                       # For each row...
           total = 0
            for j in range(n):
                                        # ...iterate through the columns.
               total += A[i,j]
            row_totals[i] = total  # Record the total.
       return row_totals
. . .
>>> def row_sum_bad(A):
        """Sum the rows of A by iterating through rows."""
        return np.array([sum(A[i,:]) for i in range(A.shape[0])])
```

```
...
>>> def row_sum_fast(A):
... """Sum the rows of A with NumPy."""
... return np.sum(A, axis=1) # Or A.sum(axis=1).
...
```

None of the functions are fundamentally different, but their run times differ dramatically.

In this experiment, row\_sum\_fast() runs several hundred times faster than row\_sum\_awful(). This is primarily because looping is expensive in Python, but NumPy handles loops in C, which is much quicker. Other NumPy functions like np.sum() with an axis argument can often be used to eliminate loops in a similar way.

**Problem 3.** Let A be an  $m \times n$  matrix with columns  $\mathbf{a}_0, \ldots, \mathbf{a}_{n-1}$ , and let  $\mathbf{x}$  be a vector of length m. The nearest neighbor problem<sup>a</sup> is to determine which of the columns of A is "closest" to  $\mathbf{x}$  with respect to some norm. That is, we compute

$$\underset{j}{\operatorname{argmin}} \|\mathbf{a}_{j} - \mathbf{x}\|.$$

The following function solves this problem naïvely for the usual Euclidean norm.

```
def nearest_column(A, x):
    """Find the index of the column of A that is closest to x."""
    distances = []
    for j in range(A.shape[1]):
        distances.append(np.linalg.norm(A[:,j] - x))
    return np.argmin(distances)
```

Write a new version of this function without any loops or list comprehensions, using array broadcasting and the axis keyword in np.linalg.norm() to eliminate the existing loop. Try to implement the entire function in a single line.

(Hint: See the NumPy Visual Guide in the Appendix for a refresher on array broadcasting.)

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Profile the old and new versions with %prun and compare the output. Finally, use %time or %timeit to verify that your new version runs faster than the original.

 $^a$ The nearest neighbor problem is a common problem in many fields of artificial intelligence. The problem can be solved more efficiently with a k-d tree, a specialized data structure for storing high-dimensional data.

# Use Data Structures Correctly

Every data structure has strengths and weaknesses, and choosing the wrong data structure can be costly. Here we consider three ways to avoid problems and use sets, dictionaries, and lists correctly.

• Membership testing. The question "is <value> a member of <container>" is common in numerical algorithms. Sets and dictionaries are implemented in a way that makes this a trivial problem, but lists are not. In other words, the in operator is near instantaneous with sets and dictionaries, but not with lists.

```
In [13]: a_list = list(range(int(1e7)))
In [14]: a_set = set(a_list)
In [15]: %timeit 12.5 in a_list
413 ms +- 48.2 ms per loop (mean+-std.dev. of 7 runs, 1 loop each)
In [16]: %timeit 12.5 in a_set
170 ns +- 3.8 ns per loop (mean+-std.dev. of 7 runs, 100000000 loops each)
```

Looking up dictionary values is also almost immediate. Use dictionaries for storing calculations to be reused, such as mappings between letters and numbers or common function outputs.

• Construction with comprehension. Lists, sets, and dictionaries can all be constructed with comprehension syntax. This is slightly faster than building the collection in a loop, and the code is highly readable.

```
# Map the integers to their squares.
In [17]: %%time
    ...: a_dict = {}
    ...: for i in range(1000000):
    ...: a_dict[i] = i**2
    ...:
CPU times: user 432 ms, sys: 54.4 ms, total: 486 ms
Wall time: 491 ms
In [18]: %time a_dict = {i:i**2 for i in range(1000000)}
CPU times: user 377 ms, sys: 58.9 ms, total: 436 ms
Wall time: 440 ms
```

• Intelligent iteration. Unlike looking up dictionary values, indexing into lists takes time. Instead of looping over the indices of a list, loop over the entries themselves. When indices and entries are both needed, use enumerate() to get the index and the item simultaneously.

#### Problem 4. This is problem 22 from https://projecteuler.net.

Using the rule  $A \mapsto 1, B \mapsto 2, \dots, Z \mapsto 26$ , the alphabetical value of a name is the sum of the digits that correspond to the letters in the name. For example, the alphabetic value of "COLIN" is 3 + 15 + 12 + 9 + 14 = 53.

The following function reads the file names.txt, containing over five-thousand first names, and sorts them in alphabetical order. The *name score* of each name in the resulting list is the alphabetic value of the name multiplied by the name's position in the list, starting at 1. "COLIN" is the 938th name alphabetically, so its name score is  $938 \times 53 = 49714$ . The function returns the total of all the name scores in the file.

Rewrite this function—removing repetition, eliminating loops, and using data structures correctly—so that it runs in less than 10 milliseconds on average.

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#### **Use Generators**

A generator is an iterator that yields multiple values, one at a time, as opposed to returning a single value. For example, range() is a generator. Using generators appropriately can reduce both the run time and the spatial complexity of a routine. Consider the following function, which constructs a list containing the entries of the sequence  $\{x_n\}_{n=1}^N$  where  $x_n = x_{n-1} + n$  with  $x_1 = 1$ .

A potential problem with this function is that all of the values in the list are computed before anything is returned. This can be a big issue if the parameter N is large. A generator, on the other hand, yields one value at a time, indicated by the keyword yield (instead of return). When the generator is asked for the next entry, the code resumes right where it left off.

```
>>> def sequence_generator(N):
        """Yield the first N entries of the sequence x_n = x_{n-1} + n."""
        for n in range(1, N+1):
            x += n
                            # "return" a single value.
            yield x
. . .
# Get the entries of the generator one at a time with next().
>>> generated = sequence_generator(10)
>>> next(generated)
>>> next(generated)
>>> next(generated)
# Put each of the generated items in a list, as in sequence_function().
>>> list(sequence_generator(10))
                                  # Or [i for i in sequence_generator(10)].
[1, 3, 6, 10, 15, 21, 28, 36, 45, 55]
# Use the generator in a for loop, like range().
>>> for entry in sequence_generator(10):
        print(entry, end=' ')
1 3 6 10 15 21 28 36 45 55
```

Many generators, like range() and sequence\_generator(), only yield a finite number of values. However, generators can also continue yielding indefinitely. For example, the following generator yields the terms of  $\{x_n\}_{n=1}^{\infty}$  forever. In this case, using enumerate() with the generator is helpful for tracking the index n as well as the entry  $x_n$ .

```
>>> def sequence_generator_forever():
        """Yield the sequence x_n = x_{n-1} + n forever."""
        x = 0
       n = 1
        while True:
            x += n
           n += 1
                           # "return" a single value.
            yield x
. . .
# Sum the entries of the sequence until the sum exceeds 1000.
>>> total = 0
>>> for i, x in enumerate(sequence_generator_forever()):
        total += x
        if total > 1000:
                            # Print the index where the total exceeds.
           print(i)
. . .
           break
                           # Break out of the for loop to stop iterating.
. . .
17
# Check that 18 terms are required (since i starts at 0 but n starts at 1).
>>> print(sum(sequence_generator(17)), sum(sequence_generator(18)))
969 1140
```

Problem 5. This is problem 25 from https://projecteuler.net.

The *Fibonacci sequence* is defined by the recurrence relation  $F_n = F_{n-1} + F_{n-2}$ , where  $F_1 = F_2 = 1$ . The 12th term,  $F_{12} = 144$ , is the first term to contain three digits.

Write a generator that yields the terms of the Fibonacci sequence indefinitely. Next, write a function that accepts an integer N. Use your generator to find the first term in the Fibonacci sequence that contains N digits. Return the index of this term.

(Hint: a generator can have more than one yield statement.)

**Problem 6.** The function in Problem 2 could be turned into a prime number generator that yields primes indefinitely, but it is not the only strategy for yielding primes. The *Sieve of Eratosthenes*<sup>a</sup> is a faster technique for finding all of the primes below a certain number.

- 1. Given a cap N, start with all of the integers from 2 to N.
- 2. Remove all integers that are divisible by the first entry in the list.

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- 3. Yield the first entry in the list and remove it from the list.
- 4. Return to step 2 until the list is empty.

Write a generator that accepts an integer N and that yields all primes (in order, one at a time) that are less than N using the Sieve of Eratosthenes. Your generator should be able to find all primes less than 100,000 in under 5 seconds.

Your generator and your fast function from Problem 2 may be helpful in solving problems 10, 35, 37, 41, 49, and 50 (for starters) of https://projecteuler.net.

```
<sup>a</sup>See https://en.wikipedia.org/wiki/Sieve_of_Eratosthenes.
```

#### Numba

Python code is simpler and more readable than many languages, but Python is also generally much slower than compiled languages like C. The numba module bridges the gap by using *just-in-time* (JIT) compilation to optimize code, meaning that the code is actually compiled right before execution.

```
>>> from numba import jit
>>> @jit
                         # Decorate a function with @jit to use Numba.
... def row_sum_numba(A):
        """Sum the rows of A by iterating through rows and columns,
        optimized by Numba.
        0.00
        m,n = A.shape
        row_totals = np.empty(m)
        for i in range(m):
            total = 0
            for j in range(n):
                total += A[i,j]
            row_totals[i] = total
        return row_totals
. . .
```

Python is a dynamically typed language, meaning variables are not defined explicitly with a datatype (x = 6 as opposed to int x = 6). This particular aspect of Python makes it flexible, easy to use, and slow. Numba speeds up Python code primarily by assigning datatypes to all the variables. Rather than requiring explicit definitions for datatypes, Numba attempts to infer the correct datatypes based on the datatypes of the input. In row\_sum\_numba(), if A is an array of integers, Numba will infer that total should also be an integer. On the other hand, if A is an array of floats, Numba will infer that total should be a double (a similar datatype to float in C).

Once all datatypes have been inferred and assigned, the original Python code is translated to machine code. Numba caches this compiled version of code for later use. The first function call takes the time to compile and then execute the code, but subsequent calls use the already-compiled code.

```
In [22]: A = np.random.random((10000, 10000))
# The first function call takes a little extra time to compile first.
In [23]: %time rows = row_sum_numba(A)
```

```
CPU times: user 408 ms, sys: 11.5 ms, total: 420 ms
Wall time: 425 ms

# Subsequent calls are consistently faster that the first call.
In [24]: %timeit row_sum_numba(A)
138 ms +- 1.96 ms per loop (mean +- std. dev. of 7 runs, 10 loops each)
```

Note that the only difference between row\_sum\_numba() and row\_sum\_awful() from a few pages ago is the @jit decorator, and yet the Numba version is about 99% faster than the original!

The inference engine within Numba does a good job, but it's not always perfect. Adding the keyword argument nopython=True to the <code>@jit</code> decorator raises an error if Numba is unable to convert each variable to explicit datatypes. The <code>inspect\_types()</code> method can also be used to check if Numba is using the desired types.

```
# Run the function once first so that it compiles.
>>> rows = row_sum_numba(np.random.random((10,10)))
>>> row_sum_numba.inspect_types()
# The output is very long and detailed.
```

Alternatively, datatypes can be specified explicitly in the <code>@jit</code> decorator as a dictionary via the <code>locals</code> keyword argument. Each of the desired datatypes must also be imported from Numba.

```
>>> from numba import int64, double
>>> @jit(nopython=True, locals=dict(A=double[:,:], m=int64, n=int64,
                                    row_totals=double[:], total=double))
... def row_sum_numba(A):
                                    # 'A' is a 2-D array of doubles.
                                    # 'm' and 'n' are both integers.
        m,n = A.shape
        row_totals = np.empty(m)
                                   # 'row_totals' is a 1-D array of doubles.
        for i in range(m):
            total = 0
                                    # 'total' is a double.
            for j in range(n):
                total += A[i,j]
            row_totals[i] = total
        return row_totals
```

While it sometimes results in a speed boost, there is a caveat to specifying the datatypes: row\_sum\_numba() no longer accepts arrays that contain anything other than floats. When datatypes are not specified, Numba compiles a new version of the function each time the function is called with a different kind of input. Each compiled version is saved, so the function can still be used flexibly.

```
Problem 7. The following function calculates the nth power of an m \times m matrix A.

def matrix_power(A, n):
    """Compute A^n, the n-th power of the matrix A."""
    product = A.copy()
```

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```
temporary_array = np.empty_like(A[0])
m = A.shape[0]
for power in range(1, n):
    for i in range(m):
        for j in range(m):
            total = 0
            for k in range(m):
                total += product[i,k] * A[k,j]
            temporary_array[j] = total
            product[i] = temporary_array
return product
```

- 1. Write a Numba-enhanced version of matrix\_power() called matrix\_power\_numba().
- 2. Write a function that accepts an integer n. Run matrix\_power\_numba() once with a small random input so it compiles. Then, for  $m = 2^2, 2^3, \ldots, 2^7$ ,
  - (a) Generate a random  $m \times m$  matrix A with np.random.random().
  - (b) Time (separately) matrix\_power(), matrix\_power\_numba(), and NumPy's np.linalg.matrix\_power() on A with the specified value of n.
     (If you are unfamiliar with timing code inside of a function, see the Additional Material section on timing code.)

Plot the times against the size m on a log-log plot (use plt.loglog()).

With n = 10, the plot should show that the Numba and NumPy versions far outperform the pure Python implementation, with NumPy eventually becoming faster than Numba.

#### ACHTUNG!

Optimizing code is an important skill, but it is also important to know when to refrain from optimization. The best approach to coding is to write unit tests, implement a solution that works, test and time that solution, **then** (and only then) optimize the solution with profiling techniques. As always, the most important part of the process is choosing the correct algorithm to solve the problem. Don't waste time optimizing a poor algorithm.

#### **Additional Material**

#### Other Timing Techniques

Though %time and %timeit are convenient and work well, some problems require more control for measuring execution time. The usual way of timing a code snippet by hand is via the time module (which %time uses). The function time.time() returns the number of seconds since the Epoch<sup>2</sup>; to time code, measure the number of seconds before the code runs, the number of seconds after the code runs, and take the difference.

```
>>> import time
>>> start = time.time()  # Record the current time.
>>> for i in range(int(1e8)):  # Execute some code.
... pass
... end = time.time()  # Record the time again.
... print(end - start)  # Take the difference.
...
4.20402193069458 # (seconds)
```

The timeit module (which %timeit uses) has tools for running code snippets several times. The code is passed in as a string, as well as any setup code to be run before starting the clock.

```
>>> import timeit
>>> timeit.timeit("for i in range(N): pass", setup="N = int(1e6)", number=200)
4.884839255013503  # Total time in seconds to run the code 200 times.
>>> _ / 200
0.024424196275067516  # Average time in seconds.
```

The primary advantages of these techniques are the ability automate timing code and being able save the results. For more documentation, see https://docs.python.org/3.6/library/time.html and https://docs.python.org/3.6/library/timeit.html.

#### Customizing the Profiler

The output from %prun is generally long, but it can be customized with the following options.

| $\operatorname{Option}$  | Description   |
|--------------------------|---|
| -1 <limit></limit>       | Include a limited number of lines in the output.                    |
| -s <key></key>           | Sort the output by call count, cumulative time, function name, etc. |
| -T <filename></filename> | Save profile results to a file (results are still printed).         |

For example, %prun -1 3 -s ncalls -T path\_profile.txt max\_path() generates a profile of max\_path() that lists the 3 functions with the most calls, then write the results to path\_profile.txt. See http://ipython.readthedocs.io/en/stable/interactive/magics.html#magic-prun for more details.

<sup>&</sup>lt;sup>2</sup>See https://en.wikipedia.org/wiki/Epoch\_(reference\_date)#Computing.

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# 1 Introduction to SymPy

Lab Objective: Most implementations of numerical algorithms focus on crunching, relating, or visualizing numerical data. However, it is sometimes convenient or necessary to represent parts of an algorithm symbolically. The SymPy module provides a way to do symbolic mathematics in Python, including algebra, differentiation, integration, and more. In this lab we introduce SymPy syntax and emphasize how to use symbolic algebra for numerical computing.

#### Symbolic Variables and Expressions

Most variables in Python refer to a number, string, or data structure. Doing computations on such variables results in more numbers, strings, or data structures. A *symbolic variable* is a variable that represents a mathematical symbol, such as x or  $\theta$ , not a number or another kind of data. Operating on symbolic variables results in an *expression*, representative of an actual mathematical expression. For example, if a symbolic variable Y refers to a mathematical variable y, the multiplication 3\*Y refers to the expression 3y. This is all done without assigning an actual numerical value to Y.

SymPy [MSP+17] is Python's library for doing symbolic algebra and calculus. It is typically imported with import sympy as sy, and symbolic variables are usually defined using sy.symbols().

```
>>> import sympy as sy
>>> x0 = sy.symbols('x0')
                                            # Define a single variable.
# Define multiple symbolic variables simultaneously.
>>> x2, x3 = sy.symbols('x2, x3')
                                            # Separate symbols by commas,
>>> m, a = sy.symbols('mass acceleration') # by spaces,
>>> x, y, z = sy.symbols('x:z')
                                            # or by colons.
>>> x4, x5, x6 = sy.symbols('x4:7')
# Combine symbolic variables to form expressions.
>>> expr = x**2 + x*y + 3*x*y + 4*y**3
>>> force = m * a
>>> print(expr, force, sep='\n')
x**2 + 4*x*y + 4*y**3
acceleration*mass
```

SymPy has its own version for each of the standard mathematical functions like  $\sin(x)$ ,  $\log(x)$ , and  $\sqrt{x}$ , and includes predefined variables for special numbers such as  $\pi$ . The naming conventions for most functions match NumPy, but some of the built-in constants are named slightly differently.

Functions 
$$\frac{\sin(x) \quad \arcsin(x) \quad \sinh(x) \quad e^x \quad \log(x) \quad \sqrt{x} }{\text{sy.sin()} \quad \text{sy.asin()} \quad \text{sy.sinh()} \quad \text{sy.exp()} \quad \text{sy.log()} \quad \text{sy.sqrt()} }$$
 Constants 
$$\frac{\pi \quad e \quad i = \sqrt{-1} \quad \infty}{\text{sy.pi} \quad \text{sy.E} \quad \text{sy.I} \quad \text{sy.oo} }$$

Other trigonometric functions like  $\cos(x)$  follow the same naming conventions. For a complete list of SymPy functions, see http://docs.sympy.org/latest/modules/functions/index.html.

#### ACHTUNG!

Always use SymPy functions and constants when creating expressions instead of using NumPy's functions and constants. Later we will show how to make NumPy and SymPy cooperate.

```
>>> import numpy as np
>>> x = sy.symbols('x')
>>> np.exp(x)  # Try to use NumPy to represent e**x.
Traceback (most recent call last):
   File "<stdin>", line 1, in <module>
AttributeError: 'Symbol' object has no attribute 'exp'
>>> sy.exp(x)  # Use SymPy's version instead.
exp(x)
```

#### NOTE

SymPy defines its own numeric types for integers, floats, and rational numbers. For example, the sy.Rational class is similar to the standard library's fractions.Fraction class, and should be used to represent fractions in SymPy expressions.

```
>>> x = sy.symbols('x')
>>> (2/3) * sy.sin(x)  # 2/3 returns a float, not a rational.

0.6666666666666667*sin(x)

>>> sy.Rational(2, 3) * sy.sin(x) # Keep 2/3 symbolic.

2*sin(x)/3
```

Always be aware of which numeric types are being used in an expression. Using rationals and integers where possible is important for simplifying expressions.

**Problem 1.** Write a function that returns the expression  $\frac{2}{5}e^{x^2-y}\cosh(x+y)+\frac{3}{7}\log(xy+1)$  symbolically. Make sure that the fractions remain symbolic.

#### Sums and Products

Expressions that can be written as a sum or a product can be constructed with sy.summation() or sy.product(), respectively. Each of these functions accepts an expression that represents one term of the sum or product, then a tuple indicating the indexing variable and which values it should take on. For example, the following code constructs the sum and product given below.

$$\sum_{i=1}^{4} x + iy \qquad \qquad \prod_{i=0}^{5} x + iy$$

```
>>> x, y, i = sy.symbols('x y i')
>>> sy.summation(x + i*y, (i, 1, 4))  # Sum over i=1,2,3,4.
4*x + 10*y
>>> sy.product(x + i*y, (i, 0, 5))  # Multiply over i=0,1,2,3,4,5.
x*(x + y)*(x + 2*y)*(x + 3*y)*(x + 4*y)*(x + 5*y)
```

#### Simplifying Expressions

The expressions for the summation and product in the previous example are automatically simplified. More complicated expressions can be simplified with one or more of the following functions.

| Function                 | Description  |
|--------------------------|--|
| sy.cancel()              | Cancel common factors in the numerator and denominator.  |
| sy.expand()              | Expand a factored expression.                            |
| <pre>sy.factor()</pre>   | Factor an expanded expression.                           |
| sy.radsimp()             | Rationalize the denominator of an expression.            |
| <pre>sy.simplify()</pre> | Simplify an expression.                                  |
| <pre>sy.trigsimp()</pre> | Simplify only the trigonometric parts of the expression. |

```
>>> x = sy.symbols('x')
>>> expr = (x**2 + 2*x + 1) / ((x+1)*((sy.sin(x)/sy.cos(x))**2 + 1))
>>> print(expr)
(x**2 + 2*x + 1)/((x + 1)*(sin(x)**2/cos(x)**2 + 1))
>>> sy.simplify(expr)
(x + 1)*cos(x)**2
```

The generic sy.simplify() tries to simplify an expression in any possible way. This is often computationally expensive; using more specific simplifiers when possible reduces the cost.

```
>>> expr = sy.product(x + i*y, (i, 0, 3))
>>> print(expr)
x*(x + y)*(x + 2*y)*(x + 3*y)
>>> expr_long = sy.expand(expr)  # Expand the product terms.
>>> print(expr_long)
x**4 + 6*x**3*y + 11*x**2*y**2 + 6*x*y**3
>>> expr_long /= (x + 3*y)
>>> print(expr_long)
(x**4 + 6*x**3*y + 11*x**2*y**2 + 6*x*y**3)/(x + 3*y)
>>> expr_short = sy.cancel(expr_long) # Cancel out the denominator.
x**3 + 3*x**2*y + 2*x*y**2
>>> sy.factor(expr_short)
                                      # Factor the result.
x*(x + y)*(x + 2*y)
# Simplify the trigonometric parts of an expression.
>>> sy.trigsimp(2*sy.sin(x)*sy.cos(x))
sin(2*x)
```

See http://docs.sympy.org/latest/tutorial/simplification.html for more examples.

#### ACHTUNG!

- 1. Simplifications return new expressions; they do not modify existing expressions in place.
- 2. The == operator compares two expressions for exact structural equality, not algebraic equivalence. Simplify or expand expressions before comparing them with ==.
- 3. Expressions containing floats may not simplify as expected. Always use integers and SymPy rationals in expressions when appropriate.

```
>>> expr = 2*sy.sin(x)*sy.cos(x)
>>> sy.trigsimp(expr)
sin(2*x)
>> print(expr)
2*sin(x)*cos(x)  # The original expression is unchanged.

>>> 2*sy.sin(x)*sy.cos(x) == sy.sin(2*x)
False  # The two expression structures differ.

>>> sy.factor(x**2.0 - 1)
x**2.0 - 1  # Factorization fails due to the 2.0.
```

**Problem 2.** Write a function that computes and simplifies the following expression.

$$\prod_{i=1}^{5} \sum_{j=i}^{5} j(\sin(x) + \cos(x))$$

#### **Evaluating Expressions**

Every SymPy expression has a subs() method that substitutes one variable for another. The result is usually still a symbolic expression, even if a numerical value is used in the substitution. The evalf() method actually evaluates the expression numerically after all symbolic variables have been assigned a value. Both of these methods can accept a dictionary to reassign multiple symbols simultaneously.

```
>>> x,y = sy.symbols('x y')
>>> expr = sy.expand((x + y)**3)
>>> print(expr)
x**3 + 3*x**2*y + 3*x*y**2 + y**3
# Replace the symbolic variable y with the expression 2x.
>>> expr.subs(y, 2*x)
27*x**3
# Replace x with pi and y with 1.
>>> new_expr = expr.subs({x:sy.pi, y:1})
>>> print(new_expr)
1 + 3*pi + 3*pi**2 + pi**3
>>> new_expr.evalf()
                                     # Numerically evaluate the expression.
71.0398678443373
# Evaluate the expression by providing values for each variable.
>>> expr.evalf(subs={x:1, y:2})
27.0000000000000
```

These operations are good for evaluating an expression at a single point, but it is typically more useful to turn the expression into a reusable numerical function. To this end, sy.lambdify() takes in a symbolic variable (or list of variables) and an expression, then returns a callable function that corresponds to the expression.

```
# Turn the expression sin(x)^2 into a function with x as the variable.
>>> f = sy.lambdify(x, sy.sin(x)**2)
>>> print(f(0), f(np.pi/2), f(np.pi), sep=' ')
0.0 1.0 1.4997597826618576e-32

# Lambdify a function of several variables.
>>> f = sy.lambdify((x,y), sy.sin(x)**2 + sy.cos(y)**2)
>>> print(f(0,1), f(1,0), f(np.pi, np.pi), sep=' ')
0.2919265817264289 1.708073418273571 1.0
```

By default, sy.lambdify() uses the math module to convert an expression to a function. For example, sy.sin() is converted to math.sin(). By providing "numpy" as an additional argument, sy.lambdify() replaces symbolic functions with their NumPy equivalents instead, so sy.sin() is converted to np.sin(). This allows the resulting function to act element-wise on NumPy arrays, not just on single data points.

#### Note

It is almost always computationally cheaper to lambdify a function than to use substitutions. According to the SymPy documentation, using sy.lambdify() to do numerical evaluations "takes on the order of hundreds of nanoseconds, roughly two orders of magnitude faster than the subs() method."

```
In [1]: import sympy as sy
In [2]: import numpy as np
# Define a symbol, an expression, and points to plug into the expression.
In [3]: x = sy.symbols('x')
In [4]: expr = sy.tanh(x)
In [5]: points = np.random.random(10000)
# Time using evalf() on each of the random points.
In [6]: %time _ = [expr.subs(x, pt).evalf() for pt in points]
CPU times: user 5.29 s, sys: 40.3 ms, total: 5.33 s
Wall time: 5.36 s
# Lambdify the expression and time using the resulting function.
In [7]: f = sy.lambdify(x, expr)
In [8]: %time _ = [f(pt) for pt in points]
CPU times: user 5.39 ms, sys: 648 micros, total: 6.04 ms
                      # About 1000 times faster than evalf().
Wall time: 7.75 ms
# Lambdify the expression with NumPy and repeat the experiment.
In [9]: f = sy.lambdify(x, expr, "numpy")
In [10]: %time _ = f(points)
CPU times: user 381 micros, sys: 63 micros, total: 444 micros
Wall time: 282 micros # About 10 times faster than regular lambdify.
```

**Problem 3.** The Maclaurin series up to order N for  $e^x$  is defined as

$$e^x \approx \sum_{n=0}^N \frac{x^n}{n!}.$$
 (10.1)

Write a function that accepts an integer N. Define an expression for (10.1), then substitute in  $-y^2$  for x to get a truncated Maclaurin series of  $e^{-y^2}$ . Lambdify the resulting expression and plot the series on the domain  $y \in [-2,2]$ . Plot  $e^{-y^2}$  over the same domain for comparison. (Hint: use sy.factorial() to compute the factorial.)

Call your function with increasing values of N to check that the series converges correctly.

#### Solving Symbolic Equations

A SymPy expression by itself is not an equation. However, sy.solve() equates an expression with zero and solves for a specified variable. In this way, SymPy can be used to solve equations.

**Problem 4.** The following equation represents a rose curve in cartesian coordinates:

$$0 = 1 - \frac{(x^2 + y^2)^{7/2} + 18x^5y - 60x^3y^3 + 18xy^5}{(x^2 + y^2)^3}.$$
 (10.2)

The curve is not the image of a single function (such a function would fail the vertical line test), so the best way to plot it is to convert (10.2) to a pair of parametric equations that depend on the angle parameter  $\theta$ .

Construct an expression for the nonzero side of (10.2) and convert it to polar coordinates with the substitutions  $x = r\cos(\theta)$  and  $y = r\sin(\theta)$ . Simplify the result, then solve it for r. There are two solutions due to the presence of an  $r^2$  term; pick one and lambdify it to get a function  $r(\theta)$ . Use this function to plot  $x(\theta) = r(\theta)\cos(\theta)$  against  $y(\theta) = r(\theta)\sin(\theta)$  for  $\theta \in [0, 2\pi]$ .

(Hint: use sy.Rational() for the fractional exponent.)

#### Linear Algebra

Sympy can also solve systems of equations. A system of linear equations  $A\mathbf{x} = \mathbf{b}$  is solved in a slightly different way than in NumPy and SciPy: instead of defining the matrix A and the vector  $\mathbf{b}$  separately, define the augmented matrix  $M = [A \mid \mathbf{b}]$  and call sy.solve\_linear\_system() on M.

SymPy matrices are defined with sy.Matrix(), with the same syntax as 2-dimensional NumPy arrays. For example, the following code solves the system given below.

SymPy matrices support the standard matrix operations of addition +, subtraction -, and multiplication @. Additionally, SymPy matrices are equipped with many useful methods, some of which are listed below. See http://docs.sympy.org/latest/modules/matrices/matrices.html for more methods and examples.

| Method                    | Returns   |
|---------------------------|---|
| det()                     | The determinant.                                      |
| eigenvals()               | The eigenvalues and their multiplicities.             |
| eigenvects()              | The eigenvectors and their corresponding eigenvalues. |
| inv()                     | The matrix inverse.                                   |
| <pre>is_nilpotent()</pre> | True if the matrix is nilpotent.                      |
| norm()                    | The Frobenius, $\infty$ , 1, or 2 norm.               |
| nullspace()               | The nullspace as a list of vectors.                   |
| <pre>rref()</pre>         | The reduced row-echelon form.                         |
| singular_values()         | The singular values.                                  |

#### ACHTUNG!

The \* operator performs matrix multiplication on SymPy matrices. To perform element-wise multiplication, use the multiply\_elementwise() method instead.

**Problem 5.** Find the eigenvalues of the following matrix by solving for  $\lambda$  in the characteristic equation  $\det(A - \lambda I) = 0$ .

$$A = \left[ \begin{array}{ccc} x - y & x & 0 \\ x & x - y & x \\ 0 & x & x - y \end{array} \right]$$

Also compute the eigenvectors by solving the linear system  $A - \lambda I = \mathbf{0}$  for each eigenvalue  $\lambda$ . Return a dictionary mapping the eigenvalues to their eigenvectors.

(Hint: the nullspace() method may be useful.)

Check that  $A\mathbf{v} = \lambda \mathbf{v}$  for each eigenvalue-eigenvector pair  $(\lambda, \mathbf{v})$ . Compare your results to the eigenvals() and eigenvects() methods for SymPy matrices.

#### Calculus

SymPy is also equipped to perform standard calculus operations, including derivatives, integrals, and taking limits. Like other elements of SymPy, calculus operations can be temporally expensive, but they give exact solutions whenever solutions exist.

#### Differentiation

The command sy.Derivative() creates a closed form, unevaluated derivative of an expression. This is like putting  $\frac{d}{dx}$  in front of an expression without actually calculating the derivative symbolically. The resulting expression has a doit() method that can be used to evaluate the actual derivative. Equivalently, sy.diff() immediately takes the derivative of an expression.

Both sy.Derivative() and sy.diff() accept a single expression, then the variable or variables that the derivative is being taken with respect to.

```
>>> x, y = sy.symbols('x y')
>>> f = sy.sin(y)*sy.cos(x)**2

# Make an expression for the derivative of f with respect to x.
>>> df = sy.Derivative(f, x)
>>> print(df)
Derivative(sin(y)*cos(x)**2, x)

>>> df.doit()  # Perform the actual differentiation.
-2*sin(x)*sin(y)*cos(x)

# Alternatively, calculate the derivative of f in a single step.
>>> sy.diff(f, x)
-2*sin(x)*sin(y)*cos(x)

# Calculate the derivative with respect to x, then y, then x again.
>>> sy.diff(f, x, y, x)
2*(sin(x)**2 - cos(x)**2)*cos(y)  # Note this expression could be simplified.
```

**Problem 6.** Let  $f: \mathbb{R} \to \mathbb{R}$  be a smooth function. A *critical point* of f is a number  $x_0 \in \mathbb{R}$  satisfying  $f'(x_0) = 0$ . The second derivative test states that a critical point  $x_0$  is a local minimum of f if  $f''(x_0) > 0$ , or a local maximum of f if  $f''(x_0) < 0$  (if  $f''(x_0) = 0$ , the test is inconclusive).

Now consider the polynomial

$$p(x) = 2x^6 - 51x^4 + 48x^3 + 312x^2 - 576x - 100.$$

Use SymPy to find all critical points of p and classify each as a local minimum or a local maximum. Plot p(x) over  $x \in [-5,5]$  and mark each of the minima in one color and the maxima in another color. Return the collections of local minima and local maxima as sets.

The Jacobian matrix of a multivariable function  $f: \mathbb{R}^n \to \mathbb{R}^m$  at a point  $\mathbf{x}_0 \in \mathbb{R}^n$  is the  $m \times n$  matrix J whose entries are given by

$$J_{ij} = \frac{\partial f_i}{\partial x_j}(\mathbf{x}_0).$$

For example, the Jacobian for a function  $f: \mathbb{R}^3 \to \mathbb{R}^2$  is defined by

$$J = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \frac{\partial f}{\partial x_3} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} \end{bmatrix}, \quad \text{where} \quad f(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}.$$

To calculate the Jacobian matrix of a multivariate function with SymPy, define that function as a symbolic matrix (sy.Matrix()) and use its jacobian() method. The method requires a list of variables that prescribes the ordering of the differentiation.

```
# Create a matrix of symbolic variables.
>>> r, t = sy.symbols('r theta')
>>> f = sy.Matrix([r*sy.cos(t), r*sy.sin(t)])
# Find the Jacobian matrix of f with respect to r and theta.
>>> J = f.jacobian([r,t])
>>> J
Matrix([
[cos(theta), -r*sin(theta)],
[sin(theta), r*cos(theta)]])
# Evaluate the Jacobian matrix at the point (1, pi/2).
>>> J.subs({r:1, t:sy.pi/2})
Matrix([
[0, -1],
[1, 0]]
# Calculate the (symbolic) determinant of the Jacobian matrix.
>>> sy.simplify(J.det())
```

#### Integration

The function sy.Integral() creates an unevaluated integral expression. This is like putting an integral sign in front of an expression without actually evaluating the integral symbolically or numerically. The resulting expression has a doit() method that can be used to evaluate the actual integral. Equivalently, sy.integrate() immediately integrates an expression.

Both sy.Derivative() and sy.diff() accept a single expression, then a tuple or tuples containing the variable of integration and, optionally, the bounds of integration.

```
# Calculate the indefinite integral of sec(x).
>>> sy.integrate(sy.sec(x), x)
-log(sin(x) - 1)/2 + log(sin(x) + 1)/2

# Integrate cos(x)^2 from 0 to pi/2.
>>> sy.integrate(sy.cos(x)**2, (x,0,sy.pi/2))
pi/4

# Compute the integral of (y^2)(x^2) dx dy with x from 0 to 2, y from -1 to 1.
>>> sy.integrate(y**2 * x**2, (x,0,2), (y,-1,1))
16/9
```

**Problem 7.** Let  $f: \mathbb{R}^3 \to \mathbb{R}$  be a smooth function. The volume integral of f over the sphere S of radius f can written in spherical coordinates as

$$\iiint_{S} f(x,y,z)dV = \int_{0}^{\pi} \int_{0}^{2\pi} \int_{0}^{r} f(h_{1}(\rho,\theta,\phi),h_{2}(\rho,\theta,\phi),h_{3}(\rho,\theta,\phi))|\det(J)| d\rho d\theta d\phi,$$

where J is the Jacobian of the function  $h: \mathbb{R}^3 \to \mathbb{R}^3$  given by

$$h(\rho, \theta, \phi) = \begin{bmatrix} h_1(\rho, \theta, \phi) \\ h_2(\rho, \theta, \phi) \\ h_3(\rho, \theta, \phi) \end{bmatrix} = \begin{bmatrix} \rho \sin(\phi) \cos(\theta) \\ \rho \sin(\phi) \sin(\theta) \\ \rho \cos(\phi) \end{bmatrix}.$$

Calculate the volume integral of  $f(x, y, z) = (x^2 + y^2 + z^2)^2$  over the sphere of radius r. Lambdify the resulting expression (with r as the independent variable) and plot the integral value for  $r \in [0, 3]$ . In addition, return the value of the integral when r = 2.

(Hint: simplify the integrand before computing the integral. In this case,  $|\det(J)| = -\det(J)$ .) To check your answer, when r = 3, the value of the integral is  $\frac{8748}{7}\pi$ .

#### ACHTUNG!

SymPy isn't perfect. It solves some integrals incorrectly, simplifies some expressions poorly, and is significantly slower than numerical computations. However, it is generally very useful for simplifying parts of an algorithm, getting exact answers, and handling tedious algebra quickly.

#### **Additional Material**

#### **Pretty Printing**

SymPy expressions, especially complicated ones, can be hard to read. Calling sy.init\_printing() changes the way that certain expressions are displayed to be more readable; in a Jupyter Notebook, the rendering is done with LaTeX, as displayed below. Furthermore, the function sy.latex() converts an expression into actual LaTeX code for use in other settings.

#### Limits

Limits can be expressed, similar to derivatives or integrals, with sy.Limit(). Alternatively, sy. limit() (lowercase) evaluates a limit directly.

```
# Define the limit of a^(1/x) as x approaches infinity.
>>> a, x = sy.symbols('a x')
>>> sy.Limit(a**(1/x), x, sy.oo)
Limit(a**(1/x), x, oo, dir='-')

# Use the doit() method or sy.limit() to evaluate a limit.
>>> sy.limit((1+x)**(1/x), x, 0)
E

# Evaluate a limit as x approaches 0 from the negative direction.
>>> sy.limit(1/x, x, 0, '-')
-oo
```

Use limits instead of the subs() method when the value to be substituted is  $\infty$  or is a singularity.

```
>>> expr = x / 2**x
>>> expr.subs(x, sy.oo)
nan
>>> sy.limit(expr, x, sy.oo)
0
```

Refer to http://docs.sympy.org/latest/tutorial/calculus.html for SymPy's official documentation on calculus operations.

#### **Numerical Integration**

Many integrals cannot be solved analytically. As an alternative to the doit() method, the as\_sum() method approximates the integral with a summation. This method accepts the number of terms to use and a string indicating which approximation rule to use ("left", "right", "midpoint", or "trapezoid").

```
>>> x = sy.symbols('x')

# Try integrating e^(x^2) from 0 to pi.
>>> I = sy.Integral(sy.exp(x**2), (x,0,sy.pi))
>>> I.doit()
sqrt(pi)*erfi(pi)/2 # The result is not very helpful.

# Instead, approximate the integral with a sum.
>>> I.as_sum(10, 'left').evalf()
1162.85031639195
```

See http://docs.sympy.org/latest/modules/integrals/integrals.html for more documentation on integration with SymPy.

#### **Differential Equations**

SymPy can be used to solve both ordinary and partial differential equations. The documentation for working with PDE functions is at http://docs.sympy.org/dev/modules/solvers/pde.html

The general form of a first-order differential equation is  $\frac{dx}{dt} = f(x(t), t)$ . To represent the unknown function x(t), use sy.Function(). Just as sy.solve() is used to solve an expression for a given variable, sy.dsolve() solves an ODE for a particular function. When there are multiple solutions, sy.dsolve() returns a list; when arbitrary constants are involved they are given as C1, C2, and so on. Use sy.checkodesol() to check that a function is a solution to a differential equation.

```
>>> t = sy.symbols('t')
>>> x = sy.Function('x')

# Solve the equation x''(t) - 2x'(t) + x(t) = sin(t).
>>> ode = x(t).diff(t, t) - 2*x(t).diff(t) + x(t) - sy.sin(t)
>>> sy.dsolve(ode, x(t))
Eq(x(t), (C1 + C2*t)*exp(t) + cos(t)/2) # C1 and C2 are arbitrary constants.
```

Since there are many types of ODEs, sy.dsolve() may also take a hint indicating what solving strategy to use. See sy.ode.allhints for a list of possible hints, or use sy.classify\_ode() to see the list of hints that may apply to a particular equation.

## Part II Appendices

## $\bigwedge$

### Getting Started

The labs in this curriculum aim to introduce computational and mathematical concepts, walk through implementations of those concepts in Python, and use industrial-grade code to solve interesting, relevant problems. Lab assignments are usually about 5–10 pages long and include code examples (yellow boxes), important notes (green boxes), warnings about common errors (red boxes), and about 3–7 exercises (blue boxes). Get started by downloading the lab manual(s) for your course from http://foundations-of-applied-mathematics.github.io/.

#### Submitting Assignments

#### Labs

Every lab has a corresponding specifications file with some code to get you started and to make your submission compatible with automated test drivers. Like the lab manuals, these materials are hosted at http://foundations-of-applied-mathematics.github.io/.

Download the .zip file for your course, unzip the folder, and move it somewhere where it won't get lost. This folder has some setup scripts and a collection of folders, one per lab, each of which contains the specifications file(s) for that lab. See Student-Materials/wiki/Lab-Index for the complete list of labs, their specifications and data files, and the manual that each lab belongs to.

#### ACHTUNG!

Do **not** move or rename the lab folders or the enclosed specifications files; if you do, the test drivers will not be able to find your assignment. Make sure your folder and file names match Student-Materials/wiki/Lab-Index.

To submit a lab, modify the provided specifications file and use the file-sharing program specified by your instructor (discussed in the next section). The instructor will drop feedback files in the lab folder after grading the assignment. For example, the Introduction to Python lab has the specifications file PythonIntro/python\_intro.py. To complete that assignment, modify PythonIntro/python\_intro.py and submit it via your instructor's file-sharing system. After grading, the instructor will create a file called PythonIntro/PythonIntro\_feedback.txt with your score and some feedback.

#### Homework

Non-lab coding homework should be placed in the \_Homework/ folder and submitted like a lab assignment. Be careful to name your assignment correctly so the instructor (and test driver) can find it. The instructor may drop specifications files and/or feedback files in this folder as well.

#### Setup

#### ACHTUNG!

We strongly recommend using a Unix-based operating system (Mac or Linux) for the labs. Unix has a true bash terminal, works well with git and python, and is the preferred platform for computational and data scientists. It is possible to do this curriculum with Windows, but expect some road bumps along the way.

There are two ways to submit code to the instructor: with git (http://git-scm.com/), or with a file-syncing service like Google Drive. Your instructor will indicate which system to use.

#### Setup With Git

Git is a program that manages updates between an online code repository and the copies of the repository, called *clones*, stored locally on computers. If git is not already installed on your computer, download it at http://git-scm.com/downloads. If you have never used git, you might want to read a few of the following resources.

- Official git tutorial: https://git-scm.com/docs/gittutorial
- Bitbucket git tutorials: https://www.atlassian.com/git/tutorials
- GitHub git cheat sheet: services.github.com/.../github-git-cheat-sheet.pdf
- GitLab git tutorial: https://docs.gitlab.com/ce/gitlab-basics/start-using-git.html
- Codecademy git lesson: https://www.codecademy.com/learn/learn-git
- Training video series by GitHub: https://www.youtube.com/playlist?list=PLg7.../

There are many websites for hosting online git repositories. Your instructor will indicate which web service to use, but we only include instructions here for setup with Bitbucket.

- 1. Sign up. Create a Bitbucket account at https://bitbucket.org. If you use an academic email address (ending in .edu, etc.), you will get free unlimited public and private repositories.
- 2. Make a new repository. On the Bitbucket page, click the + button from the menu on the left and, under CREATE, select Repository. Provide a name for the repository, mark the repository as private, and make sure the repository type is Git. For Include a README?, select No (if you accidentally include a README, delete the repository and start over). Under Advanced settings, enter a short description for your repository, select No forks under forking, and select Python as the language. Finally, click the blue Create repository button. Take note of the URL of the webpage that is created; it should be something like https://bitbucket.org/<name>/<repo>.

- 3. Give the instructor access to your repository. On your newly created Bitbucket repository page (https://bitbucket.org/<name>/<repo> or similar), go to Settings in the menu to the left and select User and group access, the second option from the top. Enter your instructor's Bitbucket username under Users and click Add. Select the blue Write button so your instructor can read from and write feedback to your repository.
- 4. Connect your folder to the new repository. In a shell application (Terminal on Linux or Mac, or Git Bash (https://gitforwindows.org/) on Windows), enter the following commands.

```
# Navigate to your folder.
$ cd /path/to/folder # cd means 'change directory'.
# Make sure you are in the right place.
$ pwd
                      # pwd means 'print working directory'.
/path/to/folder
                      # ls means 'list files'.
$1s*.md
README.md
                     # This means README.md is in the working directory.
# Connect this folder to the online repository.
$ git remote add origin https://<name>@bitbucket.org/<name>/<repo>.git
# Record your credentials.
$ git config --local user.name "your name"
$ git config --local user.email "your email"
# Add the contents of this folder to git and update the repository.
$ git add --all
$ git commit -m "initial commit"
$ git push origin master
```

For example, if your Bitbucket username is greek314, the repository is called acmev1, and the folder is called Student-Materials/ and is on the desktop, enter the following commands.

```
# Navigate to the folder.
$ cd ~/Desktop/Student-Materials

# Make sure this is the right place.
$ pwd
/Users/Archimedes/Desktop/Student-Materials
$ ls *.md
README.md

# Connect this folder to the online repository.
$ git init
$ git remote add origin https://greek314@bitbucket.org/greek314/acmev1.git

# Record credentials.
$ git config --local user.name "archimedes"
```

```
$ git config --local user.email "greek314@example.com"

# Add the contents of this folder to git and update the repository.
$ git add --all
$ git commit -m "initial commit"
$ git push origin master
```

At this point you should be able to see the files on your repository page from a web browser. If you enter the repository URL incorrectly in the git remote add origin step, you can reset it with the following line.

```
$ git remote set-url origin https://<name>@bitbucket.org/<name>/<repo>.git
```

5. Download data files. Many labs have accompanying data files. To download these files, navigate to your clone and run the download\_data.sh bash script, which downloads the files and places them in the correct lab folder for you. You can also find individual data files through Student-Materials/wiki/Lab-Index.

```
# Navigate to your folder and run the script.
$ cd /path/to/folder
$ bash download_data.sh
```

6. Install Python package dependencies. The labs require several third-party Python packages that don't come bundled with Anaconda. Run the following command to install the necessary packages.

```
# Navigate to your folder and run the script.
$ cd /path/to/folder
$ bash install_dependencies.sh
```

7. (Optional) Clone your repository. If you want your repository on another computer after completing steps 1–4, use the following commands.

```
# Navigate to where you want to put the folder.
$ cd ~/Desktop/or/something/

# Clone the folder from the online repository.
$ git clone https://<name>@bitbucket.org/<name>/<repo>.git <foldername>

# Record your credentials in the new folder.
$ cd <foldername>
$ git config --local user.name "your name"
$ git config --local user.email "your email"

# Download data files to the new folder.
$ bash download_data.sh
```

#### Setup Without Git

Even if you aren't using git to submit files, you must install it (http://git-scm.com/downloads) in order to get the data files for each lab. Share your folder with your instructor according to their directions, and follow steps 5 and 6 of the previous section to download the data files and install package dependencies.

#### **Using Git**

Git manages the history of a file system through *commits*, or checkpoints. Use git status to see the files that have been changed since the last commit. These changes are then moved to the *staging area*, a list of files to save during the next commit, with git add <filename(s)>. Save the changes in the staging area with git commit -m "<A brief message describing the changes>".

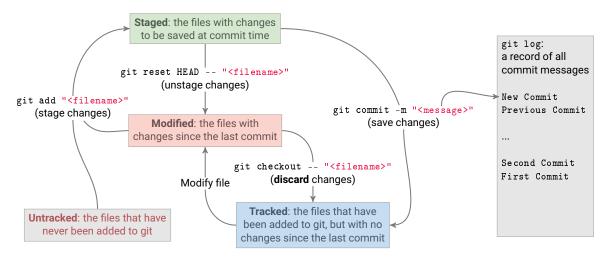


Figure A.1: Git commands to stage, unstage, save, or discard changes. Commit messages are recorded in the log.

All of these commands are done within a clone of the repository, stored somewhere on a computer. This repository must be manually synchronized with the online repository via two other git commands: git pull origin master, to pull updates from the web to the computer; and git push origin master, to push updates from the computer to the web.

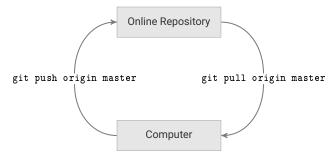


Figure A.2: Exchanging git commits between the repository and a local clone.

```
Command
                                  Explanation
git status
                                   Display the staging area and untracked changes.
git pull origin master
                                  Pull changes from the online repository.
                                  Push changes to the online repository.
git push origin master
git add <filename(s)>
                                   Add a file or files to the staging area.
                                   Add all modified, tracked files to the staging area.
git add -u
                                   Save the changes in the staging area with a given message.
git commit -m "<message>"
                                   Revert changes to an unstaged file since the last commit.
git checkout -- <filename>
git reset HEAD -- <filename>
                                   Remove a file from the staging area.
                                   See the changes to an unstaged file since the last commit.
git diff <filename>
git diff --cached <filename>
                                  See the changes to a staged file since the last commit.
                                  Record your credentials (user.name, user.email, etc.).
git config --local <option>
```

Table A.1: Common git commands.

#### Note

When pulling updates with git pull origin master, your terminal may sometimes display the following message.

```
Merge branch 'master' of https://bitbucket.org/<name>/<repo> into master

# Please enter a commit message to explain why this merge is necessary,
# especially if it merges an updated upstream into a topic branch.

#
# Lines starting with '#' will be ignored, and an empty message aborts
# the commit.
~
```

This means that someone else (the instructor) has pushed a commit that you do not yet have, while you have also made one or more commits locally that they do not have. This screen, displayed in vim (https://en.wikipedia.org/wiki/Vim\_(text\_editor)), is asking you to enter a message (or use the default message) to create a  $merge\ commit$  that will reconcile both changes. To close this screen and create the merge commit, type: wq and press enter.

#### **Example Work Sessions**

```
# Pull any updates from the online repository (such as TA feedback).
$ cd ~/Desktop/Student-Materials/
$ git pull origin master
From https://bitbucket.org/username/repo
* branch
                    master
                              -> FETCH_HEAD
Already up-to-date.
### Work on the labs. For example, modify PythonIntro/python_intro.py.
$ git status
On branch master
Your branch is up-to-date with 'origin/master'.
Changes not staged for commit:
  (use "git add <file>..." to update what will be committed)
  (use "git checkout -- <file>..." to discard changes in working directory)
    PythonIntro/python_intro.py
# Track the changes with git.
$ git add PythonIntro/python_intro.py
$ git status
On branch master
Your branch is up-to-date with 'origin/master'.
Changes to be committed:
  (use "git reset HEAD <file>..." to unstage)
    modified: PythonIntro/python_intro.py
# Commit the changes to the repository with an informative message.
$ git commit -m "Made some changes"
[master fed9b34] Made some changes
1 file changed, 10 insertion(+) 1 deletion(-)
# Push the changes to the online repository.
$ git push origin master
Counting objects: 3, done.
Delta compression using up to 2 threads.
Compressing objects: 100% (2/2), done.
Writing objects: 100% (3/3), 327 bytes | 0 bytes/s, done.
Total 3 (delta 0), reused 0 (delta 0)
To https://username@bitbucket.org/username/repo.git
   5742a1b..fed9b34 master -> master
$ git status
On branch master
Your branch is up-to-date with 'origin/master'.
nothing to commit, working directory clean
```

## B

## Installing and Managing Python

**Lab Objective:** One of the great advantages of Python is its lack of overhead: it is relatively easy to download, install, start up, and execute. This appendix introduces tools for installing and updating specific packages and gives an overview of possible environments for working efficiently in Python.

#### Installing Python via Anaconda

A *Python distribution* is a single download containing everything needed to install and run Python, together with some common packages. For this curriculum, we **strongly** recommend using the *Anaconda* distribution to install Python. Anaconda includes IPython, a few other tools for developing in Python, and a large selection of packages that are common in applied mathematics, numerical computing, and data science. Anaconda is free and available for Windows, Mac, and Linux.

Follow these steps to install Anaconda.

- 1. Go to https://www.anaconda.com/download/.
- 2. Download the **Python 3.6** graphical installer specific to your machine.
- 3. Open the downloaded file and proceed with the default configurations.

For help with installation, see https://docs.anaconda.com/anaconda/install/. This page contains links to detailed step-by-step installation instructions for each operating system, as well as information for updating and uninstalling Anaconda.

#### ACHTUNG!

This curriculum uses Python 3.6, **not** Python 2.7. With the wrong version of Python, some example code within the labs may not execute as intended or result in an error.

#### **Managing Packages**

A *Python package manager* is a tool for installing or updating Python packages, which involves downloading the right source code files, placing those files in the correct location on the machine, and linking the files to the Python interpreter. **Never** try to install a Python package without using a package manager (see https://xkcd.com/349/).

#### Conda

Many packages are not included in the default Anaconda download but can be installed via Anaconda's package manager, conda. See https://docs.anaconda.com/anaconda/packages/pkg-docs for the complete list of available packages. When you need to update or install a package, always try using conda first.

| $\operatorname{Command}$                    | Description                               |  |
|---|---|--|
| conda install <package-name></package-name> | Install the specified package.            |  |
| conda update <package-name></package-name>  | Update the specified package.             |  |
| conda update conda                          | Update conda itself.                      |  |
| conda update anaconda                       | Update all packages included in Anaconda. |  |
| condahelp                                   | Display the documentation for conda.      |  |

For example, the following terminal commands attempt to install and update matplotlib.

```
$ conda update conda  # Make sure that conda is up to date.
$ conda install matplotlib  # Attempt to install matplotlib.
$ conda update matplotlib  # Attempt to update matplotlib.
```

See https://conda.io/docs/user-guide/tasks/manage-pkgs.html for more examples.

```
NOTE

The best way to ensure a package has been installed correctly is to try importing it in IPython.

# Start IPython from the command line.
$ ipython
IPython 6.5.0 -- An enhanced Interactive Python. Type '?' for help.

# Try to import matplotlib.
In [1]: from matplotlib import pyplot as plt # Success!
```

#### ACHTUNG!

Be careful not to attempt to update a Python package while it is in use. It is safest to update packages while the Python interpreter is not running.

#### Pip

The most generic Python package manager is called pip. While it has a larger package list, conda is the cleaner and safer option. Only use pip to manage packages that are not available through conda.

| Command                         | Description   |  |
|---------------------------------|---|--|
| pip install package-name        | Install the specified package.                        |  |
| pip installupgrade package-name | Update the specified package.                         |  |
| pip freeze                      | Display the version number on all installed packages. |  |
| piphelp                         | Display the documentation for pip.                    |  |

See https://pip.pypa.io/en/stable/user\_guide/ for more complete documentation.

#### Workflows

There are several different ways to write and execute programs in Python. Try a variety of workflows to find what works best for you.

#### Text Editor + Terminal

The most basic way of developing in Python is to write code in a text editor, then run it using either the Python or IPython interpreter in the terminal.

There are many different text editors available for code development. Many text editors are designed specifically for computer programming which contain features such as syntax highlighting and error detection, and are highly customizable. Try installing and using some of the popular text editors listed below.

- Atom: https://atom.io/
- Sublime Text: https://www.sublimetext.com/
- Notepad++ (Windows): https://notepad-plus-plus.org/
- Geany: https://www.geany.org/
- Vim: https://www.vim.org/
- Emacs: https://www.gnu.org/software/emacs/

Once Python code has been written in a text editor and saved to a file, that file can be executed in the terminal or command line.

IPython is an enhanced version of Python that is more user-friendly and interactive. It has many features that cater to productivity such as tab completion and object introspection.

#### NOTE

While Mac and Linux computers come with a built-in bash terminal, Windows computers do not. Windows does come with *Powershell*, a terminal-like application, but some commands in Powershell are different than their bash analogs, and some bash commands are missing from Powershell altogether. There are two good alternatives to the bash terminal for Windows:

- Windows subsystem for linux: docs.microsoft.com/en-us/windows/wsl/.
- Git bash: https://gitforwindows.org/.

#### Jupyter Notebook

The Jupyter Notebook (previously known as IPython Notebook) is a browser-based interface for Python that comes included as part of the Anaconda Python Distribution. It has an interface similar to the IPython interpreter, except that input is stored in cells and can be modified and re-evaluated as desired. See https://github.com/jupyter/jupyter/wiki/ for some examples.

To begin using Jupyter Notebook, run the command jupyter notebook in the terminal. This will open your file system in a web browser in the Jupyter framework. To create a Jupyter Notebook, click the **New** drop down menu and choose **Python 3** under the **Notebooks** heading. A new tab will open with a new Jupyter Notebook.

Jupyter Notebooks differ from other forms of Python development in that notebook files contain not only the raw Python code, but also formatting information. As such, Juptyer Notebook files cannot be run in any other development environment. They also have the file extension .ipynb rather than the standard Python extension .py.

Jupyter Notebooks also support Markdown—a simple text formatting language—and LATEX, and can embedded images, sound clips, videos, and more. This makes Jupyter Notebook the ideal platform for presenting code.

#### Integrated Development Environments

An integrated development environment (IDEs) is a program that provides a comprehensive environment with the tools necessary for development, all combined into a single application. Most IDEs have many tightly integrated tools that are easily accessible, but come with more overhead than a plain text editor. Consider trying out each of the following IDEs.

- JupyterLab: http://jupyterlab.readthedocs.io/en/stable/
- PyCharm: https://www.jetbrains.com/pycharm/
- Spyder: http://code.google.com/p/spyderlib/
- Eclipse with PyDev: http://www.eclipse.org/, https://www.pydev.org/

See https://realpython.com/python-ides-code-editors-guide/ for a good overview of these (and other) workflow tools.

### NumPy Visual Guide

Lab Objective: NumPy operations can be difficult to visualize, but the concepts are straightforward. This appendix provides visual demonstrations of how NumPy arrays are used with slicing syntax, stacking, broadcasting, and axis-specific operations. Though these visualizations are for 1- or 2dimensional arrays, the concepts can be extended to n-dimensional arrays.

#### Data Access

The entries of a 2-D array are the rows of the matrix (as 1-D arrays). To access a single entry, enter the row index, a comma, and the column index. Remember that indexing begins with 0.

#### Slicing

A lone colon extracts an entire row or column from a 2-D array. The syntax [a:b] can be read as "the ath entry up to (but not including) the bth entry." Similarly, [a:] means "the ath entry to the end" and [:b] means "everything up to (but not including) the bth entry."

#### Stacking

np.hstack() stacks sequence of arrays horizontally and np.vstack() stacks a sequence of arrays vertically.

$$A = \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}$$

$$B = \begin{bmatrix} * & * & * \\ * & * & * \end{bmatrix}$$

$$np.hstack((A,B,A)) = \begin{bmatrix} \times & \times & \times & * & * & \times & \times \\ \times & \times & * & * & * & \times & \times \\ \times & \times & \times & * & * & * & \times & \times \end{bmatrix}$$

$$\mathtt{np.vstack((A,B,A))} = \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ * & * & * \\ * & * & * \\ * & * & * \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}$$

Because 1-D arrays are flat, np.hstack() concatenates 1-D arrays and np.vstack() stacks them vertically. To make several 1-D arrays into the columns of a 2-D array, use np.column\_stack().

$$\operatorname{np.vstack}((\mathtt{x},\mathtt{y},\mathtt{x})) = \left[ \begin{array}{ccc} \times & \times & \times & \times \\ * & * & * & * \\ \times & \times & \times & \times \end{array} \right] \quad \operatorname{np.column\_stack}((\mathtt{x},\mathtt{y},\mathtt{x})) = \left[ \begin{array}{ccc} \times & * & \times \\ \times & * & \times \\ \times & * & \times \end{array} \right]$$

The functions np.concatenate() and np.stack() are more general versions of np.hstack() and np.vstack(), and np.row\_stack() is an alias for np.vstack().

#### Broadcasting

NumPy automatically aligns arrays for component-wise operations whenever possible. See http://docs.scipy.org/doc/numpy/user/basics.broadcasting.html for more in-depth examples and broadcasting rules.

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \\ 1 & 2 & 3 \end{bmatrix} \qquad \mathbf{x} = \begin{bmatrix} 10 & 20 & 30 \end{bmatrix}$$

$$A + x = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \\ 1 & 2 & 3 \end{bmatrix} \\ + \\ \begin{bmatrix} 10 & 20 & 30 \end{bmatrix} = \begin{bmatrix} 11 & 22 & 33 \\ 11 & 22 & 33 \\ 11 & 22 & 33 \end{bmatrix}$$

A + x.reshape((1,-1)) = 
$$\begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \\ 1 & 2 & 3 \end{bmatrix} + \begin{bmatrix} 10 \\ 20 \\ 30 \end{bmatrix} = \begin{bmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{bmatrix}$$

#### Operations along an Axis

Most array methods have an axis argument that allows an operation to be done along a given axis. To compute the sum of each column, use axis=0; to compute the sum of each row, use axis=1.

$$A = \left[ \begin{array}{rrrr} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{array} \right]$$

A. sum(axis=0) = 
$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 2 & 3 \\ 1 & 2 & 2 & 3 \\ 4 & 4 & 4 \end{bmatrix} = \begin{bmatrix} 4 & 8 & 12 & 16 \end{bmatrix}$$

A.sum(axis=1) = 
$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{bmatrix} = \begin{bmatrix} 10 & 10 & 10 & 10 \end{bmatrix}$$

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