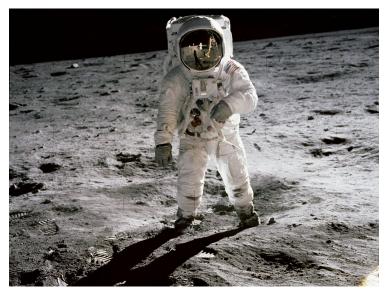
Labs for Foundations of Applied Mathematics

Data Science Essentials

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Preface

This lab manual is designed to accompany the textbook Foundations of Applied Mathematics by Humpherys and Jarvis. While the Volume 3 text focuses on statistics and rigorous data analysis, these labs aim to introduce experienced Python programmers to common tools for obtaining, cleaning, organizing, and presenting data. The reader should be familiar with Python [VD10] and its NumPy [Oli06, ADH+01, Oli07] and Matplotlib [Hun07] packages before attempting these labs. See the Python Essentials manual for introductions to these topics.

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 ${\tt https://github.com/Foundations-of-Applied-Mathematics/Labs} \ as the original source of this work.$

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Part I Labs

Unix Shell 1: Introduction

Lab Objective: Unix is a popular operating system that is commonly used for servers and the basis for most open source software. Using Unix for writing and submitting labs will develop a foundation for future software development. In this lab we explore the basics of the Unix shell, including how to navigate and manipulate files, access remote machines with Secure Shell, and use Git for basic version control.

Unix was first developed by AT&T Bell Labs in the 1970s. In the 1990s, Unix became the foundation of the Linux and MacOSX operating systems. Most servers are Linux-based, so knowing how to use Unix shells allows us to interact with servers and other Unix-based machines.

A *Unix shell* is a program that takes commands from a user and executes those commands on the operating system. We interact with the shell through a *terminal* (also called a command line), a program that lets you type in commands and gives those commands to the shell for execution.

Note

Windows is not built off Unix, but it does come with a terminal called PowerShell. This terminal uses a different command syntax. We will not cover the equivalent commands in the Windows terminal, but you could download a Unix-based terminal such as Git Bash or Cygwin to complete this lab on a Windows machine (you will still lose out on certain commands). Alternatively, Windows 10 now offers a Windows Subsystem for Linux, WSL, which is a Linux operating system downloaded onto Windows.

Note

For this lab we will be working in the UnixShell1 directory provided with the lab materials. If you have not yet downloaded the code repository, follow steps 1 through 6 in the Getting Started guide found at https://foundations-of-applied-mathematics.github.io/ before proceeding with this lab. Make sure to run the download_data.sh script as described in step 5 of Getting Started; otherwise you will not have the necessary files to complete this lab.

Basic Unix Shell

Shell Scripting

The following sections of the lab will explore several shell commands. You can execute these commands by typing these commands directly into a terminal. Sometimes, though, you will want to execute a more complicated sequence of commands, or make it easy to execute the same set of commands over and over again. In those cases, it is useful to create a *script*, which is a sequence of shell commands saved in a file. Then, instead of typing the commands in individually, you simply have to run the script, and it takes care of running all the commands.

In this lab we will be running and editing a bash script. Bash is the most commonly used Unix shell and is the default shell installed on most Unix-based systems.

The following is a very simple bash script. The command echo <string> prints <string> in the terminal.

```
#!/bin/bash
echo "Hello World!"
```

The first line, #!bin/bash, tells the computer to use the bash interpreter to run the script, and where this interpreter is located. The #! is called the *shebang* or *hashbang* character sequence. It is followed by the absolute path to the bash interpreter.

To run a bash script, type bash <script name> into the terminal. Alternatively, you can execute any script by typing ./<script name>, but note that the script must contain executable permissions for this to work. (We will learn more about permissions later in the lab.)

```
$ bash hello_world.sh
Hello World!
```

Navigation

Typically, people navigate computers by clicking on icons to open folders and programs. In the terminal, instead of point and click we use typed commands to move from folder to folder. In the Unix shell, we call folders *directories*. The file system is a set of nested directories containing files and other directories.

You can picture the file system as an tree, with directories as branches. Smaller branches stem from bigger branches, and all bigger branches eventually stem from the root of the tree. Similarly, in the Unix file system we have a "root directory", where all other directories are nested in. We denote it by using a single slash (/). All absolute paths originate at the root directory, which means all absolute path strings begin with the / character.

Begin by opening a terminal. The text you see in the upper left of the terminal is called the *prompt*. Before you start creating or deleting files, you'll want to know where you are. To see what directory you are currently working in, type pwd into the prompt. This command stands for **p**rint working directory, and it prints out a string telling you your current location.

```
~$ pwd
/home/username
```

To see the all the contents of your current directory, type the command 1s, list segments.

~\$ ls
Desktop Downloads Public Videos
Documents Pictures

The command cd, change directory, allows you to navigate directories. To change to a new directory, type the cd command followed by the name of the directory to which you want to move (if you cd into a file, you will get an error). You can move up one directory by typing cd ...

Two important directories are the root directory and the home directory. You can navigate to the home directory by typing $cd \sim or$ just cd. You can navigate to root by typing $cd \sim or$ just $cd \sim o$

Problem 1. To begin, open a terminal and navigate to the UnixShell1/ directory provided with this lab. Use 1s to list the contents. There should be a file called Shell1.zip and a script called unixshell1.sh. a

Run unixshell1.sh. This script will do the following:

- 1. Unzip Shell1.zip, creating a directory called Shell1/
- 2. Remove any previously unzipped copies of Shell1/
- 3. Execute various shell commands, to be added in the next few problems in this lab
- 4. Create a compressed version of Shell1/called UnixShell1.tar.gz.
- 5. Remove any old copies of UnixShell1.tar.gz

Now, open the unixshell1.sh script in a text editor. Add commands to the script to do the following:

- Change into the Shell1/ directory.
- Print a string telling you directory you are currently working in.

Test your commands by running the script again and checking that it prints a string ending in the location Shell1/.

^aIf the necessary data files are not in your directory, cd one directory up by typing cd .. and type bash download_data.sh to download the data files for each lab.

Documentation and Help

When you encounter an unfamiliar command, the terminal has several tools that can help you understand what it does and how to use it. Most commands have manual pages, which give information about what the command does, the syntax required to use it, and different options to modify the command. To open the manual page for a command, type man <command>. Some commands also have an option called --help, which will print out information similar to what is contained in the manual page. To use this option, type <command> --help.

\$ man ls
LS(1) User Commands LS(1)

```
NAME

ls - list directory contents

SYNOPSIS

ls [OPTION]... [FILE]...

DESCRIPTION

List information about the FILEs (the current directory by default).

-a, --all

do not ignore entries starting with .
```

The apropos <keyword> command will list all Unix commands that have <keyword> contained somewhere in their manual page names and descriptions. For example, if you forget how to copy files, you can type in apropos copy and you'll get a list of all commands that have copy in their description.

Flags

When you use man, you will see a list of options such as -a, -A, --author, etc. that modify how a command functions. These are called *flags*. You can use one flag on a command by typing <command > -<flag>, like ls -a, or combine multiple flags by typing <command> -<flag1><flag2>, etc. as in ls -alt.

For example, sometimes directories contain hidden files, which are files whose names begin with a dot character like .bash. The ls command, by default, does not list hidden files. Using the -a flag specifies that ls should not ignore hidden files. Find more common flags for ls in Table 1.1.

Flags	Description
-a	Do not ignore hidden files and folders
-1	List files and folders in long format
-r	Reverse order while sorting
-R	Print files and subdirectories recursively
-s	Print item name and size
-S	Sort by size
-t	Sort output by date modified
	'

Table 1.1: Common flags of the ls command.

```
$ ls
file1.py file2.py

$ ls -a
. .. file1.py file2.py .hiddenfile.py

$ ls -alt  # Multiple flags can be combined into one flag
total 8
drwxr-xr-x  2 c c 4096 Aug 14 10:08 .
```

```
-rw-r--r- 1 c c 0 Aug 14 10:08 .hiddenfile.py
-rw-r--r- 1 c c 0 Aug 14 10:08 file2.py
-rw-r--r- 1 c c 0 Aug 14 10:08 file1.py
drwxr-xr-x 38 c c 4096 Aug 14 10:08 ..
```

Problem 2. Within the script, add a command using 1s to print one list of the contents of Shell1/ with the following criteria:

- Include hidden files and folders
- List the files and folders in long format (include the permissions, date last modified, etc.)
- Sort the output by file size (largest files first)

Test your command by entering it into the terminal within Shell1/ or by running the script and checking for the desired output.

Manipulating Files and Directories

In this section we will learn how to create, copy, move, and delete files and folders. To create a text file, use touch <filename>. To create a new directory, use mkdir <dir_name>.

```
~$ cd Test/  # navigate to test directory

~/Test$ ls  # list contents of directory
file1.py

~/Test$ mkdir NewDirectory # create a new empty directory

~/Test$ touch newfile.py # create a new empty file

~/Test$ ls
file1.py NewDirectory newfile.py
```

To copy a file into a directory, use cp <filename> <dir_name>. When making a copy of a directory, use the -r flag to recursively copy files contained in the directory. If you try to copy a directory without the -r, the command will return an error.

Moving files and directories follows a similar format, except no -r flag is used when moving one directory into another. The command mv <filename> <dir_name> will move a file to a folder and mv <dir1> <dir2> will move the first directory into the second.

If you want to rename a file, use mv <file_old> <file_new>; the same goes for directories.

```
~/Test$ ls
file1.py NewDirectory newfile.py

~/Test$ mv newfile.py NewDirectory/  # move file into directory

~/Test$ cp file1.py NewDirectory/  # make a copy of file1 in directory
```

```
~/Test$ cd NewDirectory/
~/Test/NewDirectory$ mv file1.py newname.py # rename file1.py
~/Test/NewDirectory$ ls
newfile.py newname.py
```

When deleting files, use rm < filename>, and when deleting a directory, use $rm -r < dir_name>$. The -r flag tells the terminal to recursively remove all the files and subfolders within the targeted directory.

If you want to make sure your command is doing what you intend, the -v flag tells rm, cp, or mkdir to print strings in the terminal describing what it is doing.

When your terminal gets too cluttered, use clear to clean it up.

Commands	Description
clear	Clear the terminal screen
cp file1 dir1	Create a copy of file1 and move it to dir1/
cp file1 file2	Create a copy of file1 and name it file2
cp -r dir1 dir2	Create a copy of dir1/ and all its contents into dir2/
mkdir dir1	Create a new directory named dir1/
<pre>mkdir -p path/to/new/dir1</pre>	Create dir1/ and all intermediate directories
mv file1 dir1	Move file1 to dir1/
mv file1 file2	Rename file1 as file2
rm file1	Delete file1 [-i, -v]
rm -r dir1	Delete dir1/ and all items within dir1/ [-i, -v]
touch file1	Create an empty file named file1

Table 1.2: File Manipulation Commands

Table 1.2 contains all the commands we have discussed so far. Commonly used flags for some commands are contained in square brackets; use man or --help to see what these mean.

Problem 3. Add commands to the unixshell1.sh script to make the following changes in Shell1/:

- Delete the Audio/ directory along with all its contents
- Create Documents/, Photos/, and Python/ directories

• Change the name of the Random/ directory to Files/

Test your commands by running the script and then using 1s within Shell1/ to check that each directory was deleted, created, or changed correctly.

Wildcards

As we are working in the file system, there will be times that we want to perform the same command to a group of similar files. For example, you may need to move all text files within a directory to a new directory. Rather than copy each file one at a time, we can apply one command to several files using *wildcards*. We will use the * and ? wildcards. The * wildcard represents any string and the ? wildcard represents any single character. Though these wildcards can be used in almost every Unix command, they are particularly useful when dealing with files.

```
$ ls
File1.txt File2.txt File3.jpg text_files

$ mv -v *.txt text_files/
File1.txt -> text_files/File1.txt
File2.txt -> text_files/File2.txt

$ ls
File3.jpg text_files
```

See Table 1.3 for examples of common wildcard usage.

Command	Description
*.txt	All files that end with .txt.
image*	All files that have image as the first 5 characters.
py	All files that contain py in the name.
doc*.txt	All files of the form doc1.txt, doc2.txt, docA.txt, etc.

Table 1.3: Common uses for wildcards.

Problem 4. Within the Shell1/ directory, there are many files. Add commands to the script to organize these files into directories using wildcards. Organize by completing the following:

- Move all the .jpg files to the Photos/ directory
- Move all the .txt files to the Documents/ directory
- Move all the .py files to the Python/ directory

Working With Files

Searching the File System

There are two commands we can use for searching through our directories. The find command is used to find files or directories with a certain name; the grep command is used to find lines within files matching a certain string. When searching for a specific string, both commands allow wildcards within the string. You can use wildcards so that your search string matches a broader set of strings.

```
# Find all within files in Documents/ containing "Mary"
# -r tells grep to search all files with Documents/
# -n tells grep to print out the line number (2)

$ Shell1$ grep -nr "Mary" Documents/
Documents/people.txt:2:female,Mary,31
```

Command	Description
find dir1 -type f -name "word"	Find all files in dir1/ (and its subdirectories) called word
	(-type f is for files; -type d is for directories)
grep "word" filename	Find all occurrences of word within filename
grep -nr "word" dir1	Find all occurrences of word within the files inside dir1/
	(-n lists the line number; -r performs a recursive search)

Table 1.4: Commands using find and grep.

Table 1.4 contains basic syntax for using these two commands. There are many more variations of syntax for grep and find, however. You can use man grep and man find to explore other options for using these commands.

File Security and Permissions

A file has three levels of permissions associated with it: the permission to read the file, to write (modify) the file, and to execute the file. There are also three categories of people who are assigned permissions: the user (the owner), the group, and others.

You can check the permissions for file1 using the command ls -l <file1>. Note that your output will differ from that printed below; this is purely an example.

```
$ ls -l
-rw-rw-r-- 1 username groupname 194 Aug 5 20:20 calc.py
drw-rw-r-- 1 username groupname 373 Aug 5 21:16 Documents
-rwxr-x--x 1 username groupname 27 Aug 5 20:22 mult.py
-rw-rw-r-- 1 username groupname 721 Aug 5 20:23 project.py
```

The first character of each line denotes the type of the item whether it be a normal file, a directory, a symbolic link, etc. The next nine characters denote the permissions associated with that file.

For example, look at the output for mult.py. The first character - denotes that mult.py is a normal file. The next three characters, rwx, tell us the owner can read, write, and execute the file. The next three characters, r-x, tell us members of the same group can read and execute the file, but not edit it. The final three characters, --x, tell us other users can execute the file and nothing more.

Permissions can be modified using the chmod command. There are multiple notations used to modify permissions, but the easiest to use when we want to make small modifications to a file's permissions is *symbolic permissions* notation. See Table 1.5 for more examples of using symbolic permissions notation, as well as other useful commands for working with permissions.

```
$ ls -l script1.sh
total 0
-rw-r--r-- 1 c c 0 Aug 21 13:06 script1.sh

$ chmod u+x script1.sh  # add permission for user to execute
$ chmod o-r script1.sh  # remove permission for others to read
$ ls -l script1.sh
total 0
-rwxr---- 1 c c 0 Aug 21 13:06 script1.sh
```

Command	Description
chmod u+x file1	Add executing (x) permissions to user (u)
chmod g-w file1	Remove writing (w) permissions from group (g)
chmod o-r file1	Remove reading (r) permissions from other other users (o)
chmod a+w file1	Add writing permissions to everyone (a)
chown	change owner
chgrp	change group
getfacl	view all permissions of a file in a readable format.

Table 1.5: Symbolic permissions notation and other useful commands

Running Files

To run a file for which you have execution permissions, type the file name preceded by ./.

```
$ ./hello.sh
bash: ./hello.sh: Permission denied
$ ls -l hello.sh
```

```
-rw-r--r-- 1 username groupname 31 Jul 30 14:34 hello.sh

$ chmod u+x hello.sh  # You can now execute the file

$ ./hello.sh
Hello World!
```

Problem 5. Within Shell1/, there is a script called organize_photos.sh. First, use find to locate the script. Once you know the file location, add commands to your script so that it completes the following tasks:

- Moves organize_photos.sh to Scripts/
- Adds executable permissions to the script for the user
- Runs the script

Test that the script has been executed by checking that additional files have been moved into the Photos/directory. Check that permissions have been updated on the script by using ls -1.

Accessing Remote Machines

At times you will find it useful to perform tasks on a remote computer or server, such as running a script that requires a large amount of computing power on a supercomputer or accessing a data file stored on another machine.

Secure Shell

Secure Shell (SSH) allows you to remotely access other computers or servers securely. SSH is a network protocol encrypted using public-key cryptography. It ensures that all communication between your computer and the remote server is secure and encrypted.

The system you are connecting to is called the *host*, and the system you are connecting from is called the *client*. The first time you connect to a host, you will receive a warning saying the authenticity of the host can't be established. This warning is a default, and appears when you are connecting to a host you have not connected to before. When asked if you would like to continue connecting, select yes.

When prompted for your password, type your password as normal and press enter. No characters will appear on the screen, but they are still being logged. Once the connection is established, there is a secure tunnel through which commands and files can be exchanged between the client and host. To end a secure connection, type exit.

```
alice@mycomputer:~$ ssh alice27@acme01.byu.edu
alice27@acme01.byu.edu password:# Type password as normal
last login 7 Sept 11
```

```
[alice27@byu.local@acme01 ~]$ ls  # Commands are executed on the host
myacmeshare/

[alice27@byu.local@acme01 ~]$ exit  # End a secure connection
logout
Connection to acme01.byu.edu closed.

alice@mycomputer:~$  # Commands are executed on the client
```

Secure Copy

To copy files from one computer to another, you can use the Unix command scp, which stands for secure copy protocol. The syntax for scp is essentially the same as the syntax for cp.

To copy a file from your computer to a specific location on on a remote machine, use the syntax scp <file1> <user@remote_host:file_path>. As with cp, to copy a directory and all of its contents, use the -r flag.

```
# Make copies of file1 and dir2 in the home directory on acme01.byu.edu
alice@mycomputer:~$ scp file1 alice27@acme01.byu.edu:~/
alice@mycomputer:~$ scp -r dir1/dir2 alice27@acme01.byu.edu:~/
```

Use the syntax scp -r <user@remote_host:file_path/dir1> <file_path> to copy dir1 from a remote machine to the location specified by file_path on your current machine.

```
# Make a local copy of dir1 (from acme01.byu.edu) in the home directory
alice@mycomputer:~$ scp -r alice27@acme01.byu.edu:~/dir1 ~
```

Commands	Description	
ssh username@remote_host	Establish a secure connection with remote_host	
<pre>scp file1 user@remote_host:file_path/</pre>	Create a copy of file1 on host	
<pre>scp -r dir1 user@remote_host:file_path/</pre>	Create a copy of dir1 and its contents on host	
<pre>scp user@remote_host:file_path/file1 file_path2</pre>	Create a local copy of file on client	

Table 1.6: Basic syntax for ssh and scp.

Problem 6. On a computer with the host name acme20.byu.edu or acme21.byu.edu, there is a file called img_649.jpg. Secure copy this file to your UnixShell1/ directory. (Do not add the scp command to the script).

To ssh or scp on this computer, your username is your Net ID, and your password is your typical Net ID password. To use scp or ssh for this computer, you will have to be on campus using BYU Wifi.

Hint: To use scp, you will need to know the location of the file on the remote computer. Consider using ssh to access the machine and using find. The file is located somewhere in the directory /sshlab.

After secure copying, add a command to your script to copy the file from UnixShell1/into the directory Shell1/Photos/. (Make sure to leave a copy of the file in UnixShell1/, otherwise the file will be deleted when you run the script again.)

Git

Git is a version control system, meaning that it keeps a record of changes in a file. Git also facilitates collaboration between people working on the same code. It does both these things by managing updates between an online code repository and copies of the repository, called *clones*, stored locally on computers.

We will be using git to submit labs and return feedback on those labs. If git is not already installed on your computer, download it at http://git-scm.com/downloads.

Using Git

Git manages the history of a file system through *commits*, or checkpoints. Each time a new commit is added to the online repository, a checkpoint is created so that if need be, you can use or look back at an older version of the repository. You can use git log to see a list of previous commits. You can also use git status to see the files that have been changed in your local repository since the last commit.

Before making your own changes, you'll want to add any commits from other clones into your local repository. To do this, use the command git pull origin master.

Once you have made changes and want to make a new commit, there are normally three steps. To save these changes to the online repository, first add the changed files to the *staging area*, a list of files to save during the next commit, with git add <filename(s)>. If you want to add all changes that you have made to tracked files (files that are already included in the online repository), use git add -u.

Next, save the changes in the staging area with git commit -m "A brief message describing the changes>".

Finally, add the changes in this commit to the online repository with git push origin master.

```
$ cd MyDirectory/  # Navigate into a cloned repository
$ git pull origin master  # Pull new commits from online repository

### Make changes to file1.py ###

$ git add file1.py  # Add file to staging area
$ git commit -m "Made changes"  # Commit changes in staging area
$ git push origin master  # Push changes to online repository
```

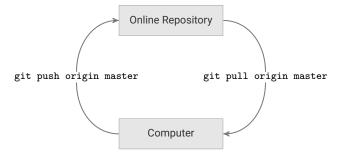


Figure 1.1: Exchanging git commits between the repository and a local clone.

Merge Conflicts

Git maintains order by raising an alert when changes are made to the same file in different clones and neither clone contains the changes made in the other. This is called a *merge conflict*, which happens when someone else 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.

ACHTUNG!

When pulling updates with git pull origin master, your terminal may sometimes display the following merge conflict 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 screen, displayed in vim (https://en.wikipedia.org/wiki/Vim_(text_editor)), is asking you to enter a message to create a *merge commit* that will reconcile both changes. If you do not enter a message, a default message is used. To close this screen and create the merge commit with the default message, type :wq (the characters will appear in the bottom left corner of the terminal) and press enter.

NOTE

Vim is a terminal text editor available on essentially any computer you will use. When working with remote machines through ssh, vim is often the only text editor available to use. To exit vim, press esc:wq To learn more about vim, visit the official documentation at https://vimhelp.org.

Command	Explanation
git status	Display the staging area and untracked changes.
git pull origin master	Pull changes from the online repository.
git push origin master	Push changes to the online repository.
<pre>git add <filename(s)></filename(s)></pre>	Add a file or files to the staging area.
git add -u	Add all modified, tracked files to the staging area.
git commit -m " <message>"</message>	Save the changes in the staging area with a given message.
git checkout <filename></filename>	Revert changes to an unstaged file since the last commit.
git reset HEAD <filename></filename>	Remove a file from the staging area, but keep changes.
git diff <filename></filename>	See the changes to an unstaged file since the last commit.
git diffcached <filename></filename>	See the changes to a staged file since the last commit.
git configlocal <option></option>	Record your credentials (user.name, user.email, etc.).

Table 1.7: Common git commands.

Problem 7. Using git commands, push unixshell1.sh and UnixShell1.tar.gz to your online git repository. Do not add anything else in the UnixShell1/ directory to the online repository.

Unix Shell 2

Lab Objective: Introduce system management, calling Unix Shell commands within Python, and other advanced topics. As in the last Unix lab, the majority of learning will not be had in finishing the problems, but in following the examples.

Archiving and Compression

In file management, the terms archiving and compressing are commonly used interchangeably. However, these are quite different. Archiving is combining a certain number of files into one file. The resulting file will be the same size as the group of files that were archived. Compressing takes a file or group of files and shrinks the file size as much as possible. The resulting compressed file will need to be extracted before being used.

The ZIP file format is common for archiving and compressing files. If the zip Unix command is not installed on your system, you can download it by running

```
>>> sudo apt-get install zip
```

Note that you will need to have administrative rights to download this package. To unzip a file, use unzip.

Note

To begin this lab, unzip the Shell2.zip file into your UnixShell2/ directory using a terminal command.

```
# Unzip a zipped file using the unzip command.
$ unzip Shell2.zip
Archive Shell2.zip
    creating: Shell2/
    creating: Shell2/Test/
    inflating: Shell2/.DS_Store
    creating: Shell2/Scripts/
```

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```
extracting: Shell2/Scripts/fiteen_secs
extracting: Shell2/Scripts/script3
extracting: Shell2/Scripts/hello.sh...
```

While the zip file format is more popular on the Windows platform, the tar utility is more common in the Unix environment.

NOTE

When submitting this lab, you will need to archive and compress your entire Shell2/directory into a file called Shell2.tar.gz and push Shell2.tar.gz as well as shell2.py to your online repository.

If you are doing multiple submissions, make sure to delete your previous Shell2.tar.gz file before creating a new one from your modified Shell2/ directory. Refer to Unix1 for more information on deleting files.

As a final note, please do not push the entire directory to your online repository. *Only* push ShellFinal.tar.gz and shell2.py.

The example below demonstrates how to archive and compress our Shell2/ directory. The -z flag calls for the gzip compression tool, the -v flag calls for a verbose output, the -p flag tells the tool to preserve file permission, and the -f flag indicates the next parameter will be the name of the archive file. Note that the -f flag must always come last.

```
# Remove your archive tar.gz file if you already have one.
$ rm -v Shell2.tar.gz
removed 'Shell2.tar.gz'

# Create a new one from your update Shell2 directory content.
# Remember that the * is the wildcard that represents all strings.
$ tar -zcpf Shell2.tar.gz Shell2/*
```

Working with Files

Displaying File Contents

The unix file system presents many opportunities for the manipulation, viewing, and editing of files. Before moving on to more complex commands, we will look at some of the commands available to view the content of a file.

The cat command, followed by the filename, will display all the contents of a file on the terminal screen. This can be problematic if you are dealing with a large file. There are a few available commands to control the output of cat in the terminal. See Table 2.1.

As an example, use less <filename> to restrict the number of lines that are shown. With this command, use the arrow keys to navigate up and down and press q to exit.

Command	Description
cat	Print all of the file contents
more	Print the file contents one page at a time, navigating forwards
less	Like more, but you navigate forward and backwards
head	Print the first 10 lines of a file
\mathtt{head} $-\mathtt{n}k$	Print the first k lines of a file
tail	Print the last 10 lines of a file
$\mathtt{tail}\ \mathtt{-n} k$	Print the last k lines of a file

Table 2.1: Commands for printing file contents

Pipes and redirects

To combine terminal commands, we can use *pipes*. When we combine or *pipe* commands, the output of one command is passed to the other. We pipe commands together using the | (bar) operator. In the example directly below, the cat command output is piped to wc -1 (wc stands for word count, and the -1 flag tells the wc command to count lines).

In the second part of the example, ls -s is piped to sort -nr. Refer to the *Unix 1* lab for explanations of ls and sort. Recall that the man command followed by an additional command will output details on the additional command's possible flags and what they mean (for example man sort).

```
$ cd Shell2/Files/Feb
# Output the number of lines in assignments.txt.
$ cat assignments.txt | wc -l
9
# Sort the files by file size and output file names and their size.
$ls -s | sort -nr
4 project3.py
4 project2.py
4 assignments.txt
4 pics
total 16
```

In addition to *piping* commands together, when working with files specifically, we can use redirects. A *redirect*, represented as < in the terminal, passes the file to a terminal command.

To save a command's output to a file, we can use > or >>. The > operator will overwrite anything that may exist in the output file whereas >> will append the output to the end of the output file. Examples of *redirects* and writing to a file are given below.

```
# Gets the same result as the first command in the above example.
$ wc -l < assignments.txt
9
# Writes the number of lines in the assignments.txt file to word_count.txt.
$ wc -l < assignments.txt >> word_count.txt
```

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Problem 1. The words.txt file in the Documents/ directory contains a list of words that are not in alphabetical order. Write an alphabetically sorted list of words in words.txt to a new file in your Documents/ called sortedwords.txt using pipes and redirects. After you write the alphabetized words to the designated file, also write the number of words in words.txt to the end of sortedwords.txt. Save this file in the Documents/ directory. Try to accomplish this with a total of two commands or fewer.

Resource Management

To be able to optimize performance, it is valuable to be aware of the resources, specifically hard drive space and computer memory, being used.

Job Control

One way to monitor and optimize performance is in job control. Any time you start a program in the terminal (you could be running a script, opening ipython, etc.,) that program is called a job. You can run a job in the foreground and also in the background. When we run a program in the foreground, we see and interact with it. Running a script in the foreground means that we will not be able to enter any other commands in the terminal while the script is running. However, if we choose to run it in the background, we can enter other commands and continue interacting with other programs while the script runs.

Consider the scenario where we have multiple scripts that we want to run. If we know that these scripts will take awhile, we can run them all in the background while we are working on something else. Table 2.2 lists some common commands that are used in job control. We strongly encourage you to experiment with some of these commands.

Command	Description
COMMAND &	Adding an ampersand to the end of a command
	runs the command in the background
bg %N	Restarts the Nth interrupted job in the background
fg %N	Brings the Nth job into the foreground
jobs	Lists all the jobs currently running
kill %N	Terminates the Nth job
ps	Lists all the current processes
Ctrl-C	Terminates current job
Ctrl-Z	Interrupts current job
nohup	Run a command that will not be killed if the user logs out

Table 2.2: Job control commands

The fifteen_secs and five_secs scripts in the Scripts/directory take fifteen seconds and five seconds to execute respectively. The python file fifteen_secs.py in the Python/directory takes fifteen seconds to execute, this file counts to fifteen and then outputs "Success!". These will be particularly useful as you are experimenting with these commands.

Remember, that when you use the ./ command in place of other commands you will probably need to change permissions. For more information on changing permissions, review *Unix 1*. Run the following command sequence from the Shell2 directory.

```
# Remember to add executing permissions to the user.
$ ./Scripts/fifteen_secs &
$ python Python/fifteen_secs.py &
$ jobs
[1]+ Running
                    ./Scripts/fifteen_secs &
[2] - Running
                   python Python/fifteen_secs.py &
$ kill %1
[1] - Terminated
                   ./Scripts/fifteen_secs &
$ jobs
                   python Python/fifteen_secs.py &
[1]+ Running
# After the python script finishes it outputs the results.
$ Success!
# To move on, click enter after "Success!" appears in the terminal.
# List all current processes
$ ps
 PID TTY
                   TIME CMD
   6 tty1
               00:00:00 bash
               00:00:00 ps
  44 tty1
$ ./Scripts/fifteen_secs &
$ ps
 PID TTY
                   TIME CMD
   6 tty1
               00:00:00 bash
  59 tty1
               00:00:00 fifteen_secs
  60 tty1
               00:00:00 sleep
  61 tty1
               00:00:00 ps
# Stop fifteen_secs
$ kill 59
$ ps
 PID TTY
                   TIME CMD
   6 tty1
               00:00:00 bash
  60 tty1
               00:00:00 sleep
  61 tty1
               00:00:00 ps
[1]+ Terminated
                              ./fifteen_secs
```

Problem 2. In addition to the five_secs and fifteen_secs scripts, the Scripts/ folder contains three scripts (named script1, script2, and script3) that each take about forty-five seconds to execute. From the Scripts directory, execute each of these commands in the background in the following order; script1, script2, and script3. Do this so all three are running at the same time. While they are all running, write the output of jobs to a new file log.txt saved in the Scripts/ directory.

(Hint: In order to get the same output as the solutions file, you need to run the ./ command and not the bash command.)

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Using Python for File Management

OS and Glob

Bash has control flow tools like if-else blocks and loops, but most of the syntax is highly unintuitive. Python, on the other hand, has extremely intuitive syntax for these control flow tools, so using Python to do shell-like tasks can result in some powerful but specific file management programs. Table 2.3 relates some of the common shell commands to Python functions, most of which come from the os module in the standard library.

Shell Command	Python Function
ls	os.listdir()
cd	os.chdir()
pwd	os.getcwd()
mkdir	os.mkdir(), os.mkdirs()
ср	shutil.copy()
mv	os.rename(), os.replace()
rm	os.remove(), shutil.rmtree()
du	os.path.getsize()
chmod	os.chmod()

Table 2.3: Shell-Python compatibility

In addition to these, Python has a few extra functions that are useful for file management and shell commands. See Table 2.4. The two functions os.walk() and glob.glob() are especially useful for doing searches like find and grep. Look at the example below and then try out a few things on your own to try to get a feel for them.

Function	Description
os.walk()	Iterate through the subfolders and subfolder files of a given directory.
os.path.isdir()	Return True if the input is a directory.
os.path.isfile()	Return True if the input is a file.
os.path.join()	Join several folder names or file names into one path.
<pre>glob.glob()</pre>	Return a list of file names that match a pattern.
<pre>subprocess.call()</pre>	Execute a shell command.
<pre>subprocess.check_output()</pre>	Execute a shell command and return its output as a string.

Table 2.4: Other useful Python functions for shell operations.

```
# Your output may differ from the example's output.
>>> import os
>>> from glob import glob

# Get the names of all Python files in the Python/ directory.
>>> glob("Python/*.py")
['Python/calc.py',
   'Python/count_files.py',
   'Python/fifteen_secs.py
   'Python/mult.py',
```

```
'Python/project.py']
# Get the names of all .jpg files in any subdirectory.
# The recursive parameter lets '**' match more than one directory.
>> glob("**/*.jpg", rescursive=True)
['Photos/IMG_1501.jpg',
 'Photos/img_1879.jpg',
 'Photos/IMG_2164.jpg',
 'Photos/IMG_2379.jpg',
 'Photos/IMG_2182.jpg',
 'Photos/IMG_1510.jpg',
 'Photos/IMG_2746.jpg',
 'Photos/IMG_2679.jpg',
 'Photos/IMG_1595.jpg',
 'Photos/IMG_2044.jpg',
 'Photos/img_1796.jpg',
 'Photos/IMG_2464.jpg',
 'Photos/img_1987.jpg',
 'Photos/img_1842.jpg']
# Walk through the directory, looking for .sh files.
>>> for directory, subdirectories, files in os.walk('.'):
        for filename in files:
            if filename.endswith(".sh"):
                print(os.path.join(directory, filename))
. . .
./Scripts/hello.sh
./Scripts/organize_photos.sh
```

Problem 3. Write a Python function <code>grep()</code> that accepts the name of a target string and a file pattern. Find all files in the current directory or its subdirectories that match the file pattern. Next, check within the contents of the matched file for the target string. For example, <code>grep("*.py", "range()")</code> should search Python files for the command <code>range()</code>. Return a list of the filenames that matched the file pattern <code>and</code> the target string.

The Subprocess module

The subprocess module allows Python to execute actual shell commands in the current working directory. Some important commands for executing shell commands from the subprocess module are listed in Table 2.5.

```
$ cd Shell2/Scripts
$ python
>>> import subprocess
>>> subprocess.call(["ls", "-1"])
```

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Function	Description
subprocess.call()	run a Unix command
<pre>subprocess.check_output()</pre>	run a Unix command and record its output
<pre>subprocess.check_output.decode()</pre>	this translates Unix command output to a string
<pre>subprocess.Popen()</pre>	use this to pipe togethether Unix commands

Table 2.5: Python subprocess module important commands

```
total 40
-rw-r--r-- 1 username groupname
                                 20 Aug 26 2016 five_secs
                                 21 Aug 26
                                            2016 script1
-rw-r--r-- 1 username
                       groupname
-rw-r--r-- 1 username groupname
                                 21 Aug 26 2016 script2
                                 21 Aug 26
                                            2016 script3
-rw-r--r- 1 username groupname
-rw-r--r-- 1 username groupname
                                 21 Aug 26
                                            2016 fiften_secs
# Decode() translates the result to a string.
>>> file_info = subprocess.check_output(["ls", "-l"]).decode()
>>> file_info.split('\n')
['total 40',
 '-rw-r--r- 1 username groupname 20 Aug 26 2016 five_secs',
 '-rw-r--r- 1 username groupname 21 Aug 26 2016 script1',
 '-rw-r--r-- 1 username groupname 21 Aug 26
                                              2016 script2',
 '-rw-r--r- 1 username groupname 21 Aug 26
                                              2016 script3',
 '-rw-r--r-- 1 username groupname 21 Aug 26 2016 fiften_secs',
 ' ']
```

Popen is a class of the subprocess module, with its own attributes and commands. It pipes together a few commands, similar to we did at the beginning of the lab. This allows for more versatility in the shell input commands. If you wish to know more about the Popen class, go to the subprocess documentation on the internet.

```
$ cd Shell2
$ python
>>> import subprocess
>>> args = ["cat Files/Feb/assignments.txt | wc -l"]
# shell = True indicates to open a new shell process
# note that task is now an object of the Popen class
>>> task = subprocess.Popen(args, shell=True)
>>> 9
```

```
ACHTUNG!
```

If shell commands depend on user input, the program is vulnerable to a *shell injection attack*. This applies to Unix Shell commands as well as other situations like web browser interaction with web servers. Be extremely careful when creating a shell process from Python. There are specific functions, like shlex.quote(), that quote specific strings that are used to construct shell commands. But, when possible, it is often better to avoid user input altogether. For example, consider the following function.

```
>>> def inspect_file(filename):
... """Return information about the specified file from the shell."""
... return subprocess.check_output(["ls", "-l", filename]).decode()
```

If $inspect_file()$ is given the input ".; rm - rf /", then ls - l . is executed innocently, and then rm - rf / destroys the computer by force deleting everything in the root directory. a Be careful not to execute a shell command from within Python in a way that a malicious user could potentially take advantage of.

 $^a\mathrm{See}$ https://en.wikipedia.org/wiki/Code_injection#Shell_injection for more example attacks.

Problem 4. Using os.path and Glob, write a Python function that accepts an integer n. Search the current directory and all subdirectories for the n largest files. Then sort the list of filenames from the largest to the smallest files. Next, write the line count of the smallest file to a file called smallest.txt into the current directory. Finally, return the list of filenames, including the file path, in order from largest to smallest.

(Hint: the shell commands ls -s shows the file size.)

As a note, to get this problem correct, you do not need to only return filenames, but the entire file path. For example, instead of returning 'data.txt' as part of your list, return 'Files/Mar/docs/data.txt'.

Downloading Files

The Unix shell has tools for downloading files from the internet. The most popular are wget and curl. At its most basic, curl is the more robust of the two while wget can download recursively. This means that wget is capable of following links and directory structure when downloading content.

When we want to download a single file, we just need the URL for the file we want to download. This works for PDF files, HTML files, and other content simply by providing the right URL.

```
\ wget https://github.com/Foundations-of-Applied-Mathematics/Data/blob/master/\leftarrow Volume1/dream.png
```

The following are also useful commands using wget.

```
# Download files from URLs listed in urls.txt.
$ wget -i list_of_urls.txt
# Download in the background.
```

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```
$ wget -b URL

# Download something recursively.
$ wget -r --no-parent URL
```

Problem 5. The file urls.txt in the Documents/directory contains a list of URLs. Download the files in this list using wget and move them to the Photos/directory.

sed and awk

sed and awk are two different scripting languages in their own right. sed is a stream editor; it perfoms basic transformations on input text. Awk is a text processing language that manipulates and reports data. Like Unix, these languages are easy to learn but difficult to master. It is very common to combine Unix commands and sed and awk commands.

Printing Specific Lines Using sed

We have already used the head and tail commands to print the beginning and end of a file respectively. What if we wanted to print lines 30 to 40, for example? We can accomplish this using sed. In the Documents/ folder, you will find the lines.txt file. We will use this file for the following examples.

```
# Same output as head -n3.
$ sed -n 1,3p lines.txt
line 1
line 2
line 3

# Same output as tail -n3.
$ sed -n 3,5p lines.txt
line 3
line 4
line 5

# Print lines 1,3,5.
$ sed -n -e 1p -e 3p -e 5p lines.txt
line 1
line 3
line 5
```

Find and Replace Using sed

Using sed, we can also find and replace. We can perform this function on the output of another commmand, or we can perform this function in place on other files. The basic syntax of this sed command is the following.

```
sed s/str1/str2/g
```

This command will replace every instance of str1 with str2. More specific examples follow.

```
$ sed s/line/LINE/g lines.txt
LINE 1
LINE 2
LINE 3
LINE 4
LINE 5
# Notice the file didn't change at all
$ cat lines.txt
line 1
line 2
line 3
line 4
line 5
# To save the changes, add the -i flag
$ sed -i s/line/LINE/g lines.txt
$ cat lines.txt
LINE 1
LINE 2
LINE 3
LINE 4
LINE 5
```

Problem 6. Problem 6. Problem 6() is a function that accepts an integer n as input and returns three different lists in the following order: a list of integers from 0 to n in increments of 1; a list of integers from n to 0 in increments of n in incre

It contains two syntax errors that are repeated in multiple locations. Look in your shell2.py file and identify the syntax errors, but do not fix them yet. After you find them, use sed commands to replace those errors with the correct commands. To test if your commands worked, you can review your lab file that you edited, or just simply run prob6().

Formatting output using awk

Earlier in this lab we mentioned 1s -1, and as we have seen, this outputs lots of information. Using awk, we can select which fields we wish to print. Suppose we only cared about the file name and the permissions. We can get this output by running the following command.

```
$ cd Shell2/Documents
$ ls -1 | awk ' {print $1, $9} '
total
```

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```
-rw-r--r- doc1.txt
-rw-r--r- doc2.txt
-rw-r--r- doc3.txt
-rw-r--r- doc4.txt
-rw-r--r- files.txt
-rw-r--r- lines.txt
-rw-r--r- newfiles.txt
-rw-r--r- people.txt
-rw-r--r- words.txt
```

Notice we pipe the output of ls -l to awk. When calling a command using awk, we have to use quotation marks. It is a common mistake to forget to add these quotation marks. Inside these quotation marks, commands always take the same format.

```
awk ' <options> {<actions>} '
```

In the remaining examples we will not be using any of the options, but we will address various actions.

In the Documents/ directory, you will find a people.txt file that we will use for the following examples. In our first example, we use the print action. The \$1 and \$9 mean that we are going to print the first and ninth fields.

Beyond specifying which fields we wish to print, we can also choose how many characters to allocate for each field. This is done using the % command within the printf command, which allows us to edit how the relevant data is printed. Look at the last part of the example below to see how it is done.

```
# contents of people.txt
$ cat people.txt
male, John, 23
female, Mary, 31
female, Sally, 37
male, Ted, 19
male, Jeff, 41
female, Cindy, 25
# Change the field separator (FS) to space at the beginning of run using BEGIN
# Printing each field individually proves we have successfully separated the \hookleftarrow
    fields
$ awk ' BEGIN{ FS = " " }; {print $1,$2,$3} ' < people.txt</pre>
male John 23
female Mary 31
female Sally 37
male Ted 19
male Jeff 41
female Cindy 25
```

The statement "%-6s %2s %s\n" formats the columns of the output. This says to set aside six characters left justified, then two characters right justified, then print the last field to its full length.

Problem 7. Inside the Documents/ directory, you should find a file named files.txt. This file contains details on approximately one hundred files. The different fields in the file are separated by tabs. Using awk, sort, pipes, and redirects, write it to a new file in the current directory named date_modified.txt with the following specifications:

- in the first column, print the date the file was modified
- in the second column, print the name of the file
- sort the file from newest to oldest based on the date last modified

All of this can be accomplished using one command.

(Hint: change the field separator to account for tab-delimited files by setting $FS = "\t"$ in the BEGIN command)

We have barely scratched the surface of what awk can do. Performing an internet search for awk one-liners will give you many additional examples of useful commands you can run using awk.

Note

Remember to archive and compress your Shell2 directory before pushing it to your online repository for grading.

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Additional Material

Customizing the Shell

Though there are multiple Unix shells, one of the most popular is the bash shell. The bash shell is highly customizable. In your home directory, you will find a hidden file named .bashrc. All customization changes are saved in this file. If you are interested in customizing your shell, you can customize the prompt using the PS1 environment variable. As you become more and more familiar with the Unix shell, you will come to find there are commands you run over and over again. You can save commands you use frequently with alias. If you would like more information on these and other ways to customize the shell, you can find many quality reference guides and tutorials on the internet.

System Management

In this section, we will address some of the basics of system management. As an introduction, the commands in Table 2.6 are used to learn more about the computer system.

Command	Description
passwd	Change user password
uname	View operating system name
uname -a	Print all system information
uname -m	Print machine hardware
W	Show who is logged in and what they are doing
whoami	Print userID of current user

Table 2.6: Commands for system administration.

3

SQL 1: Introduction

Lab Objective: Being able to store and manipulate large data sets quickly is a fundamental part of data science. The SQL language is the classic database management system for working with tabular data. In this lab we introduce the basics of SQL, including creating, reading, updating, and deleting SQL tables, all via Python's standard SQL interaction modules.

Relational Databases

A relational database is a collection of tables called relations. A single row in a table, called a tuple, corresponds to an individual instance of data. The columns, called attributes or features, are data values of a particular category. The collection of column headings is called the schema of the table, which describes the kind of information stored in each entry of the tuples.

For example, suppose a database contains demographic information for M individuals. If a table had the schema (Name, Gender, Age), then each row of the table would be a 3-tuple corresponding to a single individual, such as (Jane Doe, F, 20) or (Samuel Clemens, M, 74.4). The table would therefore be $M \times 3$ in shape. Note that including a person's age in a database means that the data would quickly be outdated since people get older every year. A better choice would be to use birth year. Another table with the schema (Name, Income) would be $M \times 2$ if it included all M individuals.

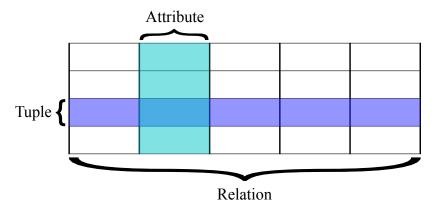


Figure 3.1: See https://en.wikipedia.org/wiki/Relational_database.

SQLite

The most common database management systems (DBMS) for relational databases are based on Structured Query Language, commonly called SQL (pronounced¹ "sequel"). Though SQL is a language in and of itself, most programming languages have tools for executing SQL routines. In Python, the most common variant of SQL is SQLite, implemented as the sqlite3 module in the standard library.

A SQL database is stored in an external file, usually marked with the file extension db or mdf. These files should **not** be opened in Python with open() like text files; instead, any interactions with the database—creating, reading, updating, or deleting data—should occur as follows.

- 1. Create a connection to the database with sqlite3.connect(). This creates a database file if one does not already exist.
- 2. Get a *cursor*, an object that manages the actual traversal of the database, with the connection's cursor() method.
- 3. Alter or read data with the cursor's execute() method, which accepts an actual SQL command as a string.
- 4. Save any changes with the cursor's commit() method, or revert changes with rollback().
- 5. Close the connection.

```
>>> import sqlite3 as sql
# Establish a connection to a database file or create one if it doesn't exist.
>>> conn = sql.connect("my_database.db")
>>> try:
        cur = conn.cursor()
                                                     # Get a cursor object.
        cur.execute("SELECT * FROM MyTable")
                                                     # Execute a SQL command.
                                                     # If there is an error,
   except sql.Error:
        conn.rollback()
                                                     # revert the changes
        raise
                                                       and raise the error.
                                                     # If there are no errors,
   else:
        conn.commit()
                                                        save the changes.
... finally:
        conn.close()
                                                     # Close the connection.
```

ACHTUNG!

Some changes, such as creating and deleting tables, are automatically committed to the database as part of the cursor's execute() method. Be extremely cautious when deleting tables, as the action is immediate and permanent. Most changes, however, do not take effect in the database file until the connection's commit() method is called. Be careful not to close the connection before committing desired changes, or those changes will not be recorded.

 $^{^1\}mathrm{See}$ https://english.stackexchange.com/questions/7231/how-is-sql-pronounced for a brief history of the somewhat controversial pronunciation of SQL.

The with statement can be used with open() so that file streams are automatically closed, even in the event of an error. Likewise, combining the with statement with sql.connect() automatically rolls back changes if there is an error and commits them otherwise. However, the actual database connection is **not** closed automatically. With this strategy, the previous code block can be reduced to the following.

```
>>> try:
... with sql.connect("my_database.db") as conn:
... cur = conn.cursor()  # Get the cursor.
... cur.execute("SELECT * FROM MyTable") # Execute a SQL command.
... finally:  # Commit or revert, then
... conn.close() # close the connection.
```

Managing Database Tables

SQLite uses five native data types (relatively few compared to other SQL systems) that correspond neatly to native Python data types.

Python Type	SQLite Type
None	NULL
int	INTEGER
float	REAL
str	TEXT
bytes	BLOB

The CREATE TABLE command, together with a table name and a schema, adds a new table to a database. The schema is a comma-separated list where each entry specifies the column name, the column data type,² and other optional parameters. For example, the following code adds a table called MyTable with the schema (Name, ID, Age) with appropriate data types.

```
>>> with sql.connect("my_database.db") as conn:
...     cur = conn.cursor()
...     cur.execute("CREATE TABLE MyTable (Name TEXT, ID INTEGER, Age REAL)")
...
>>> conn.close()
```

The DROP TABLE command deletes a table. However, using CREATE TABLE to try to create a table that already exists or using DROP TABLE to remove a nonexistent table raises an error. Use DROP TABLE IF EXISTS to remove a table without raising an error if the table doesn't exist. See Table 3.1 for more table management commands.

²Though SQLite does not force the data in a single column to be of the same type, most other SQL systems enforce uniform column types, so it is good practice to specify data types in the schema.

Operation	SQLite Command
Create a new table	<pre>CREATE TABLE (<schema>);</schema></pre>
Delete a table	DROP TABLE ;
Delete a table if it exists	DROP TABLE IF EXISTS ;
Add a new column to a table	ALTER TABLE ADD <column> <dtype></dtype></column>
Remove an existing column	ALTER TABLE DROP COLUMN <column>;</column>
Rename an existing column	ALTER TABLE ALTER COLUMN <column> <dtype>;</dtype></column>

Table 3.1: SQLite commands for managing tables and columns.

Note

SQL commands like CREATE TABLE are often written in all caps to distinguish them from other parts of the query, like the table name. This is only a matter of style: SQLite, along with most other versions of SQL, is case insensitive. In Python's SQLite interface, the trailing semicolon is also unnecessary. However, most other database systems require it, so it's good practice to include the semicolon in Python.

Problem 1. Write a function that accepts the name of a database file. Connect to the database (and create it if it doesn't exist). Drop the tables MajorInfo, CourseInfo, StudentInfo, and StudentGrades from the database if they exist. Next, add the following tables to the database with the specified column names and types.

- MajorInfo: MajorID (integers) and MajorName (strings).
- CourseInfo: CourseID (integers) and CourseName (strings).
- StudentInfo: StudentID (integers), StudentName (strings), and MajorID (integers).
- StudentGrades: StudentID (integers), CourseID (integers), and Grade (strings).

Remember to commit and close the database. You should be able to execute your function more than once with the same input without raising an error.

To check the database, use the following commands to get the column names of a specified table. Assume here that the database file is called **students.db**.

```
>>> with sql.connect("students.db") as conn:
...    cur = conn.cursor()
...    cur.execute("SELECT * FROM StudentInfo;")
...    print([d[0] for d in cur.description])
...
['StudentID', 'StudentName', 'MajorID']
```

Inserting, Removing, and Altering Data

Tuples are added to SQLite database tables with the INSERT INTO command.

```
# Add the tuple (Samuel Clemens, 1910421, 74.4) to MyTable in my_database.db.
>>> with sql.connect("my_database.db") as conn:
... cur = conn.cursor()
... cur.execute("INSERT INTO MyTable "
... "VALUES('Samuel Clemens', 1910421, 74.4);")
```

With this syntax, SQLite assumes that values match sequentially with the schema of the table. The schema of the table can also be written explicitly for clarity.

ACHTUNG!

Never use Python's string operations to construct a SQL query from variables. Doing so makes the program susceptible to a *SQL injection attack*.^a Instead, use parameter substitution to construct dynamic commands: use a ? character within the command, then provide the sequence of values as a second argument to execute().

```
>>> with sql.connect("my_database.db") as conn:
... cur = conn.cursor()
... values = ('Samuel Clemens', 1910421, 74.4)
... # Don't piece the command together with string operations!
... # cur.execute("INSERT INTO MyTable VALUES " + str(values)) # BAD!
... # Instead, use parameter substitution.
... cur.execute("INSERT INTO MyTable VALUES(?,?,?);", values) # Good.
```

To insert several rows at a time to the same table, use the cursor object's executemany() method and parameter substitution with a list of tuples. This is typically much faster than using execute() repeatedly.

```
# Insert (Samuel Clemens, 1910421, 74.4) and (Jane Doe, 123, 20) to MyTable.
>>> with sql.connect("my_database.db") as conn:
...     cur = conn.cursor()
...     rows = [('John Smith', 456, 40.5), ('Jane Doe', 123, 20)]
...     cur.executemany("INSERT INTO MyTable VALUES(?,?,?);", rows)
```

Problem 2. Expand your function from Problem 1 so that it populates the tables with the data given in Tables 3.2a–3.2d.

MajorID	MajorName
1	Math
2	Science
3	Writing
4	Art

CourseID	CourseName
1	Calculus
2	English
3	Pottery
4	History

(a) MajorInfo

(b) CourseInfo

StudentID	StudentName	MajorID
401767594	Michelle Fernandez	1
678665086	Gilbert Chapman	NULL
553725811	Roberta Cook	2
886308195	Rene Cross	3
103066521	Cameron Kim	4
821568627	Mercedes Hall	NULL
206208438	Kristopher Tran	2
341324754	Cassandra Holland	1
262019426	Alfonso Phelps	NULL
622665098	Sammy Burke	2

(c) StudentInfo

StudentID	CourseID	Grade
401767594	4	С
401767594	3	В–
678665086	4	A+
678665086	3	A+
553725811	2	C
678665086	1	В
886308195	1	A
103066521	2	C
103066521	3	C-
821568627	4	D
821568627	2	A+
821568627	1	В
206208438	2	A
206208438	1	C+
341324754	2	D–
341324754	1	A-
103066521	4	A
262019426	2	В
262019426	3	C
622665098	1	A
622665098	2	A-

(d) StudentGrades

Table 3.2: Student database.

The StudentInfo and StudentGrades tables are also recorded in student_info.csv and student_grades.csv, respectively, with NULL values represented as -1. A CSV (commaseparated values) file can be read like a normal text file or with the csv module.

```
>>> import csv
>>> with open("student_info.csv", 'r') as infile:
... rows = list(csv.reader(infile))
```

To validate your database, use the following command to retrieve the rows from a table.

```
>>> with sql.connect("students.db") as conn:
...     cur = conn.cursor()
...     for row in cur.execute("SELECT * FROM MajorInfo;"):
...         print(row)
(1, 'Math')
(2, 'Science')
(3, 'Writing')
(4, 'Art')
```

Problem 3. The data file us_earthquakes.csv^a contains data from about 3,500 earthquakes in the United States since the 1769. Each row records the year, month, day, hour, minute, second, latitude, longitude, and magnitude of a single earthquake (in that order). Note that latitude, longitude, and magnitude are floats, while the remaining columns are integers.

Write a function that accepts the name of a database file. Drop the table USEarthquakes if it already exists, then create a new USEarthquakes table with schema (Year, Month, Day, Hour, Minute, Second, Latitude, Longitude, Magnitude). Populate the table with the data from us_earthquakes.csv. Remember to commit the changes and close the connection. (Hint: using executemany() is much faster than using execute() in a loop.)

The WHERE Clause

Deleting or altering existing data in a database requires some searching for the desired row or rows. The WHERE clause is a *predicate* that filters the rows based on a boolean condition. The operators ==, !=, <, >, <=, >=, AND, OR, and NOT all work as expected to create search conditions.

```
>>> with sql.connect("my_database.db") as conn:
...     cur = conn.cursor()
...     # Delete any rows where the Age column has a value less than 30.
...     cur.execute("DELETE FROM MyTable WHERE Age < 30;")
...     # Change the Name of "Samuel Clemens" to "Mark Twain".
...     cur.execute("UPDATE MyTable SET Name='Mark Twain' WHERE ID==1910421;")</pre>
```

If the WHERE clause were omitted from either of the previous commands, every record in MyTable would be affected. Always use a very specific WHERE clause when removing or updating data.

Operation	SQLite Command
Add a new row to a table	<pre>INSERT INTO table VALUES(<values>);</values></pre>
Remove rows from a table	DELETE FROM WHERE <condition>;</condition>
Change values in existing rows	<pre>UPDATE SET <column1>=<value1>, WHERE <condition>;</condition></value1></column1></pre>

Table 3.3: SQLite commands for inserting, removing, and updating rows.

Note

SQLite treats = and == as equivalent operators. For clarity, in this lab we will always use == when comparing two values, such as in a WHERE clause. The only time we use = is in SET statements. Be aware that some flavors of SQL (such as MySQL) have no concept of ==, and typing it in a query will return an error.

 $^{{}^}a\mathrm{Retrieved}$ from https://datarepository.wolframcloud.com/resources/Sample-Data-US-Earthquakes.

Problem 4. Modify your function from Problems 1 and 2 so that in the StudentInfo table, values of -1 in the MajorID column are replaced with NULL values.

Also modify your function from Problem 3 in the following ways.

- 1. Remove rows from USEarthquakes that have a value of 0 for the Magnitude.
- 2. Replace 0 values in the Day, Hour, Minute, and Second columns with NULL values.

Reading and Analyzing Data

Constructing and managing databases is fundamental, but most time in SQL is spent analyzing existing data. A query is a SQL command that reads all or part of a database without actually modifying the data. Queries start with the SELECT command, followed by column and table names and additional (optional) conditions. The results of a query, called the result set, are accessed through the cursor object. After calling execute() with a SQL query, use fetchall() or another cursor method from Table 3.4 to get the list of matching tuples.

Method	Description
execute()	Execute a single SQL command
<pre>executemany()</pre>	Execute a single SQL command over different values
<pre>executescript()</pre>	Execute a SQL script (multiple SQL commands)
<pre>fetchone()</pre>	Return a single tuple from the result set
<pre>fetchmany(n)</pre>	Return the next n rows from the result set as a list of tuples
<pre>fetchall()</pre>	Return the entire result set as a list of tuples

Table 3.4: Methods of database cursor objects.

```
>>> conn = sql.connect("students.db")
>>> cur = conn.cursor()
# Get tuples of the form (StudentID, StudentName) from the StudentInfo table.
>>> cur.execute("SELECT StudentID, StudentName FROM StudentInfo;")
>>> cur.fetchone()
                            # List the first match (a tuple).
(401767594, 'Michelle Fernandez')
>>> cur.fetchmany(3)
                           # List the next three matches (a list of tuples).
[(678665086, 'Gilbert Chapman'),
 (553725811, 'Roberta Cook'),
 (886308195, 'Rene Cross')]
>>> cur.fetchall()
                            # List the remaining matches.
[(103066521, 'Cameron Kim'),
 (821568627, 'Mercedes Hall'),
 (206208438, 'Kristopher Tran'),
 (341324754, 'Cassandra Holland'),
 (262019426, 'Alfonso Phelps'),
 (622665098, 'Sammy Burke')]
```

```
# Use * in place of column names to get all of the columns.
>>> cur.execute("SELECT * FROM MajorInfo;").fetchall()
[(1, 'Math'), (2, 'Science'), (3, 'Writing'), (4, 'Art')]
>>> conn.close()
```

The WHERE predicate can also refine a SELECT command. If the condition depends on a column in a different table from the data that is being a selected, create a *table alias* with the AS command to specify columns in the form table.column.

```
>>> conn = sql.connect("students.db")
>>> cur = conn.cursor()
# Get the names of all math majors.
>>> cur.execute("SELECT SI.StudentName "
                "FROM StudentInfo AS SI, MajorInfo AS MI"
                "WHERE SI.MajorID == MI.MajorID AND MI.MajorName == 'Math'")
# The result set is a list of 1-tuples; extract the entry from each tuple.
>>> [t[0] for t in cur.fetchall()]
['Cassandra Holland', 'Michelle Fernandez']
# Get the names and grades of everyone in English class.
>>> cur.execute("SELECT SI.StudentName, SG.Grade "
                "FROM StudentInfo AS SI, StudentGrades AS SG "
                "WHERE SI.StudentID == SG.StudentID AND CourseID == 2;")
>>> cur.fetchall()
[('Roberta Cook', 'C'),
 ('Cameron Kim', 'C'),
 ('Mercedes Hall', 'A+'),
 ('Kristopher Tran', 'A'),
 ('Cassandra Holland', 'D-'),
 ('Alfonso Phelps', 'B'),
 ('Sammy Burke', 'A-')]
>>> conn.close()
```

Problem 5. Write a function that accepts the name of a database file. Assuming the database to be in the format of the one created in Problems 1 and 2, query the database for all tuples of the form (StudentName, CourseName) where that student has an "A" or "A+" grade in that course. Return the list of tuples.

Aggregate Functions

A result set can be analyzed in Python using tools like NumPy, but SQL itself provides a few tools for computing a few very basic statistics: AVG(), MIN(), MAX(), SUM(), and COUNT() are aggregate functions that compress the columns of a result set into the desired quantity.

```
>>> conn = sql.connect("students.db")
>>> cur = conn.cursor()

# Get the number of students and the lowest ID number in StudentInfo.
>>> cur.execute("SELECT COUNT(StudentName), MIN(StudentID) FROM StudentInfo;")
>>> cur.fetchall()
[(10, 103066521)]
```

Problem 6. Write a function that accepts the name of a database file. Assuming the database to be in the format of the one created in Problem 3, query the USEarthquakes table for the following information.

- The magnitudes of the earthquakes during the 19th century (1800–1899).
- The magnitudes of the earthquakes during the 20th century (1900–1999).
- The average magnitude of all earthquakes in the database.

Create a single figure with two subplots: a histogram of the magnitudes of the earthquakes in the 19th century, and a histogram of the magnitudes of the earthquakes in the 20th century. Show the figure, then return the average magnitude of all of the earthquakes in the database. Be sure to return an actual number, not a list or a tuple.

(Hint: use np.ravel() to convert a result set of 1-tuples to a 1-D array.)

Note

Problem 6 raises an interesting question: are the number of earthquakes in the United States increasing with time, and if so, how drastically? A closer look shows that only 3 earthquakes were recorded (in this data set) from 1700–1799, 208 from 1800–1899, and a whopping 3049 from 1900–1999. Is the increase in earthquakes due to there actually being more earthquakes, or to the improvement of earthquake detection technology? The best answer without conducting additional research is "probably both." Be careful to question the nature of your data—how it was gathered, what it may be lacking, what biases or lurking variables might be present—before jumping to strong conclusions.

See the following for more info on the sqlite3 and SQL in general.

- https://docs.python.org/3/library/sqlite3.html
- https://www.w3schools.com/sql/
- https://en.wikipedia.org/wiki/SQL_injection

Additional Material

Shortcuts for WHERE Conditions

Complicated WHERE conditions can be simplified with the following commands.

• IN: check for equality to one of several values quickly, similar to Python's in operator. In other words, the following SQL commands are equivalent.

```
SELECT * FROM StudentInfo WHERE MajorID == 1 OR MajorID == 2;
SELECT * FROM StudentInfo WHERE MajorID IN (1,2);
```

• BETWEEN: check two (inclusive) inequalities quickly. The following are equivalent.

```
SELECT * FROM MyTable WHERE AGE >= 20 AND AGE <= 60;
SELECT * FROM MyTable WHERE AGE BETWEEN 20 AND 60;</pre>
```

4

SQL 2 (The Sequel)

Lab Objective: Since SQL databases contain multiple tables, retrieving information about the data can be complicated. In this lab we discuss joins, grouping, and other advanced SQL query concepts to facilitate rapid data retrieval.

We will use the following database as an example throughout this lab, found in students.db.

MajorID	MajorName
1	Math
2	Science
3	Writing
4	Art

CourseID	CourseName
1	Calculus
2	English
3	Pottery
4	History

(a) MajorInfo

(b) CourseInfo

StudentID	StudentName	MajorID
401767594	Michelle Fernandez	1
678665086	Gilbert Chapman	NULL
553725811	Roberta Cook	2
886308195	Rene Cross	3
103066521	Cameron Kim	4
821568627	Mercedes Hall	NULL
206208438	Kristopher Tran	2
341324754	Cassandra Holland	1
262019426	Alfonso Phelps	NULL
622665098	Sammy Burke	2

(c) StudentInfo

StudentID	CourseID	Grade
401767594	4	С
401767594	3	В–
678665086	4	A+
678665086	3	A+
553725811	2	С
678665086	1	В
886308195	1	A
103066521	2	С
103066521	3	C-
821568627	4	D
821568627	2	A+
821568627	1	В
206208438	2	A
206208438	1	C+
341324754	2	D–
341324754	1	A-
103066521	4	A
262019426	2	В
262019426	3	С
622665098	1	A
622665098	2	A-

(d) StudentGrades

Table 4.1: Student database.

Joining Tables

A *join* combines rows from different tables in a database based on common attributes. In other words, a join operation creates a new, temporary table containing data from 2 or more existing tables. Join commands in SQLite have the following general syntax.

```
SELECT <alias.column, ...>
  FROM  AS <alias> JOIN  AS <alias>, ...
  ON <alias.column> == <alias.column>, ...
  WHERE <condition>;
```

The ON clause tells the query how to join tables together. Typically if there are N tables being joined together, there should be N-1 conditions in the ON clause.

Inner Joins

An *inner join* creates a temporary table with the rows that have exact matches on the attribute(s) specified in the ON clause. Inner joins **intersect** two or more tables, as in Figure 4.1a.

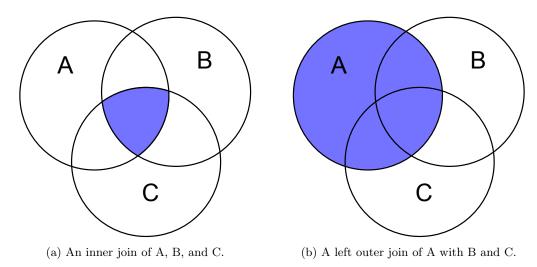


Figure 4.1

For example, Table 4.1c (StudentInfo) and Table 4.1a (MajorInfo) both have a MajorID column, so the tables can be joined by pairing rows that have the same MajorID. Such a join temporarily creates the following table.

StudentID	StudentName	MajorID	MajorID	MajorName
401767594	Michelle Fernandez	1	1	Math
553725811	Roberta Cook	2	2	Science
886308195	Rene Cross	3	3	Writing
103066521	Cameron Kim	4	4	Art
206208438	Kristopher Tran	2	2	Science
341324754	Cassandra Holland	1	1	Math
622665098	Sammy Burke	2	2	Science

Table 4.2: An inner join of StudentInfo and MajorInfo on MajorID.

Notice that this table is missing the rows where MajorID was NULL in the StudentInfo table. This is because there was no match for NULL in the MajorID column of the MajorInfo table, so the inner join throws those rows away.

Because joins deal with multiple tables at once, it is important to assign table aliases with the AS command. Join statements can also be supplemented with WHERE clauses like regular queries.

```
>>> import sqlite3 as sql
>>> conn = sql.connect("students.db")
>>> cur = conn.cursor()
>>> cur.execute("SELECT * "
                "FROM StudentInfo AS SI INNER JOIN MajorInfo AS MI "
. . .
                "ON SI.MajorID == MI.MajorID;").fetchall()
[(401767594, 'Michelle Fernandez', 1, 1, 'Math'),
 (553725811, 'Roberta Cook', 2, 2, 'Science'),
 (886308195, 'Rene Cross', 3, 3, 'Writing'),
 (103066521, 'Cameron Kim', 4, 4, 'Art'),
 (206208438, 'Kristopher Tran', 2, 2, 'Science'),
 (341324754, 'Cassandra Holland', 1, 1, 'Math'),
 (622665098, 'Sammy Burke', 2, 2, 'Science')]
# Select the names and ID numbers of the math majors.
>>> cur.execute("SELECT SI.StudentName, SI.StudentID "
                "FROM StudentInfo AS SI INNER JOIN MajorInfo AS MI "
                "ON SI.MajorID == MI.MajorID "
                "WHERE MI.MajorName == 'Math';").fetchall()
[('Cassandra Holland', 341324754), ('Michelle Fernandez', 401767594)]
```

Problem 1. Write a function that accepts the name of a database file. Assuming the database to be in the format of Tables 4.1a-4.1d, query the database for the list of the names of students who have a B grade in any course (not a B- or a B+). Be sure to return a list of strings, not a list of tuples of strings.

Outer Joins

A *left outer join*, sometimes called a *left join*, creates a temporary table with **all** of the rows from the first (left-most) table, and all the "matched" rows on the given attribute(s) from the other relations. Rows from the left table that don't match up with the columns from the other tables are supplemented with NULL values to fill extra columns. Compare the following table and code to Table 4.2.

StudentID	StudentName	MajorID	MajorID	MajorName
401767594	Michelle Fernandez	1	1	Math
678665086	Gilbert Chapman	NULL	NULL	NULL
553725811	Roberta Cook	2	2	Science
886308195	Rene Cross	3	3	Writing
103066521	Cameron Kim	4	4	Art
821568627	Mercedes Hall	NULL	NULL	NULL
206208438	Kristopher Tran	2	2	Science
341324754	Cassandra Holland	1	1	Math
262019426	Alfonso Phelps	NULL	NULL	NULL
622665098	Sammy Burke	2	2	Science

Table 4.3: A left outer join of StudentInfo and MajorInfo on MajorID.

Some flavors of SQL also support the RIGHT OUTER JOIN command, but sqlite3 does not recognize the command since T1 RIGHT OUTER JOIN T2 is equivalent to T2 LEFT OUTER JOIN T1.

Joining Multiple Tables

Complicated queries often join several different relations. If the same kind of join is being used, the relations and conditional statements can be put in list form. For example, the following code selects courses that Kristopher Tran has taken, and the grades that he got in those courses, by joining three tables together. Note that 2 conditions are required in the ON clause in this case.

To use different kinds of joins in a single query, append one join statement after another. The join closest to the beginning of the statement is executed first, creating a temporary table, and the next join attempts to operate on that table. The following example performs an additional join on Table 4.3 to find the name and major of every student who got a C in a class.

In this last example, note carefully that Alfonso Phelps would have been excluded from the result set if an inner join was performed first instead of an outer join (since he lacks a major).

Problem 2. Write a function that accepts the name of a database file. Query the database for all tuples of the form (Name, MajorName, Grade) where Name is a student's name and Grade is their grade in Calculus. Only include results for students that are actually taking Calculus, but be careful not to exclude students who haven't declared a major.

Grouping Data

Many data sets can be naturally sorted into groups. The GROUP BY command gathers rows from a table and groups them by a certain attribute. The groups are then combined by one of the aggregate functions AVG(), MIN(), MAX(), SUM(), or COUNT(). Each of these functions accepts the name of the column to be operated on. Note that the first four of these require the column to hold numerical data. Since our database has no such data, we will delay examples of using the functions other than COUNT() until later.

The following code groups the rows in Table 4.1d by studentID and counts the number of entries in each group.

GROUP BY can also be used in conjunction with joins. The join creates a temporary table like Tables 4.2 or 4.3, the results of which can then be grouped.

Just like the WHERE clause chooses rows in a relation, the HAVING clause chooses groups from the result of a GROUP BY based on some criteria related to the groupings. For this particular command, it is often useful (but not always necessary) to create an alias for the columns of the result set with the AS operator. For instance, the result set of the previous example can be filtered down to only contain students who are taking 3 courses.

```
>>> cur.execute("SELECT SI.StudentName, COUNT(*) as num_courses "
                                                                     # Alias.
                "FROM StudentGrades AS SG INNER JOIN StudentInfo AS SI "
                "ON SG.StudentID == SI.StudentID "
                "GROUP BY SG.StudentID "
                "HAVING num_courses == 3;").fetchall()
                                                         # Refer to alias later←
[('Cameron Kim', 3), ('Gilbert Chapman', 3), ('Mercedes Hall', 3)]
# Alternatively, get just the student names.
>>> cur.execute("SELECT SI.StudentName "
                                                                     # No alias.
                "FROM StudentGrades AS SG INNER JOIN StudentInfo AS SI "
                "ON SG.StudentID == SI.StudentID "
                "GROUP BY SG.StudentID "
                "HAVING COUNT(*) == 3;").fetchall()
[('Cameron Kim',), ('Gilbert Chapman',), ('Mercedes Hall',)]
```

Problem 3. Write a function that accepts a database file. Query the database for the list of the names of courses that have at least 5 student enrolled in them. Be sure to return a list of strings.

Other Miscellaneous Commands

Ordering Result Sets

The ORDER BY command sorts a result set by one or more attributes. Sorting can be done in ascending or descending order with ASC or DESC, respectively. This is always the very last statement in a query.

```
>>> cur.execute("SELECT SI.StudentName, COUNT(*) AS num_courses "
                                                                    # Alias.
                "FROM StudentGrades AS SG INNER JOIN StudentInfo AS SI "
                "ON SG.StudentID == SI.StudentID "
                "GROUP BY SG.StudentID "
. . .
                "ORDER BY num_courses DESC, SI.StudentName ASC;").fetchall()
[('Cameron Kim', 3),
                                   # The results are now ordered by the
                                # number of courses each student is in,
 ('Gilbert Chapman', 3),
 ('Mercedes Hall', 3),
                                   # then alphabetically by student name.
 ('Alfonso Phelps', 2),
 ('Cassandra Holland', 2),
 ('Kristopher Tran', 2),
 ('Michelle Fernandez', 2),
 ('Sammy Burke', 2),
 ('Rene Cross', 1),
 ('Roberta Cook', 1)]
```

Problem 4. Write a function that accepts a database file. Query the given database for tuples of the form (MajorName, N) where N is the number of students in the specified major. Sort the results in descending order by the count N, and then in alphabetic order by MajorName. Include **Null** majors.

Searching Text with Wildcards

The LIKE operator within a WHERE clause matches patterns in a TEXT column. The special characters % and _ and called *wildcards* that match any number of characters or a single character, respectively. For instance, %Z_ matches any string of characters ending in a Z then another character, and %i% matches any string containing the letter i.

Problem 5. Write a function that accepts a database file. Query the database for tuples of the form (StudentName, MajorName) where the last name of the specified student begins with the letter C. Include **Null** majors.

Case Expressions

A case expression maps the values in a column using boolean logic. There are two forms of a case expression: simple and searched. A *simple case expression* matches and replaces specified attributes.

```
# Replace the values MajorID with new custom values.
>>> cur.execute("SELECT StudentName, CASE MajorID "
                    "WHEN 1 THEN 'Mathematics' "
                    "WHEN 2 THEN 'Soft Science' "
                    "WHEN 3 THEN 'Writing and Editing' "
                    "WHEN 4 THEN 'Fine Arts' "
                    "ELSE 'Undeclared' END "
                "FROM StudentInfo "
                "ORDER BY StudentName ASC;").fetchall()
[('Alfonso Phelps', 'Undeclared'),
 ('Cameron Kim', 'Fine Arts'),
 ('Cassandra Holland', 'Mathematics'),
 ('Gilbert Chapman', 'Undeclared'),
 ('Kristopher Tran', 'Soft Science'),
 ('Mercedes Hall', 'Undeclared'),
 ('Michelle Fernandez', 'Mathematics'),
 ('Rene Cross', 'Writing and Editing'),
 ('Roberta Cook', 'Soft Science'),
 ('Sammy Burke', 'Soft Science')]
```

A searched case expression involves using a boolean expression at each step, instead of listing all of the possible values for an attribute.

```
# Change NULL values in MajorID to 'Undeclared' and non-NULL to 'Declared'.
>>> cur.execute("SELECT StudentName, CASE "
                    "WHEN MajorID IS NULL THEN 'Undeclared' "
                    "ELSE 'Declared' END "
                "FROM StudentInfo "
. . .
                "ORDER BY StudentName ASC;").fetchall()
[('Alfonso Phelps', 'Undeclared'),
 ('Cameron Kim', 'Declared'),
 ('Cassandra Holland', 'Declared'),
 ('Gilbert Chapman', 'Undeclared'),
 ('Kristopher Tran', 'Declared'),
 ('Mercedes Hall', 'Undeclared'),
 ('Michelle Fernandez', 'Declared'),
 ('Rene Cross', 'Declared'),
 ('Roberta Cook', 'Declared'),
 ('Sammy Burke', 'Declared')]
```

Chaining Queries

The result set of any SQL query is really just another table with data from the original database. Separate queries can be made from result sets by enclosing the entire query in parentheses. For these sorts of operations, it is very important to carefully label the columns resulting from a subquery.

Subqueries can also be joined with other tables, as in the following example. Note also that a subquery can be used to create numerical data out of non-numerical data, which can then be passed into any of the aggregate functions.

```
# Find the proportion of classes each student has an A+, A, or A- in.
# The inner query creates a column 'gradeisa' which is 1 if the student's grade
    is A+, A, or A-, and O otherwise.
>>> cur.execute("SELECT SI.StudentName, AVG(SG.gradeisa) "
                "FROM ("
                    "SELECT StudentID, CASE Grade "
                        "WHEN 'A+' THEN 1 "
                        "WHEN 'A' THEN 1 "
                        "WHEN 'A-' THEN 1 "
                        "ELSE 0 END AS gradeisa "
                    "FROM StudentGrades) AS SG "
                "INNER JOIN StudentInfo AS SI "
                "ON SG.StudentID == SI.StudentID "
                "GROUP BY SG.StudentID;").fetchall()
[('Cameron Kim', 0.3333333333333333),
 ('Kristopher Tran', 0.5),
 ('Alfonso Phelps', 0.0),
 ('Cassandra Holland', 0.5),
 ('Michelle Fernandez', 0.0),
 ('Roberta Cook', 0.0),
 ('Sammy Burke', 1.0),
 ('Gilbert Chapman', 0.66666666666666),
 ('Mercedes Hall', 0.333333333333333),
 ('Rene Cross', 1.0)]
```

Problem 6. Write a function that accepts the name of a database file. Query the database for tuples of the form (StudentName, N, GPA) where N is the number of courses that the specified student is enrolled in and GPA is their grade point average based on the following point system:

Order the results from greatest GPA to least.

5

Regular Expressions

Lab Objective: Cleaning and formatting data are fundamental problems in data science. Regular expressions are an important tool for working with text carefully and efficiently, and are useful for both gathering and cleaning data. This lab introduces regular expression syntax and common practices, including an application to a data cleaning problem.

A regular expression or regex is a string of characters that follows a certain syntax to specify a pattern. Strings that follow the pattern are said to match the expression (and vice versa). A single regular expression can match a large set of strings, such as the set of all valid email addresses.

ACHTUNG!

There are some universal standards for regular expression syntax, but the exact syntax varies slightly depending on the program or language. However, the syntax presented in this lab (for Python) is sufficiently similar to any other regex system. Consider learning to use regular expressions in Vim or your favorite text editor, keeping in mind that there will be slight syntactic differences from what is presented here.

Regular Expression Syntax in Python

The re module implements regular expressions in Python. The function re.compile() takes in a regular expression string and returns a corresponding *pattern* object, which has methods for determining if and how other strings match the pattern. For example, the search() method returns None for a string that doesn't match, and a *match* object for a string that does.

Note the match() method for pattern objects only matches strings that satisfy the pattern at the beginning of the string. To answer the question "does any part of my target string match this regular expression?" always use the search() method.

```
>>> import re
>>> pattern = re.compile("cat")  # Make a pattern object for finding 'cat'.
>>> bool(pattern.search("cat"))  # 'cat' matches 'cat', of course.
True
>>> bool(pattern.match("catfish"))  # 'catfish' starts with 'cat'.
```

```
True
>>> bool(pattern.match("fishcat")) # 'fishcat' doesn't start with 'cat'.
False
>>> bool(pattern.search("fishcat")) # but it does contain 'cat'.
True
>>> bool(pattern.search("hat")) # 'hat' does not contain 'cat'.
False
```

Most of the functions in the re module are shortcuts for compiling a pattern object and calling one of its methods. Using re.compile() is good practice because the resulting object is reusable, while each call to re.search() compiles a new (but redundant) pattern object. For example, the following lines of code are equivalent.

```
>>> bool(re.compile("cat").search("catfish"))
True
>>> bool(re.search("cat", "catfish"))
True
```

Problem 1. Write a function that compiles and returns a regular expression pattern object with the pattern string "python".

Literal Characters and Metacharacters

The following string characters (separated by spaces) are metacharacters in Python's regular expressions, meaning they have special significance in a pattern string: . * * + ? { } [] \ | ().

A regular expression that matches strings with one or more metacharacters requires two things.

- 1. Use raw strings instead of regular Python strings by prefacing the string with an r, such as r"cat". The resulting string interprets backslashes as actual backslash characters, rather than the start of an escape sequence like \n or \t.
- 2. Preface any metacharacters with a backslash to indicate a literal character. For example, to match the string "\$3.99? Thanks.", use r"\\$3\.99\? Thanks\.".

Without raw strings, every backslash in has to be written as a double backslash, which makes many regular expression patterns hard to read ("\\\$3\\.99\\? Thanks\\.").

Problem 2. Write a function that compiles and returns a regular expression pattern object that matches the string " $\{0\}(?)[\%]\{.\}(*)[_]\{\&\}$ ".

Hint: There are online sites like https://regex101.com/ that can help you check your answers.

The regular expressions of Problems 1 and 2 only match strings that are or include the exact pattern. The metacharacters allow regular expressions to have much more flexibility and control so that a single pattern can match a wide variety of strings, or a very specific set of strings. The line anchor metacharacters ^ and \$ are used to match the start and the end of a line of text, respectively. This shrinks the matching set, even when using the search() method instead of the match() method. For example, the only single-line string that the expression '^x\$' matches is 'x', whereas the expression 'x' can match any string with an 'x' in it.

The pipe character | is a logical OR in a regular expression: A|B matches A or B. The parentheses () create a group in a regular expression. A group establishes an order of operations in an expression. For example, in the regex "^one|two fish\$", precedence is given to the invisible string concatenation between "two" and "fish", while "^(one|two) fish\$" gives precedence to the '|' metacharacter. Notice that the pipe is inside the group.

```
>>> fish = re.compile(r"^(one|two) fish$")
>>> for test in ["one fish", "two fish", "red fish", "one two fish"]:
... print(test + ':', bool(fish.search(test)))
...
one fish: True
two fish: True
red fish: False
one two fish: False
```

Problem 3. Write a function that compiles and returns a regular expression pattern object that matches the following strings, and no other strings, even with re.search().

```
"Book store" "Mattress store" "Grocery store"
"Book supplier" "Mattress supplier" "Grocery supplier"
```

Character Classes

The hard bracket metacharacters [and] are used to create *character classes*, a part of a regular expression that can match a variety of characters. For example, the pattern [abc] matches any of the characters a, b, or c. This is different than a group delimited by parentheses: a group can match multiple characters, while a character class matches only one character. For instance, [abc] does not match ab or abc, and (abc) matches abc but not ab or even a.

Within character classes, there are two additional metacharacters. When ^ appears as the first character in a character class, right after the opening bracket [, the character class matches anything not specified instead. In other words, ^ is the set complement operation on the character class. Additionally, the dash - specifies a range of values. For instance, [0-9] matches any digit, and [a-z] matches any lowercase letter. Thus [^0-9] matches any character except for a digit, and [^a-z] matches any character except for lowercase letters. Keep in mind that the dash -, when at the beginning or end of the character class, will match the literal '-'. Note that [0-27-9] acts like [(0-2)|(7-9)].

```
>>> p1, p2 = re.compile(r"^[a-z][^0-7]$"), re.compile(r"^[^abcA-C][0-27-9]$")
>>> for test in ["d8", "aa", "E9", "EE", "d88"]:
... print(test + ':', bool(p1.search(test)), bool(p2.search(test)))
```

There are also a variety of shortcuts that represent common character classes, listed in Table 5.1. Familiarity with these shortcuts makes some regular expressions significantly more readable.

Character	Description
\b	Matches the empty string, but only at the start or end of a word.
\s	Matches any whitespace character; equivalent to [\t\n\r\f\v].
\S	Matches any non-whitespace character; equivalent to [^\s].
\d	Matches any decimal digit; equivalent to [0-9].
\ D	Matches any non-digit character; equivalent to [^\d].
\w	Matches any alphanumeric character; equivalent to [a-zA-Z0-9_].
\W	Matches any non-alphanumeric character; equivalent to [^\w].

Table 5.1: Character class shortcuts.

Any of the character class shortcuts can be used within other custom character classes. For example, <code>[_A-Z\s]</code> matches an underscore, capital letter, or whitespace character.

Finally, a period . matches **any** character except for a line break. This is a very powerful metacharacter; be careful to only use it when part of the regular expression really should match **any** character.

```
# Match any three-character string with a digit in the middle.
>>> pattern = re.compile(r"^.\d.$")
>>> for test in ["a0b", "888", "n2%", "abc", "cat"]:
        print(test + ':', bool(pattern.search(test)))
a0b: True
888: True
n2%: True
abc: False
cat: False
# Match two letters followed by a number and two non-newline characters.
>>> pattern = re.compile(r"^[a-zA-Z][a-zA-Z]\d..$")
>>> for test in ["tk421", "bb8!?", "JB007", "Boba?"]:
        print(test + ':', bool(pattern.search(test)))
tk421: True
bb8!?: True
JB007: True
Boba?: False
```

The following table is a useful recap of some common regular expression metacharacters.

Character	Description
	Matches any character except a newline.
^	Matches the start of the string.
\$	Matches the end of the string or just before the newline at the end of the string.
1	A B creates an regular expression that will match either A or B.
[]	Indicates a set of characters. A ^ as the first character indicates a complementing set.
()	Matches the regular expression inside the parentheses.
	The contents can be retrieved or matched later in the string.

Table 5.2: Standard regular expression metacharacters in Python.

Repetition

The remaining metacharacters are for matching a specified number of characters. This allows a single regular expression to match strings of varying lengths.

Character	Description
*	Matches 0 or more repetitions of the preceding regular expression.
+	Matches 1 or more repetitions of the preceding regular expression.
?	Matches 0 or 1 of the preceding regular expression.
$\{m,n\}$	Matches from m to n repetitions of the preceding regular expression.
*?, +?, ??, {m,n}?	Non-greedy versions of the previous four special characters.

Table 5.3: Repetition metacharacters for regular expressions in Python.

Each of the repetition operators acts on the expression immediately preceding it. This could be a single character, a group, or a character class. For instance, (abc)+ matches abc, abcabc, abcabcabc, and so on, but not aba or cba. On the other hand, [abc]* matches any sequence of a, b, and c, including abcabc and aabbcc.

The curly braces $\{\}$ specify a custom number of repetitions allowed. $\{,n\}$ matches **up to** n instances, $\{m,\}$ matches **at least** m instances, $\{k\}$ matches **exactly** k instances, and $\{m,n\}$ matches from m to n instances. Thus the ? operator is equivalent to $\{,1\}$ and + is equivalent to $\{1,\}$.

Be aware that line anchors are especially important when using repetition operators. Consider the following (bad) example and compare it to the previous example.

```
# Match exactly 3 'a' characters, hopefully.
```

The unexpected matches occur because "aaa" is at the beginning of each of the test strings. With the line anchors ^ and \$, the search truly only matches the exact string "aaa".

Problem 4. A valid Python identifier (a valid variable name) is any string starting with an alphabetic character or an underscore, followed by any (possibly empty) sequence of alphanumeric characters and underscores.

A valid python parameter definition is defined as the concatenation of the following strings:

- any valid python identifier
- any number of spaces
- (optional) an equals sign followed by any number of spaces and ending with one of the following: any real number, a single quote followed by any number of non-single-quote characters followed by a single quote, or any valid python identifier

Define a function that compiles and returns a regular expression pattern object that matches any valid Python parameter definition.

(Hint: Use the \w character class shortcut to keep your regular expression clean.)

To help in debugging, the following examples may be useful. These test cases are a good start, but are not exhaustive. The first table should match valid Python identifiers. The second should match a valid python parameter definition, as defined in this problem. Note that some strings which would be valid in python will not be for this problem.

```
        Matches:
        "Mouse"
        "compile"
        "_123456789"
        "__x__"
        "while"

        Non-matches:
        "3rats"
        "err*r"
        "sq(x)"
        "sleep()"
        " x"

        Matches:
        "max=4.2"
        "string= ''"
        "num_guesses"

        Non-matches:
        "300"
        "is_4=(value==4)"
        "pattern = r'^one|two fish$'"
```

Manipulating Text with Regular Expressions

So far we have been solely concerned with whether or not a regular expression and a string match, but the power of regular expressions comes with what can be done with a match. In addition to the search() method, regular expression pattern objects have the following useful methods.

Method	Description
match()	Match a regular expression pattern to the beginning of a string.
<pre>fullmatch()</pre>	Match a regular expression pattern to all of a string.
search()	Search a string for the presence of a pattern.
sub()	Substitute occurrences of a pattern found in a string.
subn()	Same as sub, but also return the number of substitutions made.
split()	Split a string by the occurrences of a pattern.
<pre>findall()</pre>	Find all occurrences of a pattern in a string.
<pre>finditer()</pre>	Return an iterator yielding a match object for each match.

Table 5.4: Methods of regular expression pattern objects.

Some substitutions require remembering part of the text that the regular expression matches. Groups are useful here: each group in the regular expression can be represented in the substitution string by n, where n is an integer (starting at 1) specifying which group to use.

```
# Find words that start with 'cat', remembering what comes after the 'cat'.
>>> pig_latin = re.compile(r"\bcat(\w*)")
>>> target = "Let's catch some catfish for the cat"

>>> pig_latin.sub(r"at\1clay", target) # \1 = (\w*) from the expression.
"Let's atchclay some atfishclay for the atclay"
```

The repetition operators ?, +, *, and $\{m,n\}$ are greedy, meaning that they match the largest string possible. On the other hand, the operators ??, +?, *?, and $\{m,n\}$? are non-greedy, meaning they match the smallest strings possible. This is very often the desired behavior for a regular expression.

```
>>> target = "<abc> <def> <ghi>"

# Match angle brackets and anything in between.
>>> greedy = re.compile(r"^<.*>$") # Greedy *
>>> greedy.findall(target)
['<abc> <def> <ghi>'] # The entire string matched!

# Try again, using the non-greedy version.
>>> nongreedy = re.compile(r"<.*?>")# Non-greedy *?
>>> nongreedy.findall(target)
['<abc>', '<def>', '<ghi>'] # Each <> set is an individual match.
```

Finally, there are a few customizations that make searching larger texts manageable. Each of these *flags* can be used as keyword arguments to re.compile().

Flag	Description
re.DOTALL	. matches any character at all, including the newline.
re.IGNORECASE	Perform case-insensitive matching.
re.MULTILINE	^ matches the beginning of lines (after a newline) as well as the string;
	\$ matches the end of lines (before a newline) as well as the end of the string.

Table 5.5: Regular expression flags.

A benefit of using 'a' and '\$' is that they allow you to search across multiple lines. For example, how would we match "World" in the string "Hello\nWorld"? Using re.MULTILINE in the re.search function will allow us to match at the beginning of each new line, instead of just the beginning of the string. The following shows how to implement multiline searching:

```
>>>pattern1 = re.compile("^W")
>>>pattern2 = re.compile("^W", re.MULTILINE)
>>>bool(pattern1.search("Hello\nWorld"))
False
>>>bool(pattern2.search("Hello\nWorld"))
True
```

Problem 5. A Python *block* is composed of several lines of code with the same indentation level. Blocks are delimited by key words and expressions, followed by a colon. Possible key words are if, elif, else, for, while, try, except, finally, with, def, and class. Some of these keywords require an expression to precede the colon (if, elif, for, etc.). Some require no expressions to precede the colon (else, finally), and except may or may not have an expression before the colon.

Write a function that accepts a string of Python code and uses regular expressions to place colons in the appropriate spots. Assume that every colon is missing in the input string. Return the string of code with colons in the correct places.

```
k, i, p = 999, 1, 0
while k > i
    i *= 2
    p += 1
    if k != 999
        print("k should not have changed")
        pass
print(p)
0.00
# The string given above should become this string.
k, i, p = 999, 1, 0
while k > i:
    i *= 2
    p += 1
    if k != 999:
        print("k should not have changed")
    else:
        pass
print(p)
```

Extracting Text with Regular Expressions

Regular expressions are useful for locating and extracting information that matches a certain format. The method pattern.findall(string) returns a list containing all non-overlapping matches of pattern found in string. The method scans the string from left to right and returns the matches in that order. If two matches overlap, the match that begins first is returned.

When at least one group, indicated by (), is present in the pattern, then only information contained in a group is returned. Each match is returned as a tuple containing the part of the string that matches each group in the pattern.

```
>>> pattern = re.compile("\w* fish")

# Without any groups, the entirety of each match is returned.
>>> pattern.findall("red fish, blue fish, one fish, two fish")
['red fish', 'blue fish', 'one fish', 'two fish']

# When a group is present, only information contained in a group is returned.
>>> pattern2 = re.compile("(\w*) (fish|dish)")
>>> pattern2.findall("red dish, blue dish, one fish, two fish")
[('red', 'dish'), ('blue', 'dish'), ('one', 'fish'), ('two', 'fish')]
```

If you wish to extract the characters that match some groups, but not others, you can choose to exclude a group from being returned using the syntax (?:)

```
>>> pattern = re.compile("(\w*) (?:fish|dish)")
>>> pattern.findall("red dish, blue dish, one fish, two fish")
['red', 'blue', 'one', 'two']
```

Problem 6. The file fake_contacts.txt contains poorly formatted contact data for 2000 fictitious individuals. Each line of the file contains data for one person, including their name and possibly their birthday, email address, and/or phone number. The formatting of the data is not consistent, and much of it is missing. Each contact name includes a first and last name. Some names have middle initials, in the form Jane C. Doe. Each birthday lists the month, then the day, and then the year, though the format varies from 1/1/11, 1/01/2011, etc. If century is not specified for birth year, as in 1/01/XX, birth year is assumed to be 20XX. Remember, not all information is listed for each contact.

Use regular expressions to extract the necessary data and format it uniformly, writing birthdays as mm/dd/yyyy and phone numbers as (xxx)xxx-xxxx. Return a dictionary where the key is the name of an individual and the value is another dictionary containing their information. Each of these inner dictionaries should have the keys "birthday", "email", and "phone". In the case of missing data, map the key to None.

The first two entries of the completed dictionary are given below.

```
{
    "John Doe": {
        "birthday": "01/01/2099",
        "email": "john_doe90@hopefullynotarealaddress.com",
        "phone": "(123)456-7890"
        },
    "Jane Smith": {
        "birthday": None,
        "email": None,
        "phone": "(222)111-3333"
        },
# ...
}
```

Additional Material

Regular Expressions in the Unix Shell

As we have seen,, regular expressions are very useful when we want to match patterns. Regular expressions can be used when matching patterns in the Unix Shell. Though there are many Unix commands that take advantage of regular expressions, we will focus on grep and awk.

Regular Expressions and grep

Recall from Lab 1 that grep is used to match patterns in files or output. It turns out we can use regular expressions to define the pattern we wish to match.

In general, we use the following syntax:

```
$ grep 'regexp' filename
```

We can also use regular expressions when piping output to grep.

```
# List details of directories within current directory.
$ ls -l | grep ^d
```

Regular Expressions and awk

By incorporating regular expressions, the awk command becomes much more robust. Before GUI spreedsheet programs like Microsoft Excel, awk was commonly used to visualize and query data from a file.

Including if statements inside awk commands gives us the ability to perform actions on lines that match a given pattern. The following example prints the filenames of all files that are owned by freddy.

```
$ ls -l | awk ' {if ($3 ~ /freddy/) print $9} '
```

Because there is a lot going on in this command, we will break it down piece-by-piece. The output of 1s -1 is getting piped to awk. Then we have an if statement. The syntax here means if the condition inside the parenthesis holds, print field 9 (the field with the filename). The condition is where we use regular expressions. The ~ checks to see if the contents of field 3 (the field with the username) matches the regular expression found inside the forward slashes. To clarify, freddy is the regular expression in this example and the expression must be surrounded by forward slashes.

Consider a similar example. In this example, we will list the names of the directories inside the current directory. (This replicates the behavior of the Unix command ls -d */)

```
$ ls -l | awk ' {if ($1 ~ /^d/) print $9} '
```

Notice in this example, we printed the names of the directories, whereas in one of the example using grep, we printed all the details of the directories as well.

ACHTUNG!

Some of the definitions for character classes we used earlier in this lab will not work in the Unix Shell. For example, \w and \d are not defined. Instead of \w, use [[:alnum:]]. Instead of \d, use [[:digit:]]. For a complete list of similar character classes, search the internet for POSIX Character Classes or Bracket Character Classes.

6

Web Technologies

Lab Objective: The Internet is a term for the collective grouping of all publicly accessible computer networks in the world. This network can be traversed to access services such as social communication, maps, video streaming, and large datasets, all of which are hosted on computers across the world. Using these technologies requires an understanding of data serialization, data transportation protocols, and how programs such as servers, clients, and APIs are created to facilitate this communication.

Data Serialization

Serialization is the process of packaging data in a form that makes it easy to transmit the data and quickly reconstruct it on another computer or in a different programming language. Many serialization metalanguages exist, such as Python's pickle, YAML, XML, and JSON. JSON, which stands for JavaScript Object Notation, is the dominant format for serialization in web applications. Despite having "JavaScript" in its name, JSON is a language-independent format and is frequently used for transmitting data between different programming languages. It stores information about objects as a specially formatted string that is easy for both humans and machines to read and write. Description is the process of reconstructing an object from the string.

JSON is built on two types of data structures: a collection of key/value pairs similar to Python's built-in dict, and an ordered list of values similar to Python's built-in list.

```
{
                                     # A family's info written in JSON format.
    "lastname": "Smith".
                                     # The outer dictionary has two keys:
    "children": [
                                     # "lastname" and "children".
        {
                                     # The "children" key maps to a list of
            "name": "Timmy",
                                     # two dictionaries, one for each of the
            "age": 8
                                     # two children.
        },
        {
            "name": "Missy",
            "age": 5
        }
```

Note

To see a longer example of what JSON looks like, try opening a Jupyter Notebook (a .ipynb file) in a plain text editor. The file lists the Notebook cells, each of which has attributes like "cell_type" (usually code or markdown) and "source" (the actual code in the cell).

The JSON libraries of various languages have a fairly standard interface. The Python standard library module for JSON is called json. If performance speed is critical, consider using the ujson or simplejson modules that are written in C. A string written in JSON format that represents a piece of data is called a JSON message. The json.dumps() function generates the JSON message for a single Python object, which can be stored and used within the Python program. Alternatively, the json encoder json.dump() generates the same object, but writes it directly to a file. To load a JSON string or file, use the json decoder json.loads() or json.load(), respectively.

```
>>> import json
# Store info about a car in a nested dictionary.
>>> my_car = {
       "car": {
            "make": "Ford".
            "color": [255, 30, 30] },
        "owner": "me" }
# Get the JSON message corresponding to my_car.
>>> car_str = json.dumps(my_car)
>>> car_str
'{"car": {"make": "Ford", "color": [255, 30, 30]}, "owner": "me"}'
# Load the JSON message into a Python object, reconstructing my_car.
>>> car_object = json.loads(car_str)
>>> for key in car_object:
                                    # The loaded object is a dictionary.
        print(key + ':', car_object[key])
car: {'make': 'Ford', 'color': [255, 30, 30]}
owner: me
# Write the car info to an external file.
>>> with open("my_car.json", 'w') as outfile:
        json.dump(my_car, outfile)
. . .
# Read the file to check that it saved correctly.
>>> with open("my_car.json", 'r') as infile:
        new_car = json.load(infile)
>>> print(new_car.keys())
                                    # This loaded object is also a dictionary.
dict_keys(['car', 'owner'])
```

Problem 1. The file nyc_traffic.json contains information about 1000 traffic accidents in New York City during the summer of 2017.^a Each entry lists one or more reasons for the accident, such as "Unsafe Speed" or "Fell Asleep."

Write a function that loads the data from the JSON file. Make a readable, sorted bar chart showing the total number of times that each of the 7 most common reasons for accidents are listed in the data set.

(Hint: the collections.Counter data structure and use plt.tight_layout() may be useful here.)

To check your work, the 6th most common reason is "Backing Unsafely," listed 59 times.

Custom Encoders and Decoders for JSON

The default JSON encoder and decoder do not support serialization for every kind of data structure. For example, a **set** cannot be serialized using only **json** functions. However, the default JSON encoder can be subclassed to handle sets or custom data structures. A custom encoder must organize the information in an object as nested lists and dictionaries. The corresponding custom decoder uses the way that the encoder organizes the information to reconstruct the original object.

For example, one way to serialize a **set** is to express it as a dictionary with one key that indicates its data type, and another key mapping to the actual data.

```
>>> class SetEncoder(json.JSONEncoder):
        """A custom JSON encoder for Python sets."""
        def default(self, obj):
            if not isinstance(obj, set):
                raise TypeError("expected a set for encoding")
            return {"dtype": "set", "data": list(obj)}
# Use the custom encoder to convert a set to its custom JSON message.
>>> set_message = json.dumps(set('abca'), cls=SetEncoder)
>>> set_message
'{"dtype": "set", "data": ["a", "b", "c"]}'
# Define a custom decoder for JSON messages generated by the SetEncoder.
>>> def set_decoder(item):
        if "dtype" in item:
            if item["dtype"] != "set" or "data" not in item:
                raise ValueError("expected a JSON message from SetEncoder")
            return set(item["data"])
        raise ValueError("expected a JSON message from SetEncoder")
# Use the custom decoder to convert a JSON message to the original object.
>>> json.loads(set_message, object_hook=set_decoder)
{'a', 'b', 'c'}
```

 $[^]a\mathrm{See}$ https://opendata.cityofnewyork.us/.

It is good practice to check for errors to ensure that custom encoders and decoders are only used when intended.

Problem 2. The following class facilitates a regular 3×3 game of tic-tac-toe, where the boxes in the board have the following coordinates.

Write a custom encoder and decoder for the TicTacToe class. If the custom encoder receives anything other than a TicTacToe object, raise a TypeError.

```
class TicTacToe:
   def __init__(self):
        """Initialize an empty board. The O's go first."""
        self.board = [[' ']*3 for _ in range(3)]
        self.turn, self.winner = "0", None
    def move(self, i, j):
        """Mark an O or X in the (i,j)th box and check for a winner."""
        if self.winner is not None:
           raise ValueError("the game is over!")
        elif self.board[i][j] != ' ':
           raise ValueError("space ({},{}) already taken".format(i,j))
        self.board[i][j] = self.turn
        # Determine if the game is over.
        b = self.board
        if any(sum(s == self.turn for s in r)==3 for r in b):
            self.winner = self.turn # 3 in a row.
        elif any(sum(r[i] == self.turn for r in b)==3 for i in range(3)):
            self.winner = self.turn # 3 in a column.
        elif b[0][0] == b[1][1] == b[2][2] == self.turn:
                                      # 3 in a diagonal.
            self.winner = self.turn
        elif b[0][2] == b[1][1] == b[2][0] == self.turn:
            self.winner = self.turn
                                       # 3 in a diagonal.
        else:
            self.turn = "0" if self.turn == "X" else "X"
    def empty_spaces(self):
        """Return the list of coordinates for the empty boxes."""
        return [(i,j) for i in range(3) for j in range(3)
                                       if self.board[i][j] == ' ' ]
    def __str__(self):
        return "\n----\n".join(" | ".join(r) for r in self.board)
```

Servers and Clients

The Internet has specific protocols that allow for standardized communication within and between computers. The most common communication protocols in computer networks are contained in the Internet Protocol Suite. Among these is *Transmission Control Protocol* (TCP), which is used to establish a connection between two computers, exchange bits of information called *packets*, and then close the connection. TCP creates the connection via network *socket* objects that are used to send and receive data packets from a computer.

Essentially, this can be thought of as a PO box at a post office. The socket is like a PO box owned by a particular program, which checks it periodically for updates. The computer can be thought of as the post office which houses the PO boxes. PO boxes, or sockets, can send mail to each other within the same post office, or computer, easily, but more work is needed when the PO boxes send mail to each other from one post office, or computer, to another.

A server is a program that interacts with and provides functionality to client programs. This can be thought of as the PO box which sends the mail. A *client* program contacts a server to receive some sort of response that assists it in fulfilling its function. This can be thought of as the PO box which receives the mail. Unlike with physical mail, in which the sender can send mail to himself, a socket being used as a server in a computer cannot also serve as a client at the same time. Servers are fundamental to modern networks and provide services such as file sharing, authentication, webpage information, databases, etc.

Creating a Server

One simple way to create a server in Python is via the **socket** module. The server socket must first be initialized by specifying the type of connection and the address at which clients can find the server. The server socket then listens and waits for a connection from a client, receives and processes data, and eventually sends a response back to the client. After exchanges between the server and the client are finished, the server closes the connection to the client.

Name	Description
socket	Create a new socket using the given address family, socket type and protocol number.
bind	Bind the socket to an address. The socket must not already be bound.
listen	Enable a server to accept connections.
accept	Accept a connection. Must be bound to an address and listening for connections.
connect	Connect to a remote socket at address.
sendall	Send data to the socket. The socket must be connected to a remote socket.
	Continues to send data until either all data has been sent or an error occurs.
recv	Receive data from the socket. Must be given a buffer size; use 1024.
close	Mark the socket closed.

Table 6.1: Socket method descriptions

The socket.socket() method receives two parameters, which specify the socket type. The server address is a (host, port) tuple. The host is the IP address, which in this case is "localhost" or "0.0.0.0"—the default address that specifies the local machine and allows connections on all interfaces. The port number is an integer from 0 to 65535. About 250 port numbers are commonly used, and certain ports have pre-defined uses. Only use port numbers greater than 1023 to avoid interrupting standard system services, such as email and system updates.

After setting up the server socket, the server program waits for a client to connect. The accept() method returns a new socket object and the client's address. Data is received through the connection socket's recv() method, which takes an integer specifying the number of bits of data to receive. The data is transferred as a raw byte stream (of type bytes), so the decode() method is necessary to translate the data into a string. Likewise, data that is sent back to the client through the connection socket's sendall() method must be encoded into a byte stream via the encode() method.

Finally, try-finally blocks in the server ensure that the connection is always closed securely. Put these blocks within an infinite while(True) block to ensure that your server will be ready for any client request. Note that the accept() method does not return until a connection is made with a client. Therefore, this server program cannot be executed in its entirety without a client. To stop a server, raise a KeyBoardInterrupt (press ctrl+c) in the terminal where it is running.

Note that server-client communication is the reason that JSON serialization and descrialization is so important. For example, information such as an image or a family tree could be sent more simply using serialized objects.

```
def mirror_server(server_address=("0.0.0.0", 33333)):
    """A server for reflecting strings back to clients in reverse order."""
   print("Starting mirror server on {}".format(server_address))
    # Specify the socket type, which determines how clients will connect.
    server_sock = socket.socket(socket.AF_INET, socket.SOCK_STREAM)
    server_sock.bind(server_address)
                                         # Assign this socket to an address.
    server_sock.listen(1)
                                         # Start listening for clients.
    while True:
        # Wait for a client to connect to the server.
        print("\nWaiting for a connection...")
        connection, client_address = server_sock.accept()
        try:
            # Receive data from the client.
            print("Connection accepted from {}.".format(client_address))
            in_data = connection.recv(1024).decode()
                                                          # Receive data.
            print("Received '{}' from client".format(in_data))
            # Process the received data and send something back to the client.
            out_data = in_data[::-1]
            print("Sending '{}' back to the client".format(out_data))
            connection.sendall(out_data.encode())
                                                          # Send data.
        finally:
                    # Make sure the connection is closed securely.
            connection.close()
            print("Closing connection from {}".format(client_address))
```

ACHTUNG!

It often takes some time for a computer to reopen a port after closing a server connection. This is due to the timeout functionality of specific protocols that check connections for errors and disruptions. While testing code, wait a few seconds before running the program again, or use different ports for each test.

Problem 3. Write a function that accepts a (host, port) tuple and starts up a tic-tac-toe server at the specified location. Wait to accept a connection, then while the connection is open, repeat the following operations.

- 1. Receive a JSON serialized TicTacToe object (serialized with your custom encoder from Problem 2) from the client.
- 2. Deserialize the TicTacToe object using your custom decoder from Problem 2.
- 3. If the client has just won the game, send "WIN" back to the client and close the connection.
- 4. If there is no winner but board is full, send "DRAW" to the client and close the connection.
- 5. If the game still isn't over, make a random move on the tic-tac-toe board and serialize the updated TicTacToe object. If this move wins the game, send "LOSE" to the client, then send the serialized object separately (as proof), and close the connection. Otherwise, send only the updated TicTacToe object back to the client but keep the connection open.

(Hint: print information at each step so you can see what the server is doing.)

Ensure that the connection closes securely even if an exception is raised. Note that you will not be able to fully test your server until you have written a client (see Problem 4).

Creating a Client

The socket module also has tools for writing client programs. First, create a socket object with the same settings as the server socket, then call the connect() method with the server address as a parameter. Once the client socket is connected to the server socket, the two sockets can transfer information between themselves.

Unlike the server socket, the client socket sends and reads the data itself instead of creating a new connection socket. When the client program is complete, close the client socket. The server will keep running, waiting for another client to serve.

To see a client and server communicate, open a terminal and run the server. Then run the client in a separate terminal. Try this with the provided examples.

```
def mirror_client(server_address=("0.0.0.0", 33333)):
    """A client program for mirror_server()."""
    print("Attempting to connect to server at {}...".format(server_address))

# Set up the socket to be the same type as the server.
```

```
client_sock = socket.socket(socket.AF_INET, socket.SOCK_STREAM)
    client_sock.connect(server_address)  # Attempt to connect to the server.

# Send some data from the client user to the server.

out_data = input("Type a message to send to the server: ")
    client_sock.sendall(out_data.encode())  # Send data.

# Wait to receive a response back from the server.

in_data = client_sock.recv(1024).decode()  # Receive data.

print("Received '{}' from the server".format(in_data))

# Close the client socket.

client_sock.close()
```

Problem 4. Write a client function that accepts a (host, port) tuple and connects to the tictac-toe server at the specified location. Start by initializing a new TicTacToe object, then repeat the following steps until the game is over.

- 1. Print the board and prompt the player for a move. Continue prompting the player until they provide valid input.
- 2. Update the board with the player's move, then serialize it using your custom encoder from Problem 2, and send the serialized version to the server.
- 3. Receive a response from the server. If the game is over, congratulate or mock the player appropriately. If the player lost, receive a second response from the server (the final game board), deserialize it, and print it out.

Close the connection once the game ends.

APIs

An Application Program Interface (API) is a particular kind of server that listens for requests from authorized users and responds with data. For example, a list of locations can be sent with the proper request syntax to a Google Maps API, and it will respond with the calculated driving time from start to end, including each location. Every API has endpoints where clients send their requests. Though standards exist for creating and communicating with APIs, most APIs have a unique syntax for authentication and requests that is documented by the organization providing the service.

The requests module is the standard way to send a download request to an API in Python.

```
>>> import requests
>>> requests.get(endpoint).json()  # Download and extract the data.
```

ACHTUNG!

Each website and API has a policy that specifies appropriate behavior for automated data retrieval and usage. If data is requested without complying with these requirements, there can be severe legal consequences. Most websites detail their policies in a file called *robots.txt* on their main page. See, for example, https://www.google.com/robots.txt.

Additional Material

Other Internet Protocols

There are many protocols in the Internet Protocol Suite other than TCP that are used for different purposes. The Protocol Suite can be divided into four categorical layers:

- 1. **Application**: Software that utilizes transport protocols to move information between computers. This layer includes protocols important for email, file transfers, and browsing the web.
- 2. **Transport**: Protocols that assist in basic high level communication between two computers in areas such as data-streaming, reliability control, and flow control.
- 3. **Internet**: Protocols that handle routing, assignment of addresses, and movement of data on a network.
- 4. Link: Protocols that communicate with local networking hardware such as routers and switches.

Although these examples are simple, every data transfer with TCP follows a similar pattern. For basic connections, these interactions are simple processes. However, requesting a webpage would require management of possibly hundreds of connections. In order to make this more feasible, there are higher level protocols that handle smaller TCP/IP details. The most predominant of these protocols is HTTP.

HTTP

HTTP stands for Hypertext Transfer Protocol, which is an application layer networking protocol. It is a higher level protocol than TCP but uses TCP protocols to manage connections and provide network capabilities. The protocol is centered around a request and response paradigm in which a client makes a request to a server and the server replies with response. There are several methods, or requests, defined for HTTP servers, the three most common of which are GET, POST, and PUT. GET requests request information from a server, POST requests modify the state of the server, and PUT requests add new pieces of data to the server.

Every HTTP request or response consists of two parts: a header and a body. The headers contain important information about the request including: the type of request, encoding, and a timestamp. Custom headers may be added to any request to provide additional information. The body of the request or response contains the appropriate data or may be empty.

An HTTP connection can be setup in Python by using the standard Python library http. Though it is the standard, the process can be greatly simplified by using an additional library called requests. The following demonstrates a simple GET request with the http library.

```
>>> import http
>>> conn = http.client.HTTPConnection("www.example.net") # Establish connection
>>> conn.request("GET", "/") # Send GET request
>>> resp = conn.getresponse() # Server response message
>>> print(resp.status)
200 # A status of 200 is the standard sign for successful communication
>>> print(resp.getheaders())
[('Cache-Control', 'max-age=604800'), ..., ('Content-Length', '1270')] # 
Header information about request
>>> print(resp.read())
```

```
b'<!doctype html>\n<html> ... n</html>\n'  # Long string with HTML from ←
  webpage
>>> conn.close() # When the request is finished, the connection is closed
```

As previously mentioned, this exchange is greatly simplified by the requests library:

```
>>> import requests
>>> r = requests.get("http://www.example.net")
>>> print(r.headers)
{'Cache-Control': 'max-age=604800', ..., 'Content-Length': '606'}
>>> print(r.content)
b'<!doctype html>\n<html> ... n</html>\n'
```

This process is how a web browser (a client program) retrieves a webpage. It first sends an HTTP request to the web server (a server program) and receives the HTML, CSS, and other code files for a webpage, which are compiled and run in the web browser.

Requests also often include parameters which are keys to tell the server what is being requested or placed. These parameters can be included in the URL that requests from the server, or in parameters that the requests library can implement. For example:

```
>>> r = requests.get("http://httpbin.org/get?key2=value2&key1=value1")
>>> print(r.text)
  "args": {
    "key1": "value1",
    "key2": "value2"
 },
 },
  "origin": "128.187.116.7",
  "url": "http://httpbin.org/get?key2=value2&key1=value1"
>>> r = requests.get("http://httpbin.org/get", params={'key1':'value1','key2':'
   value2'})
>>> print(r.url)
http://httpbin.org/get?key2=value2&key1=value1
>>> print(r.text)
  "args": {
    "key1": "value1",
    "key2": "value2"
  },
  "origin": "128.187.116.7",
  "url": "http://httpbin.org/get?key2=value2&key1=value1"
}
```

A similar format to GET requests can also be used for PUT or POST requests. These special requests alter the state of the server or send a piece of data to the server, respectively. In addition, for PUT and POST requests, a data string or dictionary may be sent as a binary stream attachment. The requests library attaches these data objects with the data parameter. For example:

Note that the data parameter accepts input in the form of a JSON string.

Frequently, when these requests arrive at the server, they are in the form of a binary stream, which can be read with similar notation to the Python open function. Below is an example of reading the previous PUT request with a data attachment as a binary stream using read.

```
>>> data = r.json()['data'] # Retrieve the sent data string
>>> print(data)
   '{key1:value1,key2:value2}'
>>> print(len(data.encode())) # Show the string's length in bytes
25
>>> with open('request.txt', 'w') as file:
>>> file.write(data) # Write the string to a file
>>> with open('request.txt', 'rb') as file: # Open the file as a binary stream
>>> file.read(25) # Read the correct number of bytes
b'{key1:value1,key2:value2}'
```

For more information on the requests library, see the documentation at http://docs.python-requests.org/.

7

Web Scraping

Lab Objective: Web Scraping is the process of gathering data from websites on the internet. Since almost everything rendered by an internet browser as a web page uses HTML, the first step in web scraping is being able to extract information from HTML. In this lab, we introduce the requests library for scraping web pages, and BeautifulSoup, Python's canonical tool for efficiently and cleanly navigating and parsing HTML.

HTTP and Requests

HTTP stands for Hypertext Transfer Protocol, which is an application layer networking protocol. It is a higher level protocol than TCP, which we used to build a server in the Web Technologies lab, but uses TCP protocols to manage connections and provide network capabilities. The HTTP protocol is centered around a request and response paradigm, in which a client makes a request to a server and the server replies with a response. There are several methods, or requests, defined for HTTP servers, the three most common of which are GET, POST, and PUT. A GET request asks for information from the server, a POST request modifies the state of the server, and a PUT request adds new pieces of data to the server.

The standard way to get the source code of a website using Python is via the requests library.¹ Calling requests.get() sends an HTTP GET request to a specified website. The website returns a response code, which indicates whether or not the request was received, understood, and accepted. If the response code is good, typically 200², then the response will also include the website source code as an HTML file.

```
>>> import requests

# Make a request and check the result. A status code of 200 is good.
>>> response = requests.get("http://www.byu.edu")
>>> print(response.status_code, response.ok, response.reason)
200 True OK
```

¹Though requests is not part of the standard library, it is recognized as a standard tool in the data science community. See http://docs.python-requests.org/.

²See https://en.wikipedia.org/wiki/List_of_HTTP_status_codes for explanation of specific response codes.

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Note that some websites aren't built to handle large amounts of traffic or many repeated requests. Most are built to identify web scrapers or crawlers that initiate many consecutive GET requests without pauses, and retaliate or block them. When web scraping, always make sure to store the data that you receive in a file and include error checks to prevent retrieving the same data unnecessarily. We won't spend much time on that in this lab, but it's especially important in larger applications.

Problem 1. Use the requests library to get the HTML source for the website http://www.example.com. Save the source as a file called example.html. If the file already exists, make sure not to scrape the website or overwrite the file. You will use this file later in the lab.

ACHTUNG!

Scraping copyrighted information without the consent of the copyright owner can have severe legal consequences. Many websites, in their terms and conditions, prohibit scraping parts or all of the site. Websites that do allow scraping usually have a file called robots.txt (for example, www.google.com/robots.txt) that specifies which parts of the website are off-limits and how often requests can be made according to the robots exclusion standard.^a

Be careful and considerate when doing any sort of scraping, and take care when writing and testing code to avoid unintended behavior. It is up to the programmer to create a scraper that respects the rules found in the terms and conditions and in ${\tt robots.txt.}^b$

We will cover this more in the next lab.

 $[^]a\mathrm{See}$ www.robotstxt.org/orig.html and en.wikipedia.org/wiki/Robots_exclusion_standard.

^bPython provides a parsing library called urllib.robotparser for reading robot.txt files. For more information, see https://docs.python.org/3/library/urllib.robotparser.html.

HTML

Hyper Text Markup Language, or HTML, is the standard markup language—a language designed for the processing, definition, and presentation of text—for creating webpages. It structures a document using pairs of tags that surround and define content. Opening tags have a tag name surrounded by angle brackets (<tag-name>). The companion closing tag looks the same, but with a forward slash before the tag name (</tag-name>). A list of all current HTML tags can be found at http://htmldog.com/reference/htmltags.

Most tags can be combined with *attributes* to include more data about the content, help identify individual tags, and make navigating the document much simpler. In the following example, the <a>a> tag has id and href attributes.

In HTML, href stands for *hypertext reference*, a link to another website. Thus the above example would be rendered by a browser as a single line of text, with here being a clickable link to http://www.example.com:

Click here for more information.

Unlike Python, HTML does not enforce indentation (or any whitespace rules), though indentation generally makes HTML more readable. The previous example can be written in a single line.

```
<html><body>Click <a id='info' href='http://www.example.com/info'>here</a>
for more information.</body></html>
```

Special tags, which don't contain any text or other tags, are written without a closing tag and in a single pair of brackets. A forward slash is included between the name and the closing bracket. Examples of these include <hr/> , which describes a horizontal line, and , the tag for representing an image.

Note

You can open .html files using a text editor or any web browser. In a browser, you can inspect the source code associated with specific elements. Right click the element and select Inspect. If you are using Safari, you may first need to enable "Show Develop menu" in "Preferences" under the "Advanced" tab.

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BeautifulSoup

BeautifulSoup (bs4) is a package³ that makes it simple to navigate and extract data from HTML documents. See http://www.crummy.com/software/BeautifulSoup/bs4/doc/index.html for the full documentation.

The bs4.BeautifulSoup class accepts two parameters to its constructor: a string of HTML code and an HTML parser to use under the hood. The HTML parser is technically a keyword argument, but the constructor prints a warning if one is not specified. The standard choice for the parser is "html.parser", which means the object uses the standard library's html.parser module as the engine behind the scenes.

Note

Depending on project demands, a parser other than "html.parser" may be useful. A couple of other options are "lxml", an extremely fast parser written in C, and "html5lib", a slower parser that treats HTML in much the same way a web browser does, allowing for irregularities. Both must be installed independently; see https://www.crummy.com/software/BeautifulSoup/bs4/doc/#installing-a-parser for more information.

A BeautifulSoup object represents an HTML document as a tree. In the tree, each tag is a node with nested tags and strings as its *children*. The prettify() method returns a string that can be printed to represent the BeautifulSoup object in a readable format that reflects the tree structure.

```
>>> from bs4 import BeautifulSoup
>>> small_example_html = """
<html><body>
    Click <a id='info' href='http://www.example.com'>here</a>
    for more information.
</body></html>
>>> small_soup = BeautifulSoup(small_example_html, 'html.parser')
>>> print(small_soup.prettify())
<html>
  <body>
    >
      <a href="http://www.example.com" id="info">
         here
      </a>
      for more information.
    </body>
</html>
```

³BeautifulSoup is not part of the standard library; install it with conda install beautifulsoup4 or with pip install beautifulsoup4.

Each tag in a BeautifulSoup object's HTML code is stored as a bs4.element.Tag object, with actual text stored as a bs4.element.NavigableString object. Tags are accessible directly through the BeautifulSoup object.

```
# Get the  tag (and everything inside of it).
>>> small_soup.p

    Click <a href="http://www.example.com" id="info">here</a>
    for more information.

# Get the <a> sub-tag of the  tag.
>>> a_tag = small_soup.p.a
>>> print(a_tag, type(a_tag), sep='\n')
<a href="http://www.example.com" id="info">here</a>
</class 'bs4.element.Tag'>

# Get just the name, attributes, and text of the <a> tag.
>>> print(a_tag.name, a_tag.attrs, a_tag.string, sep="\n")
a
{'id': 'info', 'href': 'http://www.example.com'}
here
```

Attribute	Description
name	The name of the tag
attrs	A dictionary of the attributes
string	The single string contained in the tag
strings	Generator for strings of children tags
stripped_strings	Generator for strings of children tags, stripping whitespace
text	Concatenation of strings from all children tags

Table 7.1: Data attributes of the bs4.element.Tag class.

Problem 2. The BeautifulSoup class has a find_all() method that, when called with True as the only argument, returns a list of all tags in the HTML source code.

Write a function that accepts a string of HTML code as an argument. Use BeautifulSoup to return a list of the **names** of the tags in the code.

Navigating the Tree Structure

Not all tags are easily accessible from a BeautifulSoup object. Consider the following example.

```
>>> pig_html = """
<html><head><title>Three Little Pigs</title></head>
```

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```
<body>
class="title"><b>The Three Little Pigs</b>

cp class="story">Once upon a time, there were three little pigs named
<a href="http://example.com/larry" class="pig" id="link1">Larry,</a>
<a href="http://example.com/mo" class="pig" id="link2">Mo</a>, and
<a href="http://example.com/curly" class="pig" id="link3">Curly.</a>
The three pigs had an odd fascination with experimental construction.

</body></html>
"""

>>> pig_soup = BeautifulSoup(pig_html, "html.parser")
>>> pig_soup.p
 class="title"><b>The Three Little Pigs</b>
>>> pig_soup.a
<a class="pig" href="http://example.com/larry" id="link1">Larry,</a>
```

Since the HTML in this example has several and <a> tags, only the first tag of each name is accessible directly from pig_soup. The other tags can be accessed by manually navigating through the HTML tree.

Every HTML tag (except for the topmost tag, which is usually <html>) has a parent tag. Each tag also has zero or more sibling and children tags or text. Following a true tree structure, every bs4.element.Tag in a soup has multiple attributes for accessing or iterating through parent, sibling, or child tags.

Attribute	Description
parent	The parent tag
parents	Generator for the parent tags up to the top level
next_sibling	The tag immediately after to the current tag
next_siblings	Generator for sibling tags after the current tag
<pre>previous_sibling</pre>	The tag immediately before the current tag
previous_siblings	Generator for sibling tags before the current tag
contents	A list of the immediate children tags
children	Generator for immediate children tags
descendants	Generator for all children tags (recursively)

Table 7.2: Navigation attributes of the bs4.element.Tag class.

```
# Start at the first <a> tag in the soup.
>>> a_tag = pig_soup.a
>>> a_tag
<a class="pig" href="http://example.com/larry" id="link1">Larry,</a>

# Get the names of all of <a>'s parent tags, traveling up to the top.
# The name '[document]' means it is the top of the HTML code.
>>> [par.name for par in a_tag.parents]  # <a>'s parent is , whose
['p', 'body', 'html', '[document]']  # parent is <body>, and so on.
```

Note carefully that newline characters are considered to be children of a parent tag. Therefore iterating through children or siblings often requires checking which entries are tags and which are just text. In the next example, we use a tag's attrs attribute to access specific attributes within the tag (see Table 7.1).

```
# Get to the  tag that has class="story" using these commands.
>>> p_tag = pig_soup.body.p.next_sibling.next_sibling
>>> p_tag.attrs["class"]  # Make sure it's the right tag.
['story']

# Iterate through the child tags of  and print hrefs whenever they exist.
>>> for child in p_tag.children:
...  # Skip the children that are not bs4.element.Tag objects
...  # These don't have the attribute "attrs"
...  if hasattr(child, "attrs") and "href" in child.attrs:
...  print(child.attrs["href"])
http://example.com/larry
http://example.com/mo
http://example.com/curly
```

Note that the "class" attribute of the tag is a list. This is because the "class" attribute can take on several values at once; for example, the tag is of class 'story' and of class 'book'.

The behavior of the string attribute of a bs4.element.Tag object depends on the structure of the corresponding HTML tag.

- 1. If the tag has a string of text and no other child elements, then string is just that text.
- 2. If the tag has exactly one child tag and the child tag has only a string of text, then the tag has the same string as its child tag.
- 3. If the tag has more than one child, then string is None. In this case, use strings to iterate through the child strings. Alternatively, the get_text() method returns all text belonging to a tag and to all of its descendants. In other words, it returns anything inside a tag that isn't another tag.

```
>>> pig_soup.head
<head><title>Three Little Pigs</title></head>

# Case 1: the <title> tag's only child is a string.
>>> pig_soup.head.title.string
'Three Little Pigs'
```

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```
# Case 2: The <head> tag's only child is the <title> tag.
>>> pig_soup.head.string
'Three Little Pigs'

# Case 3: the <body> tag has several children.
>>> pig_soup.body.string is None
True
>>> print(pig_soup.body.get_text().strip())
The Three Little Pigs
Once upon a time, there were three little pigs named
Larry,
Mo, and
Curly.
The three pigs had an odd fascination with experimental construction.
...
```

Problem 3. Write a function that reads a file of the same format as the output from Problem 1 and loads it into BeautifulSoup. Find the first <a> tag, and return its text along with a boolean value indicating whether or not it has a hyperlink (href attribute).

Searching for Tags

Navigating the HTML tree manually can be helpful for gathering data out of lists or tables, but these kinds of structures are usually buried deep in the tree. The find() and find_all() methods of the BeautifulSoup class identify tags that have distinctive characteristics, making it much easier to jump straight to a desired location in the HTML code. The find() method only returns the first tag that matches a given criteria, while find_all() returns a list of all matching tags. Tags can be matched by name, attributes, and/or text.

Problem 4. The file san_diego_weather.html contains the HTML source for an old page from Weather Underground.^a Write a function that reads the file and loads it into Beautiful-Soup.

Return a list of the following tags:

- 1. The tag containing the date "Thursday, January 1, 2015".
- 2. The tags which contain the links "Previous Day" and "Next Day."
- 3. The tag which contains the number associated with the Actual Max Temperature.

 $^a See \quad \texttt{http://www.wunderground.com/history/airport/KSAN/2015/1/1/DailyHistory.html?req_city=San+Diego\&req_state=CA\&req_statename=California\&reqdb.zip=92101\&reqdb.magic=1\&reqdb.wmo=99999\&MR=1$

Advanced Search Techniques: Regular Expressions

Consider the problem of finding the tag that is a link to the URL http://example.com/curly.

```
>>> pig_soup.find(href="http://example.com/curly")
<a class="pig" href="http://example.com/curly" id="link3">Curly.</a>
```

This approach works, but it requires entering in the entire URL. To perform generalized searches, the find() and find_all() method also accept compiled regular expressions from the re module. This way, the methods locate tags whose name, attributes, and/or string matches a pattern.

```
# Find the first tag with an href attribute containing 'curly'.
>>> pig_soup.find(href=re.compile(r"curly"))
<a class="pig" href="http://example.com/curly" id="link3">Curly.</a

# Find the first tag with a string that starts with 'Cu'.
>>> pig_soup.find(string=re.compile(r"^Cu")).parent
<a class="pig" href="http://example.com/curly" id="link3">Curly.</a>

# Find all tags with text containing 'Three'.
>>> [tag.parent for tag in pig_soup.find_all(string=re.compile(r"Three"))]
[<title>Three Little Pigs</tib>]
```

Finally, to find a tag that has a particular attribute, regardless of the actual value of the attribute, use True in place of search values.

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```
# Find all tags with an 'id' attribute.
>>> pig_soup.find_all(id=True)
[<a class="pig" href="http://example.com/larry" id="link1">Larry,</a>,
        <a class="pig" href="http://example.com/mo" id="link2">Mo</a>,
        <a class="pig" href="http://example.com/curly" id="link3">Curly.</a>]

# Find the names all tags WITHOUT an 'id' attribute.
>>> [tag.name for tag in pig_soup.find_all(id=False)]
['html', 'head', 'title', 'body', 'p', 'b', 'p', 'p', 'p']
```

Advanced Search Techniques: CSS Selectors

BeautifulSoup also supports the use of CSS selectors. CSS (Cascading Style Sheet) describes the style and layout of a webpage, and CSS selectors provide a useful way to navigate HTML code. Use the method soup.select() to find all elements matching an argument. The general format for an argument is tag-name[attribute-name = 'attribute value']. The table below lists symbols you can use to more precisely locate various elements.

Symbol	Meaning
=	Matches an attribute value exactly
*=	Partially matches an attribute value
^=	Matches the beginning of an attribute value
\$=	Matches the end of an attribute value
+	Next sibling of matching element
>	Search an element's children

Table 7.3: CSS symbols for use with Selenium

You can do many other useful things with CSS selectors. A helpful guide can be found at https://www.w3schools.com/cssref/css_selectors.asp. The code below gives an example using arguments described above.

```
# Find all <a> tags with id="link1"
>>> pig_soup.select("[id='link1']")
[<a class="pig" href="http://example.com/larry" id="link1">Larry,</a>]

# Find all tags with an href attribute containing 'curly'.
>>> pig_soup.select("[href*='curly']")
[<a class="pig" href="http://example.com/curly" id="link3">Curly.</a>]

# Find all <a> tags with an href attribute
>>> pig_soup.select("a[href]")
[<a class="pig" href="http://example.com/larry" id="link1">Larry,</a>,
<a class="pig" href="http://example.com/mo" id="link2">Mo</a>,
<a class="pig" href="http://example.com/curly" id="link3">Curly.</a>]

# Find all <b> tags within a  tag with class='title'
```

```
>>> pig_soup.select("p[class='title'] b")
[<b>The Three Little Pigs</b>]

# Use a comma to find elements matching one of two arguments
>>> pig_soup.select("a[href$='mo'],[id='link3']")
[<a class="pig" href="http://example.com/mo" id="link2">Mo</a>,
<a class="pig" href="http://example.com/curly" id="link3">Curly.</a>]
```

Problem 5. The file large_banks_index.html is an index of data about large banks, as recorded by the Federal Reserve.^a Write a function that reads the file and loads the source into BeautifulSoup. Return a list of the tags containing the links to bank data from September 30, 2003 to December 31, 2014, where the dates are in reverse chronological order.

^aSee https://www.federalreserve.gov/releases/lbr/.

Problem 6. The file large_banks_data.html is one of the pages from the index in Problem 5.^a Write a function that reads the file and loads the source into BeautifulSoup. Create a single figure with two subplots:

- 1. A sorted bar chart of the seven banks with the most domestic branches.
- 2. A sorted bar chart of the seven banks with the most foreign branches.

In the case of a tie, sort the banks alphabetically by name.

 $^a\mathrm{See}$ http://www.federalreserve.gov/releases/lbr/20030930/default.htm.

8

Web Crawling

Lab Objective: Gathering data from the internet often requires information from several web pages. In this lab, we present two methods for crawling through multiple web pages without violating copyright laws or straining the load on a server. We also demonstrate how to scrape data from asynchronously loaded web pages and how to interact programmatically with web pages when needed.

Scraping Etiquette

There are two main ways that web scraping can be problematic for a website owner.

- 1. The scraper doesn't respect the website's terms and conditions or gathers private or proprietary data.
- 2. The scraper imposes too much extra server load by making requests too often or in quick succession.

These are extremely important considerations in any web scraping program. Scraping copyrighted information without the consent of the copyright owner can have severe legal consequences. Many websites, in their terms and conditions, prohibit scraping parts or all of the site. Websites that do allow scraping usually have a file called robots.txt (for example, www.google.com/robots.txt) that specifies which parts of the website are off-limits, and how often requests can be made according to the robots exclusion standard.¹

ACHTUNG!

Be careful and considerate when doing any sort of scraping, and take care when writing and testing code to avoid unintended behavior. It is up to the programmer to create a scraper that respects the rules found in the terms and conditions and in robots.txt. Make sure to scrape websites legally.

Recall that consecutive requests without pauses can strain a website's server and provoke retaliation. Most servers are designed to identify such scrapers, block their access, and sometimes even blacklist the user. This is especially common in smaller websites that aren't built to handle enormous amounts of traffic. To briefly pause the program between requests, use time.sleep().

¹See www.robotstxt.org/orig.html and en.wikipedia.org/wiki/Robots_exclusion_standard.

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```
>>> import time
>>> time.sleep(3)  # Pause execution for 3 seconds.
```

The amount of necessary wait time depends on the website. Sometimes, robots.txt contains a Crawl-delay directive which gives a number of seconds to wait between successive requests. If this doesn't exist, pausing for a half-second to a second between requests is typically sufficient. An email to the site's webmaster is always the safest approach and may be necessary for large scraping operations.

Python provides a parsing library called urllib.robotparser for reading robot.txt files. Below is an example of using this library to check where robots are allowed on arxiv.org. A website's robots.txt file will often include different instructions for specific crawlers. These crawlers are identified by a User-agent string. For example, Google's webcrawler, User-agent Googlebot, may be directed to index only the pages the website wants to have listed on a Google search. We will use the default User-agent, "*".

```
>>> from urllib import robotparser
>>> rp = robotparser.RobotFileParser()
# Set the URL for the robots.txt file. Note that the URL contains `robots.txt'
>>> rp.set_url("https://arxiv.org/robots.txt")
>>> rp.read()
# Request the crawl-delay time for the default User-agent
>>> rp.crawl_delay("*")
15
# Check if User-agent "*" can access the page
>>> rp.can_fetch("*", "https://arxiv.org/archive/math/")
True
>>> rp.can_fetch("*", "https://arxiv.org/IgnoreMe/")
False
```

Problem 1. Write a program that accepts a web address defaulting to the site http://example.webscraping.com and a list of pages defaulting to ["/", "/trap", "/places/default/search"]. For each page, check if the robots.txt file permits access. Return a list of boolean values corresponding to each page. Also return the crawl delay time.

Crawling Through Multiple Pages

While web *scraping* refers to the actual gathering of web-based data, web *crawling* refers to the navigation of a program between webpages. Web crawling allows a program to gather related data from multiple web pages and websites.

Consider books.toscrape.com, a site to practice web scraping that mimics a bookstore. The page http://books.toscrape.com/catalogue/category/books/mystery_3/index.html lists mystery books with overall ratings and review. More mystery books can be accessed by clicking on the next link. The following example demonstrates how to navigate between webpages to collect all of the mystery book titles.

```
def scrape_books(start_page = "index.html"):
    """ Crawl through http://books.toscrape.com and extract mystery titles"""
    # Initialize variables, including a regex for finding the 'next' link.
   base_url="http://books.toscrape.com/catalogue/category/books/mystery_3/"
   titles = \Pi
   page = base_url + start_page
                                               # Complete page URL.
   next_page_finder = re.compile(r"next")
                                               # We need this button.
   current = None
   for _ in range(4):
       while current == None: # Try downloading until it works.
           # Download the page source and PAUSE before continuing.
           page_source = requests.get(page).text
                               # PAUSE before continuing.
           time.sleep(1)
           soup = BeautifulSoup(page_source, "html.parser")
           current = soup.find_all(class_="product_pod")
       # Navigate to the correct tag and extract title
       for book in current:
           titles.append(book.h3.a["title"])
       # Find the URL for the page with the next data.
       if "page-4" not in page:
           new_page = soup.find(string=next_page_finder).parent["href"]
           page = base_url + new_page # New complete page URL.
           current = None
    return titles
```

In this example, the for loop cycles through the pages of books, and the while loop ensures that each website page loads properly: if the downloaded page_source doesn't have a tag whose class is product_pod, the request is sent again. After recording all of the titles, the function locates the link to the next page. This link is stored in the HTML as a relative website path (page-2.html); the complete URL to the next day's page is the concatenation of the base URL http://books.toscrape.com/catalogue/category/books/mystery_3/ with this relative link.

Problem 2. Modify scrape_books() so that it gathers the price for each fiction book and returns the mean price, in \mathcal{L} , of a fiction book.

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Asynchronously Loaded Content and User Interaction

Web crawling with the methods presented in the previous section fails under a few circumstances. First, many webpages use JavaScript, the standard client-side scripting language for the web, to load portions of their content asynchronously. This means that at least some of the content isn't initially accessible through the page's source code (for example, if you have to scroll down to load more results). Second, some pages require user interaction, such as clicking buttons which aren't links (<a> tags which contain a URL that can be loaded) or entering text into form fields (like search bars).

The Selenium framework provides a solution to both of these problems. Originally developed for writing unit tests for web applications, Selenium allows a program to open a web browser and interact with it in the same way that a human user would, including clicking and typing. It also has BeautifulSoup-esque tools for searching the HTML source of the current page.

Note

Selenium requires an executable *driver* file for each kind of browser. The following examples use Google Chrome, but Selenium supports Firefox, Internet Explorer, Safari, Opera, and PhantomJS (a special browser without a user interface). See https://seleniumhq.github.io/selenium/docs/api/py or http://selenium-python.readthedocs.io/installation.html for installation instructions and driver download instructions.

If your program still can't find the driver after you've downloaded it, add the argument executable_path = "path/to/driver/file" when you call webdriver. If this doesn't work, you may need to add the location to your system PATH. On a Mac, open the file /etc/path and add the new location. On Linux, add export PATH="path/to/driver/file:\$PATH" to the file /.bashrc . For Windows, follow a tutorial such as this one: https://www.architectryan.com/2018/03/17/add-to-the-path-on-windows-10/.

To use Selenium, start up a browser using one of the drivers in selenium.webdriver. The browser has a get() method for going to different web pages, a page_source attribute containing the HTML source of the current page, and a close() method to exit the browser.

```
<meta content="text/html; charset=utf-8" http-equiv="Content-type"/>
# ...
>>> browser.close() # Close the browser.
```

Selenium can deliver the HTML page source to BeautifulSoup, but it also has its own tools for finding tags in the HTML.

Method	Returns
<pre>find_element_by_tag_name()</pre>	The first tag with the given name
<pre>find_element_by_name()</pre>	The first tag with the specified name attribute
<pre>find_element_by_class_name()</pre>	The first tag with the given class attribute
<pre>find_element_by_id()</pre>	The first tag with the given id attribute
<pre>find_element_by_link_text()</pre>	The first tag with a matching href attribute
<pre>find_element_by_partial_link_text()</pre>	The first tag with a partially matching href attribute

Table 8.1: Methods of the selenium.webdriver.Chrome class.

Each of the find_element_by_*() methods returns a single object representing a web element (of type selenium.webdriver.remote.webelement.WebElement), much like a BeautifulSoup tag (of type bs4.element.Tag). If no such element can be found, a Selenium NoSuchElementException is raised. If you want to find more than just the first matching object, each webdriver also has several find_elements_by_*() methods (elements, plural) that return a list of all matching elements, or an empty list if there are no matches.

Web element objects have methods that allow the program to interact with them: click() sends a click, send_keys() enters in text, and clear() deletes existing text. This functionality makes it possible for Selenium to interact with a website in the same way that a human would. For example, the following code opens up https://www.google.com, types "Python Selenium Docs" into the search bar, and hits enter.

```
>>> from selenium.webdriver.common.keys import Keys
>>> from selenium.common.exceptions import NoSuchElementException
>>> browser = webdriver.Chrome()
        browser.get("https://www.google.com")
            # Get the search bar, type in some text, and press Enter.
            search_bar = browser.find_element_by_name('q')
            search_bar.clear()
                                                 # Clear any pre-set text.
            search_bar.send_keys("Python Selenium Docs")
            search_bar.send_keys(Keys.RETURN)
                                                # Press Enter.
        except NoSuchElementException:
            print("Could not find the search bar!")
            raise
... finally:
        browser.close()
. . .
```

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Problem 3. The website IMDB contains a variety of information on movies. Specifically, information on the top 10 box office movies of the week can be found at https://www.imdb.com/chart/boxoffice. Using BeaufiulSoup, Selenium, or both, return a list, with each title on a new row, of the top 10 movies of the week and order the list according to the total grossing of the movies, from most money to the least. Break ties using the weekend gross, from most money to the least.

Using CSS Selectors

In addition to the methods listed in Table 8.1, you can also use CSS or XPath selectors to interact more precisely with the page source. Refer to Table 3 from the WebScraping lab for a review of CSS syntax. The following code searches Google for "Python Selenium Docs" and then clicks on the second result.

```
#As before, go to Google and type in the search bar,
# but this time we use CSS selectors
>>> from selenium.webdriver.common.keys import Keys
>>> from selenium.common.exceptions import NoSuchElementException
>>> browser = webdriver.Chrome()
>>> try:
        browser.get("https://google.com")
. . .
            search_bar = browser.find_element_by_css_selector(
                             "input[name='q']")
            search_bar.clear()
            search_bar.send_keys("Python Selenium Docs")
            search_bar.send_keys(Keys.RETURN)
            try:
                # Wait a second, then get the second search result
                time.sleep(1)
. . .
                # "+ div" returns the element's next sibling with a "div" tag
                second_result = browser.find_element_by_css_selector(
                                 "div[class='g'] + div")
                try:
                     # Get the link, which is a child of second_result
                    link = second_result.find_element_by_css_selector(
                             "div[class='r']")
                    link.click()
. . .
                    time.sleep(1)
                #Remember to handle exceptions
                except NoSuchElementException:
                    print("Could not find link")
. . .
            except NoSuchElementException:
. . .
                print("Could not find second result")
```

```
... except NoSuchElementException:
... print("Could not find the search bar")
... finally:
... browser.close()
```

In the above example, we could have used find_element_by_class_name(), but when you need more precision than that, CSS selectors can be very useful. Remember that to view specific HTML associated with an object in Chrome or Firefox, you can right click on the object and click "Inspect." For Safari, you need to first enable "Show Develop menu" in "Preferences" under "Advanced." Keep in mind that you can also search through the source code (ctrl+f or cmd+f) to make sure you're using a unique identifier.

Note

Using Selenium to access a page's source code is typically much safer, though slower, than using requests.get(), since Selenium waits for each web page to load before proceeding. For instance, some websites are somewhat defensive about scrapers, but Selenium can sometimes make it possible to gather info without offending the administrators.

Problem 4. Project Euler (https://projecteuler.net) is a collection of mathematical computing problems. Each problem is listed with an ID, a description/title, and the number of users that have solved the problem.

Using Selenium, BeautifulSoup, or both, record the number of people who have solved each of the 700+ problems in the archive at https://projecteuler.net/archives. Plot the number of people who have solved each problem against the problem IDs, using a log scale for the y-axis. Display the scatter plot, then state the IDs of which problems have been solved most and least number of times.

Problem 5. The website http://example.webscraping.com contains a list of countries of the world. Using Selenium, go to the search page, enter the letters "ca", and hit enter. Remember to use the crawl delay time you found in Problem 1 so you don't send your requests too fast. Gather the href links associated with the <a> tags of all 10 displayed results. Print each link on a different line.

9

Pandas 1: Introduction

Lab Objective: Though NumPy and SciPy are powerful tools for numerical computing, they lack some of the high-level functionality necessary for many data science applications. Python's pandas library, built on NumPy, is designed specifically for data management and analysis. In this lab we introduce pandas data structures, syntax, and explore its capabilities for quickly analyzing and presenting data.

Pandas Basics

Pandas is a python library used primarily to analyze data. It combines functionality of NumPy, MatPlotLib, and SQL to create an easy to understand library that allows for the manipulation of data in various ways. In this lab we focus on the use of Pandas to analyze and manipulate data in ways similar to NumPy and SQL.

Pandas Data Structures

Series

The first pandas data structure is a Series. A Series is a one-dimensional array that can hold any datatype, similar to a ndarray. However, a Series has an index that gives a label to each entry. An index generally is used to label the data.

Typically a Series contains information about one feature of the data. For example, the data in a Series might show a class's grades on a test and the Index would indicate each student in the class. To initialize a Series, the first parameter is the data and the second is the index.

```
>>> import pandas as pd
>>>
# Initialize Series of student grades
>>> math = pd.Series(np.random.randint(0,100,4), ['Mark', 'Barbara',
... 'Eleanor', 'David'])
>>> english = pd.Series(np.random.randint(0,100,5), ['Mark', 'Barbara',
... 'David', 'Greg', 'Lauren'])
```

DataFrame

The second key pandas data structure is a DataFrame. A DataFrame is a collection of multiple Series. It can be thought of as a 2-dimensional array, where each row is a separate datapoint and each column is a feature of the data. The rows are labeled with an index (as in a Series) and the columns are labeled in the attribute columns.

There are many different ways to initialize a DataFrame. One way to initialize a DataFrame is by passing in a dictionary as the data of the DataFrame. The keys of the dictionary will become the labels in columns and the values are the Series associated with the label.

```
# Create a DataFrame of student grades
>>> grades = pd.DataFrame({"Math": math, "English": english})
>>> grades
          Math English
Barbara
          52.0
                   73.0
David
          10.0
                   39.0
Eleanor
          35.0
                    NaN
Greg
           NaN
                   26.0
                   99.0
Lauren
           NaN
Mark
          81.0
                   68.0
```

Notice that pd.DataFrame automatically lines up data from both Series that have the same index. If the data only appears in one of the Series, the corresponding entry for the other Series is NaN.

We can also initialize a DataFrame with a NumPy array. With this method, the data is passed in as a 2-dimensional NumPy array, while the column labels and the index are passed in as parameters. The first column label goes with the first column of the array, the second with the second, and so forth. The index works similarly.

A DataFrame can also be viewed as a NumPy array using the attribute values.

```
# View the DataFrame as a NumPy array
```

Data I/O

The pandas library has functions that make importing and exporting data simple. The functions allow for a variety of file formats to be imported and exported, including CSV, Excel, HDF5, SQL, JSON, HTML, and pickle files.

Method	Description
to_csv()	Write the index and entries to a CSV file
read_csv()	Read a csv and convert into a DataFrame
to_json()	Convert the object to a JSON string
<pre>to_pickle()</pre>	Serialize the object and store it in an external file
to_sql()	Write the object data to an open SQL database
read_html()	Read a table in an html page and convert to a DataFrame

Table 9.1: Methods for exporting data in a pandas Series or DataFrame.

The CSV (comma separated values) format is a simple way of storing tabular data in plain text. Because CSV files are one of the most popular file formats for exchanging data, we will explore the read_csv() function in more detail. Some frequently-used keyword arguments include the following:

- delimiter: The character that separates data fields. It is often a comma or a whitespace character.
- header: The row number (0 indexed) in the CSV file that contains the column names.
- index_col: The column (0 indexed) in the CSV file that is the index for the DataFrame.
- skiprows: If an integer n, skip the first n rows of the file, and then start reading in the data. If a list of integers, skip the specified rows.
- names: If the CSV file does not contain the column names, or you wish to use other column names, specify them in a list.

Another particularly useful function is read_html(), which is useful when scraping data. It takes in a url or html file and an optional argument match, a string or regex, and returns a list of the tables that match the match in a DataFrame. While the resulting data will probably need to be cleaned, it is frequently much faster than scraping a website.

Data Manipulation

Accessing Data

In general, the best way to access data in a Series or DataFrame is through the indexers loc and iloc. While array slicing can be used, it is more efficient to use these indexers. Accessing Series and DataFrame objects using these indexing operations is more efficient than slicing because the bracket indexing has to check many cases before it can determine how to slice the data structure. Using loc or iloc explicitly bypasses these extra checks. The loc index selects rows and columns based on their labels, while iloc selects them based on their integer position. With these indexers, the first and second arguments refer to the rows and columns, respectively, just as array slicing.

```
# Use loc to select the Math scores of David and Greg
>>> grades.loc[['David', 'Greg'],'Math']
David 10.0
Greg NaN
Name: Math, dtype: float64

# Use iloc to select the Math scores of David and Greg
>>> grades.iloc[[1,3], 0]
David 10.0
Greg NaN
```

To access an entire column of a DataFrame, the most efficient method is to use only square brackets and the name of the column, without the indexer. This syntax can also be used to create a new column or reset the values of an entire column.

```
# Create a new History column with array of random values
>>> grades['History'] = np.random.randint(0,100,6)
>>> grades['History']
Barbara
            4
David
           92
           25
Eleanor
Greg
           79
Lauren
           82
           27
Mark
Name: History, dtype: int64
# Reset the column such that everyone has a 100
>>> grades['History'] = 100.0
>>> grades
         Math English History
Barbara 52.0
                  73.0
                          100.0
                  39.0
David
         10.0
                          100.0
Eleanor 35.0
                          100.0
                  NaN
Greg
          NaN
                  26.0
                          100.0
Lauren
         NaN
                  99.0
                          100.0
Mark
         81.0
                  68.0
                          100.0
```

Datasets can often be very large and thus difficult to visualize. Pandas has various methods to make this easier. The methods head and tail will show the first or last n data points, respectively, where n defaults to 5. The method sample will draw n random entries of the dataset, where n defaults to 1.

```
# Use head to see the first n rows
>>> grades.head(n=2)
         Math English
                       History
Barbara 52.0
                  73.0
                          100.0
         10.0
                  39.0
                          100.0
David
# Use sample to sample a random entry
>>> grades.sample()
        Math English History
Lauren
         NaN
                 99.0
                         100.0
```

It may also be useful to re-order the columns or rows or sort according to a given column.

```
# Re-order columns
>>> grades.reindex(columns=['English','Math','History'])
         English Math History
Barbara
            73.0 52.0
                          100.0
            39.0 10.0
David
                           100.0
Eleanor
             NaN 35.0
                          100.0
                          100.0
Greg
            26.0
                   NaN
Lauren
            99.0
                   NaN
                          100.0
Mark
            68.0 81.0
                          100.0
# Sort descending according to Math grades
>>> grades.sort_values('Math', ascending=False)
         Math English History
         81.0
                  68.0
Mark
                          100.0
Barbara 52.0
                  73.0
                          100.0
         35.0
Eleanor
                   NaN
                          100.0
David
         10.0
                  39.0
                          100.0
                  26.0
                          100.0
Greg
          {\tt NaN}
                  99.0
                          100.0
Lauren
          NaN
```

Other methods used for manipulating DataFrame and Series panda structures can be found in Table 9.2.

Method	Description
append()	Concatenate two or more Series.
drop()	Remove the entries with the specified label or labels
<pre>drop_duplicates()</pre>	Remove duplicate values
dropna()	Drop null entries
fillna()	Replace null entries with a specified value or strategy
reindex()	Replace the index
<pre>sample()</pre>	Draw a random entry
<pre>shift()</pre>	Shift the index
unique()	Return unique values

Table 9.2: Methods for managing or modifying data in a pandas Series or DataFrame.

Problem 1. The file budget.csv contains the budget of a college student over the course of 4 years. Write a function that performs the following operations in this order:

- 1. Read in budget.csv as a DataFrame with the index as column 0. Hint: Use index_col=0 to set the first column as the index when reading in the csv.
- 2. Reindex the columns such that amount spent on groceries is the first column and all other columns maintain the same ordering.
- 3. Sort the DataFrame in descending order by how much money was spent on Groceries.
- 4. Reset all values in the 'Rent' column to 800.0.
- 5. Reset all values in the first 5 data points to 0.0.

Return the values of the updated DataFrame as a NumPy array.

Basic Data Manipulation

Because the primary pandas data structures are based off of ndarray, most NumPy functions work with pandas structures. For example, basic vector operations work as would be expected:

```
# Sum history and english grades of all students
>>> grades['English'] + grades['History']
Barbara
           173.0
David
           139.0
Eleanor
             NaN
Greg
           126.0
           199.0
Lauren
Mark
           168.0
dtype: float64
# Double all Math grades
>>> grades['Math']*2
           104.0
Barbara
David
            20.0
```

```
Eleanor 70.0
Greg NaN
Lauren NaN
Mark 162.0
Name: Math, dtype: float64
```

In addition to arithmetic, Series has a variety of other methods similar to NumPy arrays. A collection of these methods is found in Table 9.3.

Method	Returns		
abs()	Object with absolute values taken (of numerical data)		
<pre>idxmax()</pre>	The index label of the maximum value		
<pre>idxmin()</pre>	The index label of the minimum value		
<pre>count()</pre>	The number of non-null entries		
<pre>cumprod()</pre>	The cumulative product over an axis		
<pre>cumsum()</pre>	The cumulative sum over an axis		
max()	The maximum of the entries		
mean()	The average of the entries		
median()	The median of the entries		
min()	The minimum of the entries		
mode()	The most common element(s)		
<pre>prod()</pre>	The product of the elements		
sum()	The sum of the elements		
<pre>var()</pre>	The variance of the elements		

Table 9.3: Numerical methods of the Series and DataFrame pandas classes.

Basic Statistical Functions

The pandas library allows us to easily calculate basic summary statistics of our data, which can be useful when we want a quick description of the data. The describe() function outputs several such summary statistics for each column in a DataFrame:

```
# Use describe to better understand the data
>>> grades.describe()
            Math
                   English
                            History
                   5.00000
count
        4.000000
                                 6.0
                               100.0
       44.500000 61.00000
mean
       29.827281
                  28.92231
                                 0.0
std
       10.000000
                  26.00000
                               100.0
min
       28.750000
                  39.00000
                               100.0
25%
50%
       43.500000
                  68.00000
                               100.0
       59.250000
75%
                  73.00000
                               100.0
max
       81.000000
                  99.00000
                               100.0
```

Functions for calculating means and variances, the covariance and correlation matrices, and other basic statistics are also available.

```
# Find the average grade for each student
```

```
>>> grades.mean(axis=1)
Barbara
           75.000000
David
           49.666667
Eleanor
           67.500000
           63.000000
Greg
Lauren
           99.500000
           83.000000
Mark
dtype: float64
# Give correlation matrix between subjects
>>> grades.corr()
            Math English
                            History
Math
         1.00000
                  0.84996
                                 NaN
         0.84996
                   1.00000
English
                                 NaN
History
              NaN
                       NaN
                                 NaN
```

The method rank() can be used to rank the values in a data set, either within each entry or with each column. This function defaults ranking in ascending order: the least will be ranked 1 and the greatest will be ranked the highest number.

```
# Rank each student's performance in their classes in descending order
# (best to worst)
# The method keyword specifies what rank to use when ties occur.
>>> grades.rank(axis=1,method='max',ascending=False)
         Math English History
          3.0
                    2.0
Barbara
                             1.0
          3.0
David
                    2.0
                             1.0
Eleanor
          2.0
                    NaN
                             1.0
Greg
                    2.0
                             1.0
          NaN
Lauren
          NaN
                    2.0
                             1.0
Mark
          2.0
                    3.0
                             1.0
```

These methods can be very effective in interpreting data. For example, the rank() example above shows use that Barbara does best in History, then English, and then Math.

Dealing with Missing Data

Missing data is a ubiquitous problem in data science. Fortunately, pandas is particularly well-suited to handling missing or anomalous data. As we have already seen, the pandas default for a missing value is NaN. In basic arithmetic operations, if one of the operands is NaN, then the output is also NaN. If we are not interested in the missing values, we can simply drop them from the data altogether, or we can fill them with some other value, such as the mean. NaN might also mean something specific, such as some default value, which should inform what to do with NaN values.

```
Mark
         81.0
                  68.0
                           100.0
# fill missing data with 50.0
>>> grades.fillna(50.0)
         Math English History
Barbara
         52.0
                  73.0
                           100.0
         10.0
                  39.0
David
                           100.0
Eleanor 35.0
                  50.0
                           100.0
Greg
         50.0
                  26.0
                           100.0
         50.0
                  99.0
                           100.0
Lauren
         81.0
Mark
                  68.0
                           100.0
```

When dealing with missing data, make sure you are aware of the behavior of the pandas functions you are using. For example, sum() and mean() ignore NaN values in the computation.

ACHTUNG!

Always consider missing data carefully when analyzing a dataset. It may not always be helpful to drop the data or fill it in with a random number. Consider filling the data with the mean of surrounding data or the mean of the feature in question. Overall, the choice for how to fill missing data should make sense with the dataset.

Problem 2. Write a function which uses budget.csv to answer the questions "Which category affects living expenses the most?" Which affects other expenses the most?" Perform the following manipulations:

- 1. Fill all NaN values with 0.0.
- 2. Create two new columns, 'Living Expenses' and 'Other'. Set the value of 'Living Expenses' to be the sum of the columns 'Rent', 'Groceries', 'Gas' and 'Utilities '. Set the value of 'Other' to be the sum of the columns 'Dining Out', 'Out With Friends' and 'Netflix'.
- 3. Identify which column, other than 'Living Expenses', correlates most with 'Living Expenses' and which column, other than 'Other', correlates most with 'Other'. This can indicate which columns in the budget affect the overarching categories the most.

Return the names of each of those columns as a tuple. The first should be of the column corresponding to 'Living Expenses' and the second to 'Other'.

Complex Operations in Pandas

Often times, the data that we have is not exactly the data we want to analyze. In cases like this we use more complex data manipulation tools to access only the data that we need.

For the examples below, we will use the following data:

```
>>> name = ['Mylan', 'Regan', 'Justin', 'Jess', 'Jason', 'Remi', 'Matt',
       'Alexander', 'JeanMarie']
>>> age = [20, 21, 18, 22, 19, 20, 20, 19, 20]
>>> rank = ['Sp', 'Se', 'Fr', 'Se', 'Sp', 'J', 'J', 'J', 'Se']
>>> ID = range(9)
>>> aid = ['y', 'n', 'n', 'y', 'n', 'n', 'n', 'y', 'n']
>>> GPA = [3.8, 3.5, 3.0, 3.9, 2.8, 2.9, 3.8, 3.4, 3.7]
>>> mathID = [0, 1, 5, 6, 3]
>>>  mathGd = [4.0, 3.0, 3.5, 3.0, 4.0]
>>> major = ['y', 'n', 'y', 'n', 'n']
>>> studentInfo = pd.DataFrame({'ID': ID, 'Name': name, 'Sex': sex, 'Age': age,
       'Class': rank})
>>> otherInfo = pd.DataFrame({'ID': ID, 'GPA': GPA, 'Financial_Aid': aid})
>>> mathInfo = pd.DataFrame({'ID': mathID, 'Grade': mathGd, 'Math_Major':
       major})
```

Before querying our data, it is helpful to know some of its basic properties, such as number of columns, number of rows, and the datatypes of the columns. This can be done by simply calling the info() method on the desired DataFrame:

Masks

Sometimes, we only want to access data from a single column. For example if we want to only access the ID of the students in the studentInfo DataFrame, then we would use the following syntax.

```
# Get the ID column from studentInfo
>>> studentInfo.ID # or studentInfo['ID']
   ID
0
    0
1
    1
2
    2
3
    3
4
    4
5
    5
6
    6
7
    7
```

If we want to access multiple columns at once we can use a list of column names.

```
# Get the ID and Age columns.
>>> studentInfo[['ID', 'Age']]
   ID
       Age
    0
         20
0
         21
1
    1
2
         18
3
    3
         22
4
    4
         19
5
    5
         20
6
    6
         20
7
    7
         19
8
    8
         29
```

Now we can access the specific columns that we want. However, some of these columns may still contain data points that we don't want to consider. In this case we can build a mask. Each mask that we build will return a pandas Series object with a bool value at each index indicating if the condition is satisfied.

```
# Create a mask for all student receiving financial aid.
>>> mask = otherInfo['Financial_Aid'] == 'y'

# Access other info where the mask is true and display the ID and GPA ← columns.
>>> otherInfo[mask][['ID', 'GPA']]

ID GPA
0 0 3.8
3 3 3.9
7 7 3.4
```

We can also create compound masks with multiple statements. We do this using the same syntax you would use for a compound mask in a normal NumPy array. Useful operators are &, the AND operator; |, the OR operator; and \sim , the NOT operator.

```
# Get all student names where Class = 'J' OR Class = 'Sp'.
>>> mask = (studentInfo.Class == 'J') | (studentInfo.Class == 'Sp')
    studentInfo[mask].Name
>>>
        Mylan
0
4
        Jason
5
         Remi
6
         Matt
    Alexander
Name: Name, dtype: object
# This can also be acomplished with the following command:
# studentInfo['Class'].isin(['J','Sp'])]['Name']
```

Problem 3. Read in the file crime_data.csv as a pandas object. The file contains data on types of crimes in the U.S. from 1960 to 2016. Set the index as the column 'Year'. Answer the following questions using the pandas methods learned in this lab. The answer of each question should be saved as indicated. Return the answers to all three questions as a tuple (i.e. (answer_1,answer_2,answer_3)).

- 1. Identify the three crimes that have a mean yearly number of occurences over 1,500,000. Of these three crimes, which two are very correlated? Which of these two crimes has a greater maximum value? Save the title of this column as a variable to return as the answer.
- 2. Examine the data from 2000 and later. Sort this data (in ascending order) according to number of murders. Find the years where aggravated assault is greater than 850,000. Save the indices (the years) of the masked and reordered DataFrame as a NumPy array to return as the answer.
- 3. What year had the highest crime rate? In this year, which crime was committed the most? What percentage of the total crime that year was it? Save this value as a float.

Working with Dates and Times

The datetime module in the standard library provides a few tools for representing and operating on dates and times. The datetime object represents a *time stamp*: a specific time of day on a certain day. Its constructor accepts a four-digit year, a month (starting at 1 for January), a day, and, optionally, an hour, minute, second, and microsecond. Each of these arguments must be an integer, with the hour ranging from 0 to 23.

```
>>> from datetime import datetime

# Represent November 18th, 1991, at 2:01 PM.
>>> bday = datetime(1991, 11, 18, 14, 1)
>>> print(bday)
1991-11-18 14:01:00

# Find the number of days between 11/18/1991 and 11/9/2017.
>>> dt = datetime(2017, 11, 9) - bday
>>> dt.days
9487
```

The datetime.datetime object has a parser method, strptime(), that converts a string into a new datetime.datetime object. The parser is flexible so the user must specify the format that the dates are in. For example, if the dates are in the format "Month/Day//Year::Hour", specify format "=\m/\m/d//\m/Y::\m/H" to parse the string appropriately. See Table 9.4 for formatting options.

Pattern	Description
%Y	4-digit year
%у	2-digit year
%m	1- or 2-digit month
%d	1- or 2-digit day
%Н	Hour (24-hour)
%I	Hour (12-hour)
%M	2-digit minute
%S	2-digit second

Table 9.4: Formats recognized by datetime.strptime()

```
>>> print(datetime.strptime("1991-11-18 / 14:01", "%Y-%m-%d / %H:%M"),
... datetime.strptime("1/22/1996", "%m/%d/%Y"),
... datetime.strptime("19-8, 1998", "%d-%m, %Y"), sep='\n')
1991-11-18 14:01:00  # The date formats are now standardized.
1996-01-22 00:00:00  # If no hour/minute/seconds data is given,
1998-08-19 00:00:00  # the default is midnight.
```

Converting Dates to an Index

The TimeStamp class is the pandas equivalent to a datetime.datetime object. A pandas index composed of TimeStamp objects is a DatetimeIndex, and a Series or DataFrame with a DatetimeIndex is called a *time series*. The function pd.to_datetime() converts a collection of dates in a parsable format to a DatetimeIndex. The format of the dates is inferred if possible, but it can be specified explicitly with the same syntax as datetime.strptime().

```
>>> import pandas as pd
# Convert some dates (as strings) into a DatetimeIndex.
>>> dates = ["2010-1-1", "2010-2-1", "2012-1-1", "2012-1-2"]
>>> pd.to_datetime(dates)
DatetimeIndex(['2010-01-01', '2010-02-01', '2012-01-01', '2012-01-02'],
                dtype='datetime64[ns]', freq=None)
# Create a time series, specifying the format for the DatetimeIndex.
>>> dates = ["1/1, 2010", "1/2, 2010", "1/1, 2012", "1/2, 2012"]
>>> date_index = pd.to_datetime(dates, format="%m/%d, %Y")
>>> pd.Series([x**2 for x in range(4)], index=date_index)
2010-01-01
2010-01-02
              1
2012-01-01
              4
2012-01-02
              9
dtype: int64
```

Problem 4. The file DJIA.csv contains daily closing values of the Dow Jones Industrial Average from 2006–2016. Read the data into a Series or DataFrame with a DatetimeIndex as the index. Drop any rows without numerical values, cast the "VALUE" column to floats, then return the updated DataFrame.

Hint: You can change the column type the same way you'd change a numpy array type.

Generating Time-based Indices

Some time series datasets come without explicit labels but have instructions for deriving timestamps. For example, a list of bank account balances might have records from the beginning of every month, or heart rate readings could be recorded by an app every 10 minutes. Use pd.date_range() to generate a DatetimeIndex where the timestamps are equally spaced. The function is analogous to np.arange() and has the following parameters:

Parameter	Description
start	Starting date
end	End date
periods	Number of dates to include Amount of time between consecutive dates
freq	Amount of time between consecutive dates
normalize	Normalizes the start and end times to midnight

Table 9.5: Parameters for pd.date_range().

Exactly three of the parameters start, end, periods, and freq must be specified to generate a range of dates. The freq parameter accepts a variety of string representations, referred to as offset aliases. See Table 9.6 for a sampling of some of the options. For a complete list of the options, see https://pandas.pydata.org/pandas-docs/stable/user_guide/timeseries.html#timeseries-offset-aliases1.

Parameter	Description	
"D"	calendar daily (default)	
"B"	business daily (every business day)	
"H"	hourly	
"T"	minutely	
"S"	secondly	
"MS"	first day of the month (Month Start)	
"BMS"	first business day of the month (Business Month Start)	
"W-MON"	every Monday (Week-Monday)	
"WOM-3FRI"	every 3rd Friday of the month (Week of the Month - 3rd Friday)	

Table 9.6: Options for the freq parameter to pd.date_range().

```
# Create a DatetimeIndex for 5 consecutive days starting on September 28, 2016. >>> pd.date_range(start='9/28/2016 16:00', periods=5) DatetimeIndex(['2016-09-28 16:00:00', '2016-09-29 16:00:00',
```

```
'2016-09-30 16:00:00', '2016-10-01 16:00:00',
               '2016-10-02 16:00:00'],
              dtype='datetime64[ns]', freq='D')
# Create a DatetimeIndex with the first weekday of every other month in 2016.
>>> pd.date_range(start='1/1/2016', end='1/1/2017', freq="2BMS")
DatetimeIndex(['2016-01-01', '2016-03-01', '2016-05-02', '2016-07-01',
               '2016-09-01', '2016-11-01'],
              dtype='datetime64[ns]', freq='2BMS')
# Create a DatetimeIndex for 10 minute intervals between 4:00 PM and 4:30 PM on\hookleftarrow
     September 9, 2016.
>>> pd.date_range(start='9/28/2016 16:00',
            end='9/28/2016 16:30', freq="10T")
DatetimeIndex(['2016-09-28 16:00:00', '2016-09-28 16:10:00',
                '2016-09-28 16:20:00', '2016-09-28 16:30:00'],
              dtype='datetime64[ns]', freq='10T')
# Create a DatetimeIndex for 2 hour 30 minute intervals between 4:30 PM and \hookleftarrow
   2:30 AM on September 29, 2016.
>>> pd.date_range(start='9/28/2016 16:30', periods=5, freq="2h30min")
DatetimeIndex(['2016-09-28 16:30:00', '2016-09-28 19:00:00',
               '2016-09-28 21:30:00', '2016-09-29 00:00:00',
               '2016-09-29 02:30:00'],
              dtype='datetime64[ns]', freq='150T')
```

Problem 5. The file paychecks.csv contains values of an hourly employee's last 93 paychecks. Paychecks are given every other Friday, starting on March 14, 2008, and the employee started working on March 13, 2008.

Read in the data, using pd.date_range() to generate the DatetimeIndex. Set this as the new index of the DataFrame and return the DataFrame.

Elementary Time Series Analysis

Shifting

DataFrame and Series objects have a shift() method that allows you to move data up or down relative to the index. When dealing with time series data, we can also shift the DatetimeIndex relative to a time offset.

```
2016-10-08 0.811226
2016-10-09 0.656711
2016-10-10 0.351431
2016-10-11 0.608767
>>> df.shift(1)
               VALUE
2016-10-07
                 NaN
2016-10-08 0.127895
2016-10-09 0.811226
2016-10-10 0.656711
2016-10-11 0.351431
>>> df.shift(-2)
               VALUE
2016-10-07 0.656711
2016-10-08 0.351431
2016-10-09 0.608767
2016-10-10
                 NaN
2016-10-11
                 NaN
>>> df.shift(14, freq="D")
               VALUE
2016-10-21 0.127895
2016-10-22 0.811226
2016-10-23 0.656711
2016-10-24 0.351431
2016-10-25 0.608767
```

Shifting data makes it easy to gather statistics about changes from one timestamp or period to the next.

Problem 6. Compute the following information about the DJIA dataset from Problem 4 that has a DateTimeIndex.

- $\bullet\,$ The single day with the largest gain.
- The single day with the largest loss.

Return the DateTimeIndex of the day with the largest gain and the day with the largest loss. (Hint: Call your function from Problem 4 to get the DataFrame already cleaned and with DatetimeIndex).

More information on how to use datetime with Pandas is in the additional material section. This includes working with Periods and more analysis with time series.

Additional Material

SQL Operations in pandas

DataFrames are tabular data structures bearing an obvious resemblance to a typical relational database table. SQL is the standard for working with relational databases; however, pandas can accomplish many of the same tasks as SQL. The SQL-like functionality of pandas is one of its biggest advantages, eliminating the need to switch between programming languages for different tasks. Within pandas, we can handle both the querying and data analysis.

For the examples below, we will use the following data:

```
>>> name = ['Mylan', 'Regan', 'Justin', 'Jess', 'Jason', 'Remi', 'Matt',
       'Alexander', 'JeanMarie']
>>> age = [20, 21, 18, 22, 19, 20, 20, 19, 20]
>>> rank = ['Sp', 'Se', 'Fr', 'Se', 'Sp', 'J', 'J', 'J', 'Se']
>>> ID = range(9)
>>> aid = ['y', 'n', 'n', 'y', 'n', 'n', 'n', 'y', 'n']
>>> GPA = [3.8, 3.5, 3.0, 3.9, 2.8, 2.9, 3.8, 3.4, 3.7]
>>> mathID = [0, 1, 5, 6, 3]
>>>  mathGd = [4.0, 3.0, 3.5, 3.0, 4.0]
>>> major = ['y', 'n', 'y', 'n', 'n']
>>> studentInfo = pd.DataFrame({'ID': ID, 'Name': name, 'Sex': sex, 'Age': age,
        'Class': rank})
>>> otherInfo = pd.DataFrame({'ID': ID, 'GPA': GPA, 'Financial_Aid': aid})
>>> mathInfo = pd.DataFrame({'ID': mathID, 'Grade': mathGd, 'Math_Major':
       major})
```

SQL SELECT statements can be done by column indexing. WHERE statements can be included by adding masks (just like in a NumPy array). The method isin() can also provide a useful WHERE statement. This method accepts a list, dictionary, or Series containing possible values of the DataFrame or Series. When called upon, it returns a Series of booleans, indicating whether an entry contained a value in the parameter pass into isin().

```
# SELECT ID, Age FROM studentInfo
>>> studentInfo[['ID', 'Age']]
   ID
       Age
0
    0
        20
1
    1
        21
    2
        18
3
        22
    3
4
    4
        19
5
    5
        20
6
    6
        20
7
    7
        19
8
    8
# SELECT ID, GPA FROM otherInfo WHERE Financial_Aid = 'y'
>>> mask = otherInfo['Financial_Aid'] == 'y'
>>> otherInfo[mask][['ID', 'GPA']]
```

```
ID
       GPA
    0
       3.8
    3
       3.9
7
    7 3.4
# SELECT Name FROM studentInfo WHERE Class = 'J' OR Class = 'Sp'
>>> studentInfo[studentInfo['Class'].isin(['J','Sp'])]['Name']
         Mylan
4
         Jason
5
          Remi
6
          Matt
7
     Alexander
Name: Name, dtype: object
```

Next, let's look at JOIN statements. In pandas, this is done with the merge function. merge takes the two DataFrame objects to join as parameters, as well as keyword arguments specifying the column on which to join, along with the type (left, right, inner, outer).

```
# SELECT * FROM studentInfo INNER JOIN mathInfo ON studentInfo.ID = mathInfo.ID
>>> pd.merge(studentInfo, mathInfo, on='ID') # INNER JOIN is the default
   Age Class ID
                    Name Sex Grade Math_Major
    20
                   Mylan
          Sp
               0
                           M
                                4.0
                           F
1
    21
          Se
               1
                   Regan
                                3.0
                                             n
2
    22
          Se
                    Jess
                                4.0
                                             n
3
    20
           J
                           F
               5
                    Remi
                                3.5
                                             У
    20
           J
               6
                    Matt
                                3.0
                                             n
[5 rows x 7 columns]
# SELECT GPA, Grade FROM otherInfo FULL OUTER JOIN mathInfo ON otherInfo.
# ID = mathInfo.ID
>>> pd.merge(otherInfo, mathInfo, on='ID', how='outer')[['GPA', 'Grade']]
0 3.8
          4.0
1 3.5
          3.0
2 3.0
          NaN
3 3.9
          4.0
4 2.8
          NaN
5 2.9
          3.5
6 3.8
          3.0
7 3.4
          NaN
8 3.7
          NaN
[9 rows x 2 columns]
```

More Datetime with Pandas

Periods

A pandas Timestamp object represents a precise moment in time on a given day. Some data, however, is recorded over a time interval, and it wouldn't make sense to place an exact timestamp on any of the measurements. For example, a record of the number of steps walked in a day, box office earnings per week, quarterly earnings, and so on. This kind of data is better represented with the pandas Period object and the corresponding PeriodIndex.

The Period class accepts a value and a freq. The value parameter indicates the label for a given Period. This label is tied to the end of the defined Period. The freq indicates the length of the Period and in some cases can also indicate the offset of the Period. The default value for freq is "M" for months. The freq parameter accepts the majority, but not all, of frequencies listed in Table 9.6.

```
# Creates a period for month of Oct, 2016.
>>> p1 = pd.Period("2016-10")
>>> p1.start_time
                                    # The start and end times of the period
Timestamp('2016-10-01 00:00:00') # are recorded as Timestamps.
>>> p1.end_time
Timestamp('2016-10-31 23:59:59.999999999')
# Represent the annual period ending in December that includes 10/03/2016.
>>> p2 = pd.Period("2016-10-03", freq="A-DEC")
>>> p2.start_time
Timestamp('2016-01-01 00:00:00')
> p2.end_time
Timestamp('2016-12-31 23:59:59.999999999')
# Get the weekly period ending on a Saturday that includes 10/03/2016.
>>> print(pd.Period("2016-10-03", freq="W-SAT"))
2016-10-02/2016-10-08
```

Like the pd.date_range() method, the pd.period_range() method is useful for generating a PeriodIndex for unindexed data. The syntax is essentially identical to that of pd.date_range(). When using pd.period_range(), remember that the freq parameter marks the end of the period. After creating a PeriodIndex, the freq parameter can be changed via the asfreq() method.

The bounds of a PeriodIndex object can be shifted by adding or subtracting an integer. PeriodIndex will be shifted by $n \times \text{freq}$.

If for any reason you need to switch from periods to timestamps, pandas provides a very simple method to do so. The how parameter can be start or end and determines if the timestamp is the beginning or the end of the period. Similarly, you can switch from timestamps to periods.

Operations on Time Series

There are certain operations only available to Series and DataFrames that have a DatetimeIndex. A sampling of this functionality is described throughout the remainder of this lab.

Slicing

Slicing is much more flexible in pandas for time series. We can slice by year, by month, or even use traditional slicing syntax to select a range of dates.

Resampling

Some datasets do not have datapoints at a fixed frequency. For example, a dataset of website traffic has datapoints that occur at irregular intervals. In situations like these, *resampling* can help provide insight on the data.

The two main forms of resampling are *downsampling*, aggregating data into fewer intervals, and *upsampling*, adding more intervals.

To downsample, use the resample() method of the Series or DataFrame. This method is similar to groupby() in that it groups different entries together. Then aggregation produces a new data set. The first parameter to resample() is an offset string from Table 9.6: "D" for daily, "H" for hourly, and so on.

```
>>> import numpy as np
# Get random data for every day from 2000 to 2010.
>>> dates = pd.date_range(start="2000-1-1", end='2009-12-31', freq='D')
>>> df = pd.Series(np.random.random(len(days)), index=dates)
>>> df
2000-01-01
              0.559
2000-01-02
              0.874
2000-01-03
              0.774
                . . .
2009-12-29
              0.837
              0.472
2009-12-30
2009-12-31
              0.211
Freq: D, Length: 3653, dtype: float64
# Group the data by year.
>>> years = df.resample("A")
                                    # 'A' for 'annual'.
>>> years.agg(len)
                                    # Number of entries per year.
2000-12-31
              366.0
2001-12-31
              365.0
2002-12-31
              365.0
                . . .
2007-12-31
              365.0
2008-12-31
              366.0
2009-12-31
              365.0
```

```
Freq: A-DEC, dtype: float64
>>> years.mean()
                                    # Average entry by year.
2000-12-31
             0.491
2001-12-31
             0.514
2002-12-31
             0.484
               . . .
2007-12-31
             0.508
2008-12-31
             0.521
2009-12-31
             0.523
Freq: A-DEC, dtype: float64
# Group the data by month.
>>> months = df.resample("M")
>>> len(months.mean())
                                    # 12 months x 10 years = 120 months.
120
```

Elementary Time Series Analysis

Rolling Functions and Exponentially-Weighted Moving Functions

Many time series are inherently noisy. To analyze general trends in data, we use *rolling functions* and *exponentally-weighted moving (EWM)* functions. Rolling functions, or *moving window functions*, perform a calculation on a window of data. There are a few rolling functions that come standard with pandas.

Rolling Functions (Moving Window Functions)

One of the most commonly used rolling functions is the *rolling average*, which takes the average value over a window of data.

The function call s.rolling(window=200) creates a pd.core.rolling.Window object that can be aggregated with a function like mean(), std(), var(), min(), max(), and so on.

Exponentially-Weighted Moving (EWM) Functions

Whereas a moving window function gives equal weight to the whole window, an *exponentially-weighted* moving function gives more weight to the most recent data points.

In the case of a exponentially-weighted moving average (EWMA), each data point is calculated as follows.

$$z_i = \alpha \bar{x}_i + (1 - \alpha)z_{i-1},$$

where z_i is the value of the EWMA at time i, \bar{x}_i is the average for the i-th window, and α is the decay factor that controls the importance of previous data points. Notice that $\alpha = 1$ reduces to the rolling average.

More commonly, the decay is expressed as a function of the window size. In fact, the span for an EWMA is nearly analogous to window size for a rolling average.

Notice the syntax for EWM functions is very similar to that of rolling functions.

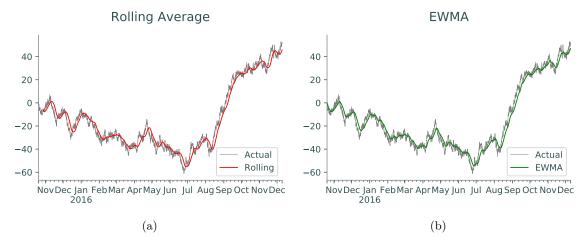


Figure 9.1: Rolling average and EWMA.

```
ax2 = plt.subplot(122)
s.plot(color="gray", lw=.3, ax=ax2)
s.ewm(span=200).mean().plot(color='g', lw=1, ax=ax2)
ax2.legend(["Actual", "EWMA"], loc="lower right")
ax2.set_title("EWMA")
```

1 Pandas 2: Plotting

Lab Objective: Clear, insightful visualizations are a crucial part of data analysis. To facilitate quick data visualization, pandas includes several tools that wrap around matplotlib. These tools make it easy to compare different parts of a data set, explore the data as a whole, and spot patterns and correlations in the data.

Overview of Plotting Tools

The main tool for visualization in pandas is the plot() method for Series and DataFrames. The method has a keyword argument kind that specifies the type of plot to draw. The valid options for kind are detailed below.

Plot Type	plot() ID	Uses and Advantages
Line plot	"line"	Show trends ordered in data; easy to compare multiple data sets
Scatter plot	"scatter"	Compare exactly two data sets, independent of ordering
Bar plot	"bar", "barh"	Compare categorical or sequential data
Histogram	"hist"	Show frequencies of one set of values, independent of ordering
Box plot	"box"	Display min, median, max, and quartiles; compare data distributions
Hexbin plot	"hexbin"	2D histogram; reveal density of cluttered scatter plots

Table 10.1: Types of plots in pandas. The plot ID is the value of the keyword argument kind. That is, df.plot(kind="scatter") creates a scatter plot. The default kind is "line".

The plot() method calls plt.plot(), plt.hist(), plt.scatter(), and other matplotlib plotting functions, but it also assigns axis labels, tick marks, legends, and a few other things based on the index and the data. Most calls to plot() specify the kind of plot and which Series to use as the x and y axes. By default, the index of the Series or DataFrame is used for the x axis.

```
>>> import pandas as pd
>>> from matplotlib import pyplot as plt

>>> budget = pd.read_csv("budget.csv", index_col="Date")
>>> budget.plot(y="Rent") # Plot rent against the index (date).
```



In this case, the call to the plot() method is essentially equivalent to the following code.

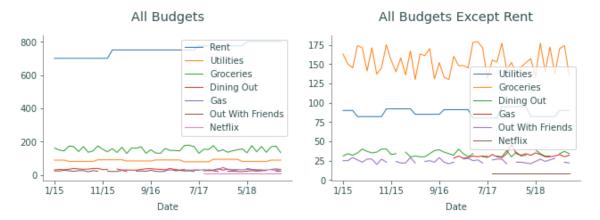
```
>>> plt.plot(budget.index, budget['Rent'], label='Rent')
>>> plt.xlabel(budget.index.name)
>>> plt.xlim(min(budget.index), max(budget.index))
>>> plt.legend(loc='best')
```

The plot() method also takes in many keyword arguments for matplotlib plotting and annotation functions. For example, setting legend=False disables the legend, providing a value for title sets the figure title, grid=True turns a grid on, and so on. For more customizations, see https://pandas.pydata.org/pandas-docs/stable/generated/pandas.DataFrame.plot.html.

Visualizing an Entire Data Set

A good way to start analyzing an unfamiliar data set is to visualize as much of the data as possible to determine which parts are most important or interesting. For example, since the columns in a DataFrame share the same index, the columns can all be graphed together using the index as the x-axis. By default, the plot() method attempts to plot every Series (column) in a DataFrame. This is especially useful with sequential data, like the budget data set.

```
# Plot all columns together against the index.
>>> budget.plot(title="All Budgets",linewidth=1)
>>> budget.drop(["Rent"], axis=1).plot(linewidth=1,title="All Budgets Except ← Rent")
```



- (a) All columns of the budget data set on the same figure, using the index as the *x*-axis.
- (b) All columns of the budget data set except "Living Expenses" and "Rent".

Figure 10.1

While plotting every **Series** at once can give an overview of all the data, the resulting plot is often difficult for the reader to understand. For example, the budget data set has 9 columns, so the resulting figure, Figure 10.1a, is fairly cluttered.

One way to declutter a visualization is to examine less data. Notice that 'Living Expenses' has values much bigger than the other columns. Dropping this column, as well as 'Rent', gives a better overview of the data, shown in Figure 10.1b.

ACHTUNG!

Often plotting all data at once is unwise because columns have **different units of measure**. Be careful not to plot parts of a data set together if those parts do not have the same units or are otherwise incomparable.

Another way to declutter a plot is to use subplots. To quickly plot several columns in separate subplots, use subplots=True and specify a shape tuple as the layout for the plots. Subplots automatically share the same x-axis. Set sharey=True to force them to share the same y-axis as well.

```
>>> budget.plot(y=['Dining Out','Gas','Out With Friends', 'Netflix'],
... subplots=True, layout=(2,2), sharey=True,
... style=['-','--','-.',':'],title="Plots of Dollars Spent for Different \( \to \) Budgets")
```





As mentioned previously, the plot() method can be used to plot different kinds of plots. One possible kind of plot is a histogram. Since plots made by the plot() method share an x-axis by default, histograms turn out poorly whenever there are columns with very different data ranges or when more than one column is plotted at once.

```
# Plot three histograms together.
>>> budget.plot(kind='hist',y=['Gas','Dining Out','Out With Friends'],
... alpha=.7,bins=10,title="Frequency of Amount (in dollars) Spent")

# Plot three histograms, stacking one on top of the other.
>>> budget.plot(kind='hist',y=['Gas','Dining Out','Out With Friends'],
... bins=10,stacked=True,title="Frequency of Amount (in dollars) Spent")
```

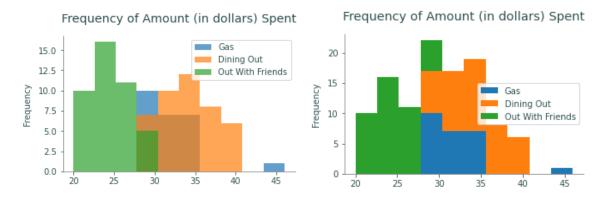


Figure 10.2: Two examples of histograms that are difficult to understand because multiple columns are plotted.

Thus, histograms are good for examining the distribution of a **single** column in a data set. For histograms, use the hist() method of the DataFrame instead of the plot() method. Specify the number of bins with the bins parameter. Choose a number of bins that accurately represents the data; the wrong number of bins can create a misleading or uninformative visualization.

```
>>> budget[["Dining Out", "Gas"]].hist(grid=False,bins=10)
```

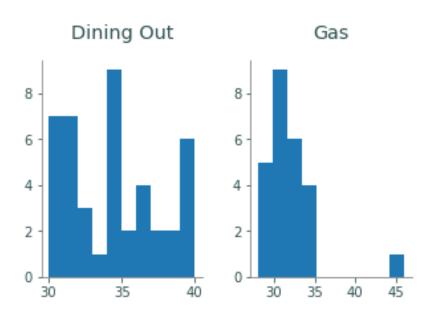


Figure 10.3: Histograms of "Dining Out" and "Gas".

Problem 1. Create 3 visualizations for the data in crime_data.csv. Make one of the visualizations a histogram. The visualizations should be well labeled and easy to understand.

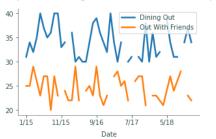
Patterns and Correlations

After visualizing the entire data set initially, a good next step is to closely compare related parts of the data. This can be done with different types of visualizations. For example, Figure 10.1b suggests that the "Dining Out" and "Out With Friends" columns are roughly on the same scale. Since this data is sequential (indexed by time), start by plotting these two columns against the index. Next, create a scatter plot of one of the columns versus the other to investigate correlations that are independent of the index. Unlike other types of plots, using kind="scatter" requires both x and y columns as arguments.

```
# Plot 'Dining Out' and 'Out With Friends' as lines against the index.
>>> budget.plot(y=["Dining Out", "Out With Friends"],title="Amount Spent on ←
Dining Out and Out with Friends per Day")
```

```
# Make a scatter plot of 'Dining Out' against 'Out With Friends'
>>> budget.plot(kind="scatter", x="Dining Out", y="Out With Friends",
... alpha=.8,xlim=(0,max(budget['Dining Out'])+1),
... ylim=(0,max(budget['Out With Friends'])+1))
```

Amount Spent on Dining Out and Out with Friends per Day



Correlation between Dining Out and Out with Friends

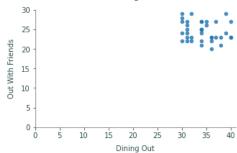


Figure 10.4: Correlations between "Dining Out" and "Out With Friends".

The first plot shows us that more money is spent on dining out than being out with friends overall. However, both categories stay in the same range for most of the data. This is confirmed in the scatter plot by the block in the upper right corner, indicating the common range spent on dining out and being out with friends.

ACHTUNG!

When analyzing data, especially while searching for patterns and correlations, **always** ask yourself if the data makes sense and is trustworthy. What lurking variables could have influenced the data measurements as they were being gathered?

The crime data set from Problem 1 is somewhat suspect in this regard. The murder rate is likely accurate, since murder is conspicuous and highly reported, but what about the rape rate? Are the number of rapes increasing, or is the percentage of rapes being reported increasing? It's probably both! Be careful about drawing conclusions for sensitive or questionable data.

Another useful visualization used to understand correlations in a data set is a scatter matrix. The function pd.plotting.scatter_matrix() produces a table of plots where each column is plotted against each other column in separate scatter plots. The plots on the diagonal, instead of plotting a column against itself, displays a histogram of that column. This provides a very quick method for an initial analysis of the correlation between different columns.

```
>>> pd.plotting.scatter_matrix(budget[['Living Expenses','Other']])
```

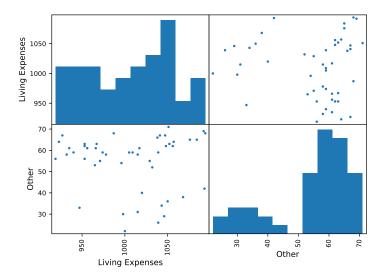


Figure 10.5: Scatter matrix comparing "Living Expenses" and "Other".

Bar Graphs

Different types of graphs help to identify different patterns. Note that the data set budget gives monthly expenses. It may be beneficial to look at one specific month. Bar graphs are a good way to compare small portions of the data set.

As a general rule, horizontal bar charts (kind="barh") are better than the default vertical bar charts (kind="bar") because most humans can detect horizontal differences more easily than vertical differences. If the labels are too long to fit on a normal figure, use plt.tight_layout() to adjust the plot boundaries to fit the labels in.

```
# Plot all data for the last month in the budget
>>> budget.iloc[-1,:].plot(kind='barh')
>>> plt.tight_layout()

# Plot all data for the last month without 'Rent' and 'Living Expenses'
>>> budget.drop(['Rent','Living Expenses'],axis=1).iloc[-1,:].plot(kind='barh')
>>> plt.tight_layout()
```

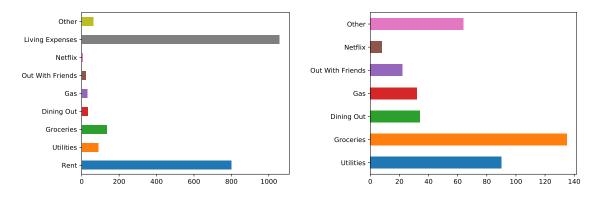


Figure 10.6: Bar graphs showing expenses paid in the last month of budget.

Problem 2. Using the crime data from the previous problem, identify if a trend exists between Forcible Rape and the following variables:

- 1. Violent
- 2. Burglary
- 3. Aggravated Assault

Make sure each graph is clearly labelled and readable. Return a tuple of booleans describing whether Forcible Rape correlates with each of the other variables.

Distributional Visualizations

While histograms are good at displaying the distributions for one column, a different visualization is needed to show the distribution of an entire set. A box plot, sometimes called a "cat-and-whisker" plot, shows the five number summary: the minimum, first quartile, median, third quartile, and maximum of the data. Box plots are useful for comparing the distributions of relatable data. However, box plots are a basic summary, meaning that they are susceptible to miss important information such as how many points were in each distribution.

```
# Compare the distributions of four columns.
>>> budget.plot(kind="box", y=["Gas","Dining Out","Out With Friends","Other"])
# Compare the distributions of all columns but 'Rent' and 'Living Expenses'.
>>> budget.drop(["Rent", "Living Expenses"], axis=1).plot(kind="box",
... vert=False)
```

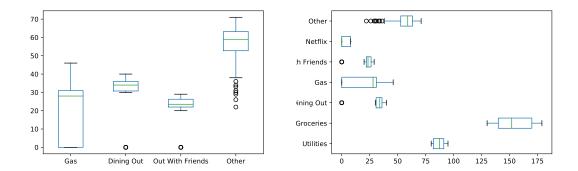


Figure 10.7: Vertical and horizontal box plots of budget dataset.

Hexbin Plots

A scatter plot is essentially a plot of samples from the joint distribution of two columns. However, scatter plots can be uninformative for large data sets when the points in a scatter plot are closely clustered. *Hexbin plots* solve this problem by plotting point density in hexagonal bins—essentially creating a 2-dimensional histogram.

The file sat_act.csv contains 700 self reported scores on the SAT Verbal, SAT Quantitative and ACT, collected as part of the Synthetic Aperture Personality Assessment (SAPA) web based personality assessment project. The obvious question with this data set is "how correlated are ACT and SAT scores?" The scatter plot of ACT scores versus SAT Quantitative scores, Figure 10.8a, is highly cluttered, even though the points have some transparency. A hexbin plot of the same data, Figure 10.8b, reveals the **frequency** of points in binned regions.

```
>>> satact = pd.read_csv("sat_act.csv", index_col="ID")
>>> list(satact.columns)
['gender', 'education', 'age', 'ACT', 'SATV', 'SATQ']

# Plot the ACT scores against the SAT Quant scores in a regular scatter plot.
>>> satact.plot(kind="scatter", x="ACT", y="SATQ", alpha=.8)

# Plot the densities of the ACT vs. SATQ scores with a hexbin plot.
>>> satact.plot(kind="hexbin", x="ACT", y="SATQ", gridsize=20)
```

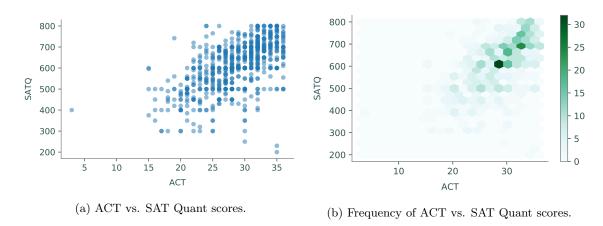


Figure 10.8: Scatter plots and hexbin plot of SAT and ACT scores.

Just as choosing a good number of bins is important for a good histogram, choosing a good gridsize is crucial for an informative hexbin plot. A large gridsize creates many small bins and a small gridsize creates fewer, larger bins.

Note

Since hexbins are based on frequencies, they are prone to being misleading if the dataset is not understood well. For example, when plotting information that deals with geographic position, increases in frequency may be results in higher populations rather than the actual information being plotted.

See http://pandas.pydata.org/pandas-docs/stable/visualization.html for more types of plots available in Pandas and further examples.

Problem 3. Use crime_data.csv to display the following distributions.

- 1. The distributions of Burglary, Violent, and Vehicle Theft,
- 2. The distributions of Vehicle Thefts against the values of Robbery.

As usual, all plots should be labeled and easy to read.

Hint: To get the x-axis label to display, you might need to set the sharex parameter of plot() to False.

Principles of Good Data Visualization

Data visualization is a powerful tool for analysis and communication. When writing a paper or report, the author must make many decisions about how to use graphics effectively to convey useful information to the reader. Here we will go over a simple process for making deliberate, effective, and efficient design decisions.

Attention to Detail

Consider the plot in Figure 10.9. It is a scatter plot of positively correlated data of some kind, with temp-likely temperature—on the x axis and cons on the y axis. However, the picture is not really communicating anything about the dataset. It has not specified the units for the x or the y axis, nor does it tell what cons is. There is no title, and the source of the data is unknown.

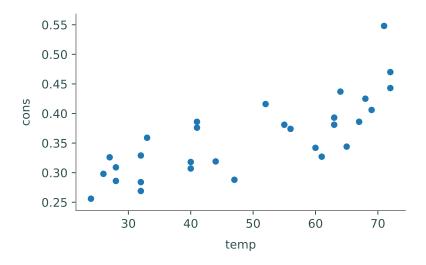


Figure 10.9: Non-specific data.

Labels and Citations

In a homework or lab setting, we sometimes (mistakenly) think that it is acceptable to leave off appropriate labels, legends, titles, and sourcing. In a published report or presentation, this kind of carelessness is confusing at best and, when the source is not included, even plagiaristic. Data needs to be explained in a useful manner that includes all of the vital information.

Consider again Figure 10.9. This figure comes from the Icecream dataset within the pydataset package, which we store here in a dataframe and then plot:

```
>>> from pydataset import data
>>> icecream = data("Icecream")
```

```
>>> icecream.plot(kind="scatter", x="temp", y="cons")
```

This code produces the rather substandard plot in Figure 10.9. Examining the source of the dataset can give important details to create better plots. When plotting data, make sure to understand what the variable names represent and where the data was taken from. Use this information to create a more effective plot.

The ice cream data used in Figure 10.9 is better understood with the following information:

- 1. The dataset details ice cream consumption via 30 four-week periods from March 1951 to July 1953 in the United States.
- 2. cons corresponds to "consumption of ice cream per capita" and is measured in pints.
- 3. income is the family's weekly income in dollars.
- 4. price is the price of a pint of ice cream.
- 5. temp corresponds to temperature, degrees Fahrenheit.
- 6. The listed source is: "Hildreth, C. and J. Lu (1960) Demand relations with autocorrelated disturbances, Technical Bulletin No 2765, Michigan State University."

This information gives important details that can be used in the following code. As seen in previous examples, pandas automatically generates legends when appropriate. Pandas also automatically labels the x and y axes, however our data frame column titles may be insufficient. Appropriate titles for the x and y axes must also list appropriate units. For example, the y axis should specify that the consumption is in units of *pints per head*, in place of the ambiguous label **cons**.

```
>>> icecream = data("Icecream")
# Set title via the title keyword argument
>>> icecream.plot(kind="scatter", x="temp", y="cons",
... title="Ice Cream Consumption in the U.S., 1951-1953")
# Override pandas automatic labelling using xlabel and ylabel
>>> plt.xlabel("Temp (Fahrenheit)")
>>> plt.ylabel("Consumption per head (pints)")
```

To add the necessary text to the figure, use either plt.annotate() or plt.text(). Alternatively, add text immediately below wherever the figure is displayed. The first two parameters of plt.text are the x and y coordinates to place the text. The third parameter is the text to write. For instance, using plt.text(0.5, 0.5, "Hello World") will center the Hello World string in the axes.

```
>>> plt.text(20, .1, r"Source: Hildreth, C. and J. Lu (1960) \emph{Demand" ... "relations with autocorrelated disturbances}\nTechnical Bulletin No" ... "2765, Michigan State University.", fontsize=7)
```

Both of these methods are imperfect but can normally be easily replaced by a caption attached to the figure. Again, we reiterate how important it is that you source any data you use; failing to do so is plagiarism.

Finally, we have a clear and demonstrative graphic in Figure 10.10.

Ice Cream Consumption in the U.S., 1951--1953

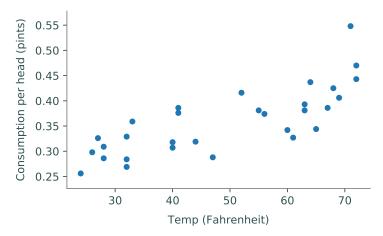


Figure 10.10: Source: Hildreth, C. and J. Lu (1960) Demand relations with autocorrelated disturbances, Technical Bulletin No 2765, Michigan State University.

ACHTUNG!

Visualizing data can inherit many biases of the visualizer and as a result can be intentionally misleading. Examples of this include, but are not limited to, visualizing subsets of data that do not represent the whole of the data and having purposely misconstrued axes. Every data visualizer has the responsibility to avoid including biases in their visualizations to ensure data is being represented informatively and accurately.

Problem 4. The dataset college.csv contains information from 1995 on universities in the United States. To access information on variable names, go to https://cran.r-project.org/web/packages/ISLR/ISLR.pdf. Create 3 plots that compare variables or universities. These plots should answer questions about the data, e.g. what is the distribution of graduation rates or do schools with lower student to faculty ratios have higher tuition costs. These three plots should be easy to understand and have clear variable names and citations.

11

Pandas 3: Grouping

Lab Objective: Many data sets contain categorical values that naturally sort the data into groups. Analyzing and comparing such groups is an important part of data analysis. In this lab we explore pandas tools for grouping data and presenting tabular data more compactly, primarily through groupby and pivot tables.

Groupby

The file mammal_sleep.csv¹ contains data on the sleep cycles of different mammals, classified by order, genus, species, and diet (carnivore, herbivore, omnivore, or insectivore). The "sleep_total" column gives the total number of hours that each animal sleeps (on average) every 24 hours. To get an idea of how many animals sleep for how long, we start off with a histogram of the "sleep_total" column.

```
>>> import pandas as pd
>>> from matplotlib import pyplot as plt
# Read in the data and print a few random entries.
>>> msleep = pd.read_csv("mammal_sleep.csv")
>>> msleep.sample(5)
      name
               genus
                       vore
                                    order sleep_total sleep_rem
51
   Jaguar Panthera carni
                                Carnivora
                                                  10.4
                                                              NaN
                                                                            NaN
77
   Tenrec
                       omni Afrosoricida
                                                  15.6
                                                              2.3
                                                                            NaN
              Tenrec
      Goat
               Capri herbi
                             Artiodactyla
                                                   5.3
                                                              0.6
                                                                            NaN
80
     Genet
             Genetta carni
                                Carnivora
                                                   6.3
                                                              1.3
                                                                            NaN
33
                                                   8.0
                                                                            1.5
     Human
                Homo
                                 Primates
                                                              1.9
                       omni
# Plot the distribution of the sleep_total variable.
>>> msleep.plot(kind="hist", y="sleep_total", title="Mammalian Sleep Data")
>>> plt.xlabel("Hours")
```

¹Proceedings of the National Academy of Sciences, 104 (3):1051–1056, 2007. Updates from V. M. Savage and G. B. West, with additional variables supplemented by Wikipedia. Available in pydataset (with a few more columns) under the key "msleep".

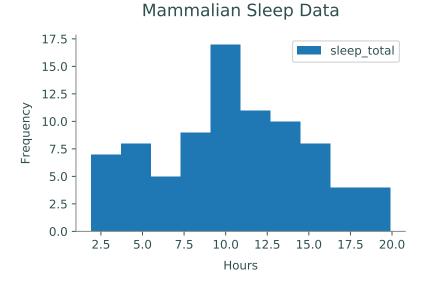


Figure 11.1: "sleep_total" frequencies from the mammalian sleep data set.

While this visualization is a good start, it doesn't provide any information about how different kinds of animals have different sleeping habits. How long do carnivores sleep compared to herbivores? Do mammals of the same genus have similar sleep patterns?

A powerful tool for answering these kinds of questions is the groupby() method of the pandas DataFrame class, which partitions the original DataFrame into groups based on the values in one or more columns. The groupby() method does **not** return a new DataFrame; it returns a pandas GroupBy object, an interface for analyzing the original DataFrame by groups.

For example, the columns "genus", "vore", and "order" in the mammal sleep data all have a discrete number of categorical values that could be used to group the data. Since the "vore" column has only a few unique values, we start by grouping the animals by diet.

```
# List all of the unique values in the 'vore' column.
>>> set(msleep["vore"])
{nan, 'herbi', 'omni', 'carni', 'insecti'}
# Group the data by the 'vore' column.
>>> vores = msleep.groupby("vore")
>>> list(vores.groups)
['carni', 'herbi', 'insecti', 'omni']
                                              # NaN values for vore were dropped.
# Get a single group and sample a few rows. Note vore='carni' in each entry.
>>> vores.get_group("carni").sample(5)
                 genus
       name
                         vore
                                    order
                                           sleep_total
                                                         sleep_rem
                                                                    sleep_cycle
80
      Genet
              Genetta
                       carni
                               Carnivora
                                                   6.3
                                                               1.3
                                                                             NaN
50
                                                  15.8
                                                                             NaN
      Tiger
             Panthera
                        carni
                               Carnivora
                                                               NaN
                                                               2.9
8
        Dog
                 Canis
                        carni
                               Carnivora
                                                   10.1
                                                                           0.333
0
    Cheetah
                               Carnivora
                                                   12.1
                                                               {\tt NaN}
                                                                             NaN
             Acinonyx
                        carni
82
   Red fox
               Vulpes
                        carni
                               Carnivora
                                                   9.8
                                                               2.4
                                                                           0.350
```

As shown above, groupby() is useful for filtering a DataFrame by column values; the command df.groupby(col).get_group(value) returns the rows of df where the entry of the col column is value. The real advantage of groupby(), however, is how easily it compares groups of data. Standard DataFrame methods like describe(), mean(), std(), min(), and max() all work on GroupBy objects to produce a new data frame that describes the statistics of each group.

```
# Get averages of the numerical columns for each group.
>>> vores.mean()
         sleep_total sleep_rem sleep_cycle
vore
                                          0.373
               10.379
                           2.290
carni
herbi
                9.509
                           1.367
                                          0.418
insecti
               14.940
                           3.525
                                          0.161
               10.925
                           1.956
omni
                                          0.592
# Get more detailed statistics for 'sleep_total' by group.
>>> vores["sleep_total"].describe()
                                       25%
          count
                   mean
                            std
                                              50%
                                                      75%
                                                             max
vore
                 10.379
                         4.669
                                 2.7
                                      6.25
                                             10.4
                                                   13.000
                                                            19.4
          19.0
carni
          32.0
                  9.509
                         4.879
                                 1.9
                                      4.30
                                             10.3
                                                   14.225
                                                            16.6
herbi
insecti
           5.0
                14.940
                         5.921
                                 8.4
                                      8.60
                                             18.1
                                                   19.700
                                                            19.9
          20.0
                 10.925
                         2.949
                                 8.0
                                      9.10
                                              9.9
                                                   10.925
                                                            18.0
omni
```

Multiple columns can be used simultaneously for grouping. In this case, the get_group() method of the GroupBy object requires a tuple specifying the values for each of the grouping columns.

```
>>> msleep_small = msleep.drop(["sleep_rem", "sleep_cycle"], axis=1)
>>> vores_orders = msleep_small.groupby(["vore", "order"])
>>> vores_orders.get_group(("carni", "Cetacea"))
                                   genus
                     name
                                                    order
                                                           sleep_total
                                            vore
30
             Pilot whale
                           Globicephalus
                                           carni
                                                  Cetacea
                                                                    2.7
59
                                                                    5.6
         Common porpoise
                                Phocoena
                                           carni
                                                  Cetacea
79
   Bottle-nosed dolphin
                                                                    5.2
                                Tursiops
                                           carni
                                                  Cetacea
```

Problem 1. Read in the data college.csv containing information on various United States universities in 1995. To access information on variable names, go to https://cran.r-project.org/web/packages/ISLR/ISLR.pdf. Use a groupby object to group the colleges by private and public universities. Read in the data as a DataFrame object and use groupby and describe to examine the following columns by group:

- 1. Student to faculty ratio
- 2. Percent of students from the top 10% of their high school class
- 3. Percent of students from the top 25% of their high school class

Determine whether private or public universities have a higher mean for each of these columns. For the type of university with the higher mean, save the values of the describe function on said column as an array using .values. Return a tuple with these arrays in the order described above.

For example, if we were comparing whether the average number of professors with PhDs was higher at private or public universities, we would find that public universities have a higher average, and we would return the following array:

```
array([212., 76.83490566, 12.31752531, 33., 71., 78.5 , 86., 103.])
```

Visualizing Groups

There are a few ways that groupby() can simplify the process of visualizing groups of data. First of all, groupby() makes it easy to visualize one group at a time using the plot method. The following visualization improves on Figure 11.1 by grouping mammals by their diets.

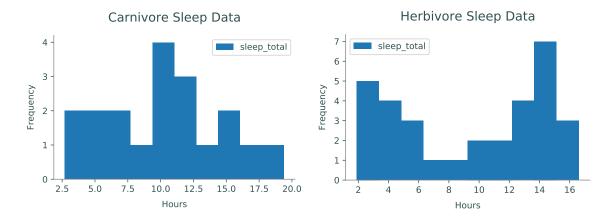
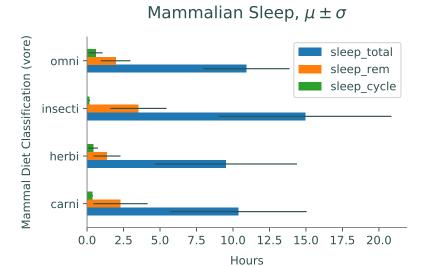


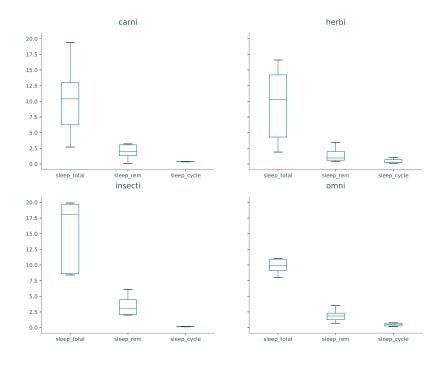
Figure 11.2: "sleep_total" histograms for two groups in the mammalian sleep data set.

The statistical summaries from the GroupBy object's mean(), std(), or describe() methods also lend themselves well to certain visualizations for comparing groups.



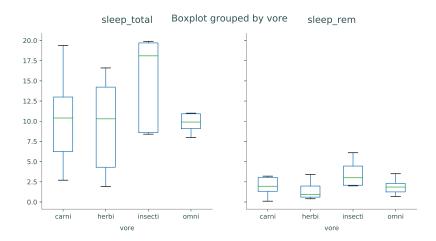
Box plots are well suited for comparing similar distributions. The boxplot() method of the GroupBy class creates one subplot **per group**, plotting each of the columns as a box plot.

```
# Use GroupBy.boxplot() to generate one box plot per group.
>>> vores.boxplot(grid=False)
>>> plt.tight_layout()
```



Alternatively, the boxplot() method of the DataFrame class creates one subplot **per column**, plotting each of the columns as a box plot. Specify the by keyword to group the data appropriately.

```
# Use DataFrame.boxplot() to generate one box plot per column.
>>> msleep.boxplot(["sleep_total", "sleep_rem"], by="vore", grid=False)
```



Like groupby(), the by argument can be a single column label or a list of column labels. Similar methods exist for creating histograms (GroupBy.hist() and DataFrame.hist() with by keyword), but generally box plots are better for comparing multiple distributions.

Problem 2. Create visualizations that give relevant information answering the following questions (using college.csv):

- 1. How do the number of applicants, number of accepted students, and number of enrolled students compare between private and public universities?
- 2. How does the range of money spent on room and board compare between private and public universities?

Pivot Tables

One of the downfalls of <code>groupby()</code> is that a typical <code>GroupBy</code> object has too much information to display coherently. A *pivot table* intelligently summarizes the results of a <code>groupby()</code> operation by aggregating the data in a specified way. The standard tool for making a pivot table is the <code>pivot_table()</code> method of the <code>DataFrame</code> class. As an example, consider the <code>"HairEyeColor"</code> data set from <code>pydataset</code>.

```
Black
           Brown
                    Male
                             32
    Brown
           Green
                    Male
                             15
                              7
31
      Red
           Green
                  Female
21
   Black
            Blue
                  Female
                              9
>>> for col in ["Hair", "Eye", "Sex"]:
                                             # Get unique values per column.
        print("{}: {}".format(col, ", ".join(set(str(x) for x in hec[col]))))
Hair: Brown, Black, Blond, Red
Eye: Brown, Blue, Hazel, Green
Sex: Male, Female
```

There are several ways to group this data with groupby(). However, since there is only one entry per unique hair-eye-sex combination, the data can be completely presented in a pivot table.

```
>>> hec.pivot_table(values="Freq", index=["Hair", "Eye"], columns="Sex")
Sex
              Female Male
Hair Eye
                    9
Black Blue
                         11
      Brown
                   36
                         32
      Green
                    2
                          3
      Hazel
                    5
                         10
Blond Blue
                   64
                         30
      Brown
                    4
                          3
      Green
                    8
                          8
                    5
                          5
      Hazel
Brown Blue
                   34
                         50
      Brown
                   66
                         53
      Green
                   14
                         15
      Hazel
                   29
                         25
                   7
                         10
Red
      Blue
      Brown
                   16
                         10
                    7
                          7
      Green
                    7
                          7
      Hazel
```

Listing the data in this way makes it easy to locate data and compare the female and male groups. For example, it is easy to see that brown hair is more common than red hair and that about twice as many females have blond hair and blue eyes than males.

Unlike "HairEyeColor", many data sets have more than one entry in the data for each grouping. An example in the previous dataset would be if there were two or more rows in the original data for females with blond hair and blue eyes. To construct a pivot table, data of similar groups must be aggregated together in some way.

By default entries are aggregated by averaging the non-null values. You can use the keyword argument aggfunc to choose among different ways to aggregate the data. For example, if you use aggfunc='min', the value displayed will be the minimum of all the values. Other arguments include 'max', 'std' for standard deviation, 'sum', or 'count' to count the number of occurrences. You also may pass in any function that reduces to a single float, like np.argmax or even np.linalg.norm if you wish. A list of functions can also be passed into the aggfunc keyword argument.

Consider the Titanic data set found in titanic.csv². For this analysis, take only the "Survived", "Pclass", "Sex", "Age", "Fare", and "Embarked" columns, replace null age values with the average age, then drop any rows that are missing data. To begin, we examine the average survival rate grouped by sex and passenger class.

```
>>> titanic = pd.read_csv("titanic.csv")
>>> titanic = titanic[["Survived", "Pclass", "Sex", "Age", "Fare", "Embarked"]]
>>> titanic["Age"].fillna(titanic["Age"].mean(),)

>>> titanic.pivot_table(values="Survived", index="Sex", columns="Pclass")
Pclass    1.0    2.0    3.0
Sex
female    0.965    0.887    0.491
male    0.341    0.146    0.152
```

Note

The pivot_table() method is a convenient way of performing a potentially complicated groupby() operation with aggregation and some reshaping. The following code is equivalent to the previous example.

```
>>> titanic.groupby(["Sex", "Pclass"])["Survived"].mean().unstack()
Pclass 1.0 2.0 3.0
Sex
female 0.965 0.887 0.491
male 0.341 0.146 0.152
```

The stack(), unstack(), and pivot() methods provide more advanced shaping options.

Among other things, this pivot table clearly shows how much more likely females were to survive than males. To see how many entries fall into each category, or how many survived in each category, aggregate by counting or summing instead of taking the mean.

```
# See how many entries are in each category.
>>> titanic.pivot_table(values="Survived", index="Sex", columns="Pclass",
                        aggfunc="count")
Pclass 1.0 2.0 3.0
Sex
       144
            106 216
female
male
        179
            171 493
# See how many people from each category survived.
>>> titanic.pivot_table(values="Survived", index="Sex", columns="Pclass",
                        aggfunc="sum")
Pclass
                       3.0
          1.0
                2.0
```

²There is a "Titanic" data set in pydataset, but it does not contain as much information as the data in titanic.csv.

```
Sex
female 137.0 94.0 106.0
male 61.0 25.0 75.0
```

Problem 3. The file Ohio_1999.csv contains data on workers in Ohio in the year 1999. Use pivot tables to answer the following questions:

- 1. Which race/sex combination has the highest Usual Weekly Earnings in total?
- 2. Which race/sex combination has the lowest cumulative Usual Hours Worked?
- 3. What race/sex combination has the highest average Usual Hours Worked?

Return a tuple for each question (in order of the questions) where the first entry is the numerical code corresponding to the race and the second entry is corresponding to the sex.

Some useful keys in understand the data are as follows:

- 1. In column Sex, {1: male, 2: female}.

Discretizing Continuous Data

In the Titanic data, we examined survival rates based on sex and passenger class. Another factor that could have played into survival is age. Were male children as likely to die as females in general? We can investigate this question by *multi-indexing*, or pivoting, on more than just two variables, by adding in another index.

In the original dataset, the "Age" column has a floating point value for the age of each passenger. If we add "Age" as another pivot, then the table would create a new row for **each** age present. Instead, we partition the "Age" column into intervals with pd.cut(), thus creating a categorical that can be used for grouping. Notice that when creating the pivot table, the index uses the categorical age instead of the column name "Age".

```
# pd.cut() maps continuous entries to discrete intervals.
>>> pd.cut([1, 2, 3, 4, 5, 6, 7], [0, 4, 8])
[(0, 4], (0, 4], (0, 4], (0, 4], (0, 4], (4, 8], (4, 8], (4, 8]]
Categories (2, interval[int64]): [(0, 4] < (4, 8]]
# Partition the passengers into 3 categories based on age.
>>> age = pd.cut(titanic['Age'], [0, 12, 18, 80])
>>> titanic.pivot_table(values="Survived", index=["Sex", age],
                        columns="Pclass", aggfunc="mean")
Pclass
                   1.0
                          2.0
                                 3.0
Sex
       Age
                 0.000 1.000 0.467
female (0, 12]
```

```
(12, 18]
                 1.000 0.875
                               0.607
       (18, 80]
                 0.969
                        0.871
                               0.475
       (0, 12]
                        1.000
                               0.343
male
                 1.000
       (12, 18]
                 0.500 0.000
                               0.081
       (18, 80]
                 0.322 0.093 0.143
```

From this table, it appears that male children (ages 0 to 12) in the 1st and 2nd class were very likely to survive, whereas those in 3rd class were much less likely to. This clarifies the claim that males were less likely to survive than females. However, there are a few oddities in this table: zero percent of the female children in 1st class survived, and zero percent of teenage males in second class survived. To further investigate, count the number of entries in each group.

```
>>> titanic.pivot_table(values="Survived", index=["Sex", age],
                          columns="Pclass", aggfunc="count")
Pclass
                  1.0 2.0
                            3.0
Sex
       Age
female (0, 12]
                        13
                              30
                    1
       (12, 18]
                   12
                         8
                              28
                  129
       (18, 80]
                        85
                             158
       (0, 12]
                    4
                        11
                              35
male
       (12, 18]
                    4
                        10
                              37
       (18, 80]
                       150
                             420
                  171
```

This table shows that there was only 1 female child in first class and only 10 male teenagers in second class, which sheds light on the previous table.

ACHTUNG!

The previous pivot table brings up an important point about partitioning datasets. The Titanic dataset includes data for about 1300 passengers, which is a somewhat reasonable sample size, but half of the groupings include less than 30 entries, which is **not** a healthy sample size for statistical analysis. Always carefully question the numbers from pivot tables before making any conclusions.

Pandas also supports multi-indexing on the columns. As an example, consider the price of a passenger tickets. This is another continuous feature that can be discretized with pd.cut(). Instead, we use pd.qcut() to split the prices into 2 equal quantiles. Some of the resulting groups are empty; to improve readability, specify fill_value as the empty string or a dash.

		;	aggfunc='	'coun	t", f	ill_value='-')			
Fare		(-0.001,	14.454]			(14.454, 512.329]			
Pclass			1.0	2.0	3.0	1.0	2.0	3.0	
Sex	Age								
female	(0, 12]		-	-	7	1	13	23	
	(12, 18]		-	4	23	12	4	5	
	(18, 80]		-	31	101	129	54	57	
male	(0, 12]		-	-	8	4	11	27	
	(12, 18]		-	5	26	4	5	11	
	(18, 80]		8	94	350	163	56	70	

Not surprisingly, most of the cheap tickets went to passengers in 3rd class.

Problem 4. Use the employment data from Ohio in 1999 to answer the following questions:

- 1. The column Educational Attainment contains numbers 0-46. Any number less than 39 means the person did not get any form of degree. 39-42 refers to either a high-school or associate's degree. A number greater than or equal to 43 means the person got at least a bachelor's degree. Out of these categories, which degree type is the most common among these workers?
- 2. Partition the Age column into 6 equally-sized groups using pd.qcut(). Which interval has the highest average Usual Hours Worked?
- 3. Using the partitions from the first two parts, what age/degree combination has the lowest yearly salary on average?

Return the answer to each question (in order) as an Interval. For part three, the answer should be a tuple where the first entry in the Interval of the age and the second is the Interval of the degree.

An Interval is the object returned by pd.cut() and pd.qcut(). These can also be obtained from a pivot table, as in the example below.

Problem 5. Examine the college dataset using pivot tables and groupby objects. Determine the answer to the following questions. If the answer is yes, save the answer as True. If the answer the no, save the answer as False. For the last question, save the answer as a string giving your explanation. Return a tuple containing your answers to the questions in order.

- 1. Is there a correlation between the percent of alumni that donate and the amount the school spends per student in BOTH private and public universities?
- 2. Partition Grad.Rate into evenly spaced intervals of 20%. Is the partition with the greatest number of schools the same for private and public universities?
- 3. Does having a lower acceptance rate correlate with having more students from the top 10 percent of their high school class being admitted on average for BOTH private and public universities?
- 4. Why is the average percentage of students admitted from the top 10 percent of their high school class so high in private universities with very low acceptance rates? Use only the data to explain why; do not extrapolate.

12 GeoPandas

Lab Objective: GeoPandas is a package designed to organize and manipulate geographic data, It combines the data manipulation tools of pandas with the geometric capabilities of the Shapely package. In this lab, we explore the basic data structures of GeoSeries and GeoDataFrames and their functionalities.

Installation

GeoPandas is a new package designed to combine the functionality of pandas with Shapely, a package used for geometric manipulation. Using GeoPandas with geographic data is very useful as it allows the user to not only compare numerical data, but also geometric attributes. GeoPandas can be installed via pip:

>>> pip install geopandas

However, Geopandas can be notoriously difficult to install. This is especially the case if the python environment is not carefully maintained. Some of its dependencies can also be very difficult to install on certain systems. Because of this, using Colab for this lab is recommended; its environment is set up in a way that makes GeoPandas very easy to install. Otherwise, the GeoPandas documentation contains some additional options that can be used if installation difficulties occur: https://geopandas.org/install.html.

GeoSeries

A GeoSeries is a pandas Series where each entry is a set of geometric objects. There are three classes of geometric objects inherited from the Shapely package:

- 1. Points / Multi-Points
- 2. Lines / Multi-Lines
- 3. Polygons / Multi-Polygons

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A point is used to identify objects like coordinates, where there is one small instance of the object. A line could be used to describe objects such as roads. A polygon could be used to identify regions, such as a country. Multipoints, multilines, and multipolygons contain lists of points, lines, and polygons, respectively.

Since each object in the GeoSeries is also a Shapely object, the GeoSeries inherits many methods and attributes of Shapely objects. Some of the key attributes and methods are listed in Table 12.1. These attributes and methods can be used to calculate distances, find the sizes of countries, and determine whether coordinates are within country's boundaries. The example below uses the attribute bounds to find the maximum and minimum coordinates of Egypt in a built-in GeoDataFrame.

${\bf Method/Attribute}$	Description				
distance(other)	returns minimum distance from GeoSeries to other				
<pre>contains(other)</pre>	returns True if shape contains other				
<pre>intersects(other)</pre>	returns True if shape intersects other				
area	returns shape area				
convex_hull	returns convex shape around all points in the object				
bounds	returns the bounding x- and y-coordinates of the object				

Table 12.1: Attributes and Methods for GeoSeries

Creating GeoDataFrames

The main structure used in GeoPandas is a GeoDataFrame, which is similar to a pandas DataFrame. A GeoDataFrame has one special column called geometry, which must be a GeoSeries. This GeoSeries column is used when a spatial method, like distance(), is used on the GeoDataFrame.

A GeoDataFrame can be made from a pandas DataFrame. At least one of the columns in the DataFrame should contain geometric information. This column containing geometric information can be converted to a GeoSeries using the apply() method. At this point, the Pandas DataFrame can be cast as a GeoDataFrame. Assign which column will be the geometry using either the geometry keyword in the constructor or the set_geometry() method afterwards.

```
>>> import pandas as pd
>>> import geopandas as gpd
>>> from shapely.geometry import Point, Polygon
# Create a Pandas DataFrame
```

```
>>> df = pd.DataFrame({'City': ['Seoul', 'Lima', 'Johannesburg'],
                      'Country': ['South Korea', 'Peru', 'South Africa'],
. . .
                      'Latitude': [37.57, -12.05, -26.20],
. . .
                      'Longitude': [126.98, -77.04, 28.04]})
# Create geometry column
>>> df['Coordinates'] = list(zip(df.Longitude, df.Latitude))
# Make geometry column Shapely objects
>>> df['Coordinates'] = df['Coordinates'].apply(Point)
# Cast as GeoDataFrame
>>> gdf = gpd.GeoDataFrame(df, geometry='Coordinates')
# Equivalently, specify the geometry after construction
# Note that set_geometry() returns a new GeoDataFrame
>>> gdf = gpd.GeoDataFrame(df)
>>> gdf = gdf.set_geometry('Coordinates')
# Display the GeoDataFrame
>>> gdf
           City
                      Country Latitude Longitude
                                                                    Coordinates
                                                     POINT (126.98000 37.57000)
0
          Seoul
                  South Korea
                                 37.57 126.98
          Lima
                        Peru
                                 -12.05
                                            -77.04 POINT (-77.04000 -12.05000)
2 Johannesburg South Africa
                                -26.20
                                             28.04 POINT (28.04000 -26.20000)
# Create a polygon with all three cities as points
>>> city_polygon = Polygon(list(zip(df.Longitude, df.Latitude)))
```

A GeoDataFrame can also be made directly from a dictionary. If the dictionary already contains geometric objects, the corresponding column can be directly set as the geometry in the constructor. Otherwise, a column containing geometry data can be created as in the above example and then set as the geometry with the set_geometry() method.

```
# Both of these methods create the same GeoDataFrame as above
# Directly create the GeoDataFrame from the dictionary
>>> gdf = gpd.GeoDataFrame({'City': ['Seoul', 'Lima', 'Johannesburg'],
                      'Country': ['South Korea', 'Peru', 'South Africa'],
. . .
                      'Latitude': [37.57, -12.05, -26.20],
. . .
                      'Longitude': [126.98, -77.04, 28.04]})
# Create geometry column and set as the geometry
>>> gdf['Coordinates'] = list(zip(df.Longitude, df.Latitude))
>>> gdf['Coordinates'] = df['Coordinates'].apply(Point)
# inplace=True modifies gdf itself rather than returning a copy
>>> gdf.set_geometry('Coordinates', inplace=True)
# Equivalently, using a dictionary that already contains geometry objects
>>> gdf = gpd.GeoDataFrame({'City': ['Seoul', 'Lima', 'Johannesburg'],
                      'Country': ['South Korea', 'Peru', 'South Africa'],
```

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```
... 'Coordinates': [Point(126.98,37.57),
... Point(-77.04,-12.05), Point(28.04,-12.05)]},
... geometry='Coordinates')
```

Note

Longitude is the angular measurement starting at the Prime Meridian, 0° , and going to 180° to the east and -180° to the west. Latitude is the angle between the equatorial plane and the normal line at a given point; a point along the Equator has latitude 0, the North Pole has latitude $+90^{\circ}$ or $90^{\circ}N$, and the South Pole has latitude -90° or $90^{\circ}S$.

Plotting GeoDataFrames

Information from a GeoDataFrame is plotted based on the geometry column. Data points are displayed as geometry objects. The following example plots the shapes in the world GeoDataFrame.

```
# Plot world GeoDataFrame
>>> world.plot()
```

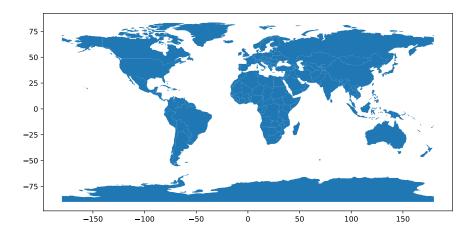


Figure 12.1: World map

Multiple GeoDataFrames can be plotted at once. This can be done by by setting one GeoDataFrame as the base of the plot and ensuring that each layer uses the same axes. In the following example, the file airports.csv, containing the coordinates of world airports, is loaded into a GeoDataFrame and plotted on top of the boundary of the world GeoDataFrame.

```
# Set outline of world countries as base
>>> fig,ax = plt.subplots(figsize=(10,7), ncols=1, nrows=1)
>>> base = world.boundary.plot(edgecolor='black', ax=ax, linewidth=1)
# Load airport data and convert to a GeoDataFrame
```

```
>>> airports = pd.read_csv('airports.csv')
>>> airports['Coordinates'] = list(zip(airports.Longitude, airports.Latitude))
>>> airports['Coordinates'] = airports.Coordinates.apply(Point)
>>> airports = gpd.GeoDataFrame(airports, geometry='Coordinates')

# Plot airports on top of world map
>>> airports.plot(ax=base, marker='o', color='green', markersize=1)
>>> ax.set_xlabel('Longitude')
>>> ax.set_ylabel('Latitude')
>>> ax.set_title('World Airports')
```

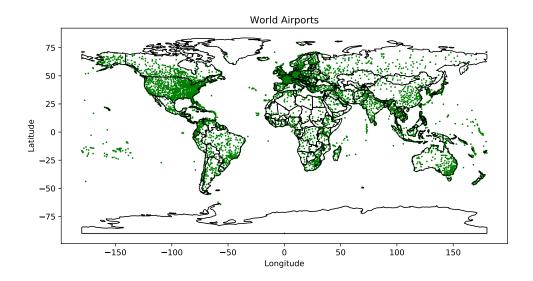


Figure 12.2: Airport map

Problem 1. Read in the file airports.csv as a pandas DataFrame. Create three convex hulls around the three sets of airports listed below. This can be done by passing in lists of the airports' coordinates to a shapely.geometry.Polygon object.

Create a new GeoDataFrame with these three Polygons as entries. Plot this GeoDataFrame on top of an outlined world map.

- Maio Airport, Scatsta Airport, Stokmarknes Skagen Airport, Bekily Airport, K. D. Matanzima Airport, RAF Ascension Island
- Oiapoque Airport, Maio Airport, Zhezkazgan Airport, Walton Airport, RAF Ascension Island, Usiminas Airport, Piloto Osvaldo Marques Dias Airport
- Zhezkazgan Airport, Khanty Mansiysk Airport, Novy Urengoy Airport, Kalay Airport, Biju Patnaik Airport, Walton Airport

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Working with GeoDataFrames

As previously mentioned, GeoDataFrames contain many of the functionalities of pandas DataFrames. For example, to create a new column, define a new column name in the GeoDataFrame with the needed information for each GeoSeries.

```
# Create column in the world GeoDataFrame for gdp_per_capita
>>> world['gdp_per_cap'] = world.gdp_md_est / world.pop_est
```

GeoDataFrames can utilize many pandas functionalities, and they can also be parsed by geometric manipulations. For example, a useful way to index GeoDataFrames is with the cx indexer. This splits the GeoDataFrame by the coordinates of each geometric object. It is used by calling the method cx on a GeoDataFrame, followed by a slicing argument, where the first element refers to the longitude and the second refers to latitude.

```
# Create a GeoDataFrame containing the northern hemisphere
>>> north = world.cx[:, 0:]

# Create a GeoDataFrame containing the southeastern hemisphere
>>> south_east = world.cx[0:, :0]
```

GeoSeries objects in a GeoDataFrame can also be dissolved, or merged, together into one GeoSeries based on their geometry data. For example, all countries on one continent could be merged to create a GeoSeries containing the information of that continent. The method designed for this is called dissolve. It receives two parameters, by and aggfunc. by indicates which column to dissolve along, and aggfunc tells how to combine the information in all other columns. The default aggfunc is first, which returns the first application entry. In the following example, we use sum as the aggfunc so that each continent is the combination of its countries.

```
>>> world = world[['continent', 'geometry', 'gdp_per_cap']]
# Dissolve world GeoDataFrame by continent
>>> continent = world.dissolve(by = 'continent', aggfunc='sum')
```

Projections and Coloring

When plotting, GeoPandas uses the CRS (coordinate reference system) of a GeoDataFrame. This reference system indicates how coordinates should be spaced on a plot. Two of the most commonly used CRSs are EPSG:4326 and EPSG:3395. EPSG:4326 is the standard latitude-longitude projection used by GPS. EPSG:3395, also known as the Mercator projection, is the standard navigational projection.

When creating a new GeoDataFrame, it is important to set the crs attribute of the GeoDataFrame. This allows any plots to be shown correctly. Furthermore, GeoDataFrames being layered need to have the same CRS. To change the CRS, use the method to_crs().

```
# Check CRS of world GeoDataFrame
>>> print(world.crs)
epsg:4326
```

```
# Change CRS of world to Mercator
# inplace=True ensures that we modify world instead of returning a copy
>>> world.to_crs(3395, inplace=True)
>>> print(world.crs)
epsg:3395
```

GeoPandas accepts many different CRSs; a reference can be found at www.spatialreference. org. Additionally, inspecting a given CRS object in the terminal without using print() or str() can be used to get additional information about a specific CRS:¹

```
>>> world.crs
<Projected CRS: EPSG:3395>
Name: WGS 84 / World Mercator
Axis Info [cartesian]:
- E[east]: Easting (metre)
- N[north]: Northing (metre)
Area of Use:
- name: World between 80°S and 84°N.
- bounds: (-180.0, -80.0, 180.0, 84.0)
Coordinate Operation:
- name: World Mercator
- method: Mercator (variant A)
Datum: World Geodetic System 1984
- Ellipsoid: WGS 84
- Prime Meridian: Greenwich
```

GeoDataFrames can also be plotted using the values in the the other attributes of the GeoSeries. The map plots the color of each geometry object according to the value of the column selected. This is done by passing in the parameter column into the plot() method.

```
>>> fig, ax = plt.subplots(1, figsize=(10,4))
# Plot world based on gdp
>>> world.plot(column='gdp_md_est', cmap='OrRd', legend=True, ax=ax)
>>> ax.set_title('World Map based on GDP')
>>> ax.set_xlabel('Longitude')
>>> ax.set_ylabel('Latitude')
>>> plt.show()
```

¹This can also be accomplished using print(repr(crs)).

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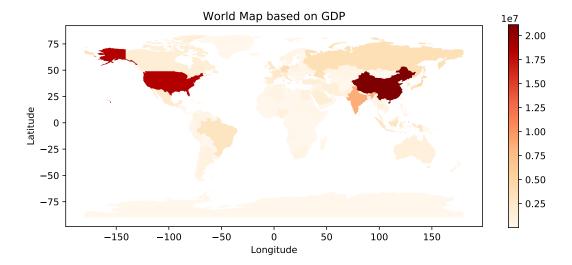


Figure 12.3: World Map Based on GDP

Problem 2. The file county_data.gpkg.zip contains information about US counties.^a After unzipping, use the command gpd.read_file('county_data.gpkg') to create a GeoDataFrame of this information. Each county's shape is stored in the geometry column. Use this to plot all US counties two times, first using the default CRS and then using EPSG:5071.

Next, create a new GeoDataFrame that merges all counties within a single state. Drop regions with the following STATEFP codes: 02, 15, 60, 66, 69, 72, 78. Plot this GeoDataFrame to see an outline of all 48 contiguous states. Ensure a CRS of EPSG:5071.

 ${\it ^a} Source: \ \texttt{http://www2.census.gov/geo/tiger/GENZ2016/shp/cb_2016_us_county_5m.zip}$

Note

.gpkg files are actually structured as a directory that contains several files that each contain parts of the data. For instance, county_data.gpkg consists of the files county_data.cpg, county_data.dbf, county_data.prj, county_data.shp, and county_data.shx. Be sure that these files are placed directly in the first level of folders, and not in further subdirectories. To use this file in Google Colab, upload the zipped file and extract it with the following code:

```
county = files.upload()
!unzip county_data.gpkg.zip
```

It then can be loaded:

```
county_df = gpd.read_file('county_data.gpkg')
```

Merging GeoDataFrames

Just as multiple pandas DataFrames can be merged, multiple GeoDataFrames can be merged with attribute joins or spatial joins. An attribute join is similar to a merge in pandas. It combines two GeoDataFrames on a column (not the geometry column) and then combines the rest of the data into one GeoDataFrame.

```
>>> world = gpd.read_file(geopandas.datasets.get_path('naturalearth_lowres'))
>>> cities = gpd.read_file(geopandas.datasets.get_path('naturalearth_cities'))

# Create subsets of the world and cities GeoDataFrames
>>> world = world[['continent', 'name', 'iso_a3']]
>>> cities = cities[['name', 'iso_a3']]

# Merge the GeoDataFrames on their iso_a3 code
>>> countries = world.merge(cities, on='iso_a3')
```

A spatial join merges two GeoDataFrames based on their geometry data. The function used for this is sjoin accepts two GeoDataFrames and then direction on how to merge. It is imperative that two GeoDataFrames have the same CRS. In the example below, we merge using an inner join with the option intersects. The inner join means that we will only use keys in the intersection of both geometry columns, and we will retain only the left geometry column. intersects tells the GeoDataFrames to merge on GeoSeries that intersect each other. Other options include contains and within.

```
# Combine countries and cities on their geographic location
>>> countries = gpd.sjoin(world, cities, how='inner', op='intersects')
```

Problem 3. Load in the file nytimes.csv^a as a DataFrame. This file includes county-level data for the cumulative cases and deaths of Covid-19 in the US, starting with the first case in Snohomish County, Washington, on January 21, 2020. Begin by converting the date column into a DatetimeIndex.

Next, use county FIPS codes to merge your GeoDataFrame from Problem 2 with the DataFrame you just created. A FIPS code is a 5-digit unique identifier for geographic locations. Ignore rows in the Covid-19 DataFrame with unknown FIPS codes as well as all data from Hawaii and Alaska.

Note that the fips column of the Covid-19 DataFrame stores entries as floats, but the county GeoDataFrame stores FIPS codes as strings, with the first two digits in the STATEFP column and the last three in the COUNTYFP column.

Once you have completed the merge, plot the cases from March 21, 2020 on top of your state outline map from Problem 2, using the CRS of EPSG:5071. Finally, print out the name of the county with the most cases on March 21, 2020 along with its case count.

^aSource: https://raw.githubusercontent.com/nytimes/covid-19-data/master/us-counties.csv

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Logarithmic Plotting Techniques

The color scheme of a graph can also help to communicate information clearly. A good list of available colormaps can be found at https://matplotlib.org/3.2.1/gallery/color/colormap_reference.html. Note also that you can reverse any colormap by adding _r to the end. The following example demonstrates some plotting features, using country GDP as in Figure 12.3.

```
>>> fig, ax = plt.subplots(figsize=(15,7), ncols=1, nrows=1)
>>> world.plot(column='gdp_md_est', cmap='plasma_r',
... ax=ax, legend=True, edgecolor='gray')

# Add title and remove axis tick marks
>>> ax.set_title('GDP on Linear Scale')
>>> ax.set_yticks([])
>>> ax.set_xticks([])
>>> plt.show()
```

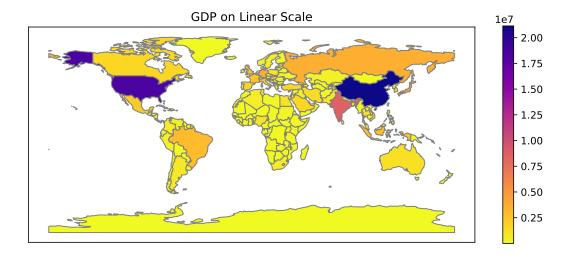


Figure 12.4: World map showing country GDP

Sometimes data can be much more informative when plotted on a logarithmic scale. See how the world map changes when we add a norm argument in the code below. Depending on the purpose of the graph, Figure 12.5 may be more informative than Figure 12.4.

```
>>> from matplotlib.colors import LogNorm
>>> from matplotlib.cm import ScalarMappable
>>> fig, ax = plt.subplots(figsize=(15,6), ncols=1, nrows=1)

# Set the norm using data bounds
>>> data = world.gdp_md_est
>>> norm = LogNorm(vmin=min(data), vmax=max(data))

# Plot the graph using the norm
>>> world.plot(column='gdp_md_est', cmap='plasma_r', ax=ax,
```

```
# Create a custom colorbar
>>> cbar = fig.colorbar(ScalarMappable(norm=norm, cmap='plasma_r'),
... ax=ax, orientation='horizontal', pad=0, label='GDP')

>>> ax.set_title('Country Area on a Log Scale')
>>> ax.set_yticks([])
>>> ax.set_xticks([])
>>> plt.show()
```

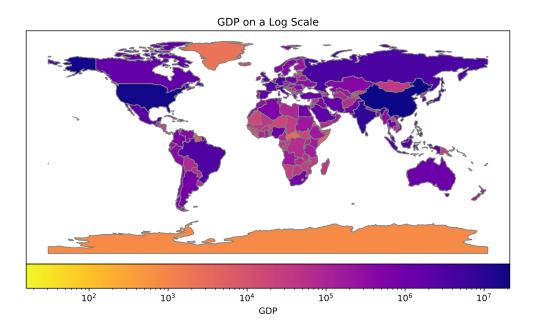


Figure 12.5: World map showing country GDP using a log scale

Problem 4. As in Problem 3, plot your state outline map from Problem 2 on top of a map of the Covid-19 cases from March 21, 2020. This time, however, use a log scale. Use EPSG:5071 for the CRS. Pick a good colormap (the counties with the most cases should generally be darkest) and be sure to display a colorbar.

Problem 5. In this problem, you will create an animation of the spread of Covid-19 through US counties from January 21, 2020 to June 21, 2020. Use a log scale and a good colormap, and be sure that you're using the same norm and colorbar for the whole animation. Use EPSG:5071 for the projection.

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As a reminder, below is a summary of what you will need in order to animate this map. You may also find it helpful to refer to the animation section included with the Volume 4 lab manual.

- 1. Set up your figure and norm. Be sure to use the highest case count for your vmax so that the scale remains uniform.
- 2. Write your update function. This should plot the cases from a given day.
- 3. Set up your colorbar. Do this outside the update function to avoid adding a new colorbar each day.
- 4. Create the animation and embed it.

13 Data Cleaning

Lab Objective: The quality of a data analysis or model is limited by the quality of the data used. In this lab we learn techniques for cleaning data, creating features, and determining feature importance.

Almost every dataset has problems that make it unsuitable for regression or other modeling. At a basic level, these problems might cause simple functions to error out. More substantially, data problems could significantly change the result of your model or analysis.

Data cleaning is the process of identifying and correcting bad data. This could be data that is missing, duplicated, irrelevant, inconsistent, incorrect, in the wrong format, or does not make sense. Though it can be tedious, data cleaning is the most important step of data analysis. Without accurate and legitimate data, any results or conclusions are suspect and may be incorrect.

We will demonstrate common issues with data and how to correct them using the following dataset. It consists of family members and some basic details.

```
# Example dataset
>>> df = pd.read_csv('toy_dataset.csv')
>>>
                                            DOB Marital_Status
           Name
                  Age
                              name
0
      John Doe
                   30
                              john
                                    01/01/2010
                                                       Divorcee
1
      Jane Doe
                   29
                                    12/02/1990
                                                       Divorced
                              jane
2
    Jill smith
                   40
                                    03/04/1980
                                                        married
                               {\tt NaN}
3
    Jill smith
                   40
                              jill
                                    03/04/1980
                                                        married
    jack smith
                  100
                              jack
                                       4/4/1980
                                                       marrieed
5
   Jenny Smith
                    5
                               NaN
                                    05/05/2015
                                                             NaN
6
   JAmes Smith
                    2
                                    20/06/2018
                               NaN
                                                          single
          Rover
                               NaN
                                    05/05/2018
                                                             NaN
   Height
            Weight
                       Marriage_Len
                                           Spouse
0
     72.0
               175
                                   5
                                              NaN
                                   5
1
      5.5
               125
                                         John Doe
2
     64.0
               120
                                  10
                                      Jack Smith
```

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3	64.0	120	NaN	jack smith
4	1.8	220	10	jill smith
5	105.0	40	NaN	NaN
6	27.0	25	Not Applicable	NaN
7	36.0	50	NaN	NaN

Inspection

The first step of data cleaning is to analyze the quality of the data. If the quality is poor, the data might not be worth using. Knowing the quality of the data will also give you an idea of how long it will take to clean it. A quality dataset is one in which the data is valid, accurate, complete, consistent, and uniform. Some of these issues, like uniformity, are fairly easy to fix during cleaning, while other aspects like accuracy are more difficult, if not impossible.

Validity is the degree that the data conforms to given rules. If a column corresponds to the temperature in Salt Lake City, measured in degrees Farenheit, then a value over 110 or below 0 should make you suspicious, since those would be extreme values for Salt Lake City. In fact, checking the all-time temperature records for Salt Lake shows that the values in this column should never be more than 107 and never less than -30. Any values outside that range are almost certainly errors and should probably be reset to NaN, unless you have special information that allows you to impute more accurate values.

Some standard rules are

- data type: The data types of each column should all be the same.
- data range: The data of a column, typically numbers or dates, should all be in the same range.
- mandatory constraints: Certain columns cannot have missing data.
- unique constraint: Certain columns must be unique.
- regular expression patterns: A text column must be in the same format, like phone numbers must in the form 999-999-9999.
- **cross-field validation**: Conditions must hold across multiple columns, a hospital discharge date can't be earlier than the admittance date.
- duplicated data: Rows or columns that are repeated. In some cases, they may not be exact.

We can check the data type in Pandas using dtype. A dytpe of object means that the data in that column contains either strings or mixed dtypes. These fields should be investigated to determine if they contain mixed datatypes. In our toy example, we would expect that Marriage_Len is numerical, so an object dtype is suspicious. Looking at the data, we see that James has Not Applicable, which is a string.

```
name object

DOB object

Marital_Status object

Height float64

Weight int64

Marriage_Len object

Spouse object

dtype: object
```

Duplicates can be easily identified in Pandas using the duplicated() function. When no parameters are passed, it returns a DataFrame of the first duplicates. We can identify rows that are duplicated in only some columns by passing in the column names. The keep parameter has three possible values, first, last, and False. False keeps all duplicated values, while first and last only keep one of the duplicated values, the first and last ones respectively.

```
# Display duplicated rows
>>> df[df.duplicated()]
Empty DataFrame
Columns: [Name, Age, name, DOB, Marital_Status, Height, Weight, Marriage_Len, ←
   Spouse]
Index: []
# Display rows that have duplicates in some columns
>>> df[df.duplicated(['Name','DOB','Marital_Status'],keep=False)]
                                DOB Marital_Status Height Weight ←
         Name Age name
            Marriage_Len
                              Spouse
 Jill smith
               40
                    NaN 03/04/1980
                                           married
                                                      64.0
                                                                120
   10 Jack Smith
               40 jill 03/04/1980
  Jill smith
                                           married
                                                      64.0
                                                                120
   NaN jack smith
```

We can check the range of values in a numeric column using the min and max attributes. Other options for looking at the values include line plots, histograms, and boxplots. Some other useful Pandas commands for evaluating data include pd.unique() and df.nunique(), which identify and count unique values. value_counts() counts the number of values in each item of a column, like a histogram.

```
# Count the number of unique values in each row
>>> df.nunique()
                   7
Name
                   6
Age
                   2
name
                   7
DOB
Marital_Status
                   5
                   7
Height
                   7
Weight
Marriage_Len
                   4
                   4
Spouse
dtype: int64
```

The accuracy of the data, how close the data is to reality, is harder to confirm. Just because a data point is valid, doesn't mean that it is true. For example, a valid street address doesn't have to exist, or a person might lie about their weight. The first case could be checked using mapping software, but the second could be unverifiable.

The percentage of missing data is the completeness of the data. All uncleaned data will have missing values, but datasets with large amounts of missing data, or lots of missing data in key columns, are not going to be as useful. Pandas has several functions to help identify and count missing values. In Pandas, all missing data is considered a NaN and does not affect the dtype of a column. df.isna () returns a boolean DataFrame indicating whether each value is missing. df.notnull() returns a boolean DataFrame with True where a value is not missing.

```
# Count number of missing data points in each column
>>> df.isna().sum()
Name
                   0
Age
                   6
name
                   0
DOB
                   2
Marital_Status
Height
                   0
                   0
Weight
                   2
Marriage_Len
Spouse
                   4
dtype: int64
```

Consistency measures how consistent the data is in the dataset and across multiple datasets. For example, in our toy dataset, Jack Smith is 100 years old, but his birth year is 1980. Data is inconsistent across datasets when the data points should be the same and are different. This could be due to incorrect entries or syntax. An example is using multiple finance dataset to build a predictive model. The dates in each dataset should have the same format so that they can all be used equally in the model. Any columns that have monetary data should all be in the same unit, like dollars or pesos.

Lastly, uniformity is the measure of how similarly the data is formatted. Data that has the same units of measure and syntax are considered uniform. Looking at the Height column in our dataset, we see values ranging from 1.8 to 105. This is likely the result of different units of measure.

When looking at the quality of the data, there are no set rules on how to measure these concepts or at what point the data is considered bad data. Sometimes, even if the data is bad, it is the only data available and has to be used. Having an idea of the quality of the data will help you know what cleaning steps are needed and help with analyzing the results. Creating a summary statistics, also known as data profiling is a good way to get a general idea of the quality of the data. The summary statistics should be specific to the dataset and describe aspects of the data discussed in this section. It could also include visualizations and basic statistics, like the mean and standard deviation.

Visualization is an important aspect of the inspection phase. Using histograms, box plots, and hexbins can identify outliers in the data. Outliers should be investigated to determine if they are accurate. Removing outliers will improve your model, but you should only remove an outlier if you have a legitimate reason. Columns that have a small distribution or variance, or consist of one value, could be worth removing since they might contribute little to the model.

Problem 1. The g_t_results.csv file is a set of parent-reported scores on their child's Gifted and Talented tests. The two tests, OLSAT and NNAT, are used by NYC to determine if children are qualified for gifted programs. The OLSAT Verbal has 16 questions for Kindergartners and 30 questions for first, second, and third graders. The NNAT has 48 questions. Using this dataset, answer the following questions.

- 1) What column has the highest number of null values and what percent of its values are null? Print the answer as a tuple with (column name, percentage). Make sure the second value is a percent.
 - 2) List the columns that should be numeric that aren't. Print the answer as a tuple.
- 3) How many third graders have scores outside the valid range for the OLSAT Verbal Score? Print the answer
 - 4) How many data values are missing (NaN)? Print the number. Each part is one point.

Cleaning

After the data has been inspected, it's time to start cleaning. There are many aspects and methods of cleaning; not all of them will be used in every dataset. Which ones you choose should be based on your dataset and the goal of the project.

Unwanted Data

Removing unwanted data typically falls into two categories, duplicated data and irrelevant data. Duplicated observations usually occur when data is scraped, combined from multiple datasets, or a user submits the data twice. Irrelevant data consists of observations that don't fit the specific problem you are trying to solve or don't have enough variation to affect the model. We can drop duplicated data using the duplicated() function described above with drop() or using drop_duplicates, which has the same parameters as duplicated.

Validity Errors

After moving unwanted data, we correct any validity errors found during inspection. All features should have a consistent type, standard formatting (like capitalization), and the same units. Syntax errors should be fixed, and white space at the beginning and ends of strings should be removed. Some data might need to be padded so that it's all the same length.

Method	Description
series.str.lower()	Convert to all lower case
series.str.upper()	Convert to all upper case
series.str.strip()	Remove all leading and trailing white space
series.str.lstrip()	Remove leading white space
series.str.replace(" ","")	Remove all spaces
series.str.pad()	Pad strings

Table 13.1: Pandas String Formatting Methods

Validity also includes correcting or removing contradicting values. This might be two values in a row or values across datasets. For example, a child shouldn't have a marital status of married. Another example is if two columns should sum to a third but don't for a specific row.

Missing Data

There will always be missing data in any uncleaned dataset. Some commonly suggested methods for handling data are removing the missing data and setting the missing values to some value based on other observations. However, missing data can be informative and removing or replacing missing data erases that information. Also, removing missing values from a dataset might result in significant amounts of data being lost. Removing missing data could also make your model less accurate if you need to predict on data with missing values, so retaining the missing values can help increase accuracy.

So how can we handle missing data? Dropping missing data is the easiest method. Dropping rows should only be done if the are a small number of missing data points in a column or if the row is missing a significant amount of data. If a column is very sparse, consider dropping the entire column. Another option is to estimate the missing data's value and replace it. There are many ways to do this, including mean, mode, median, randomly choosing from the distribution, linear regression, and hot-decking.

Hot-deck is when you fill in the data based on similar observations. It can be applied to numerical and categorical data, unlike most of the other options listed above. The easiest hot-deck method is to fill in the data with random numbers after dividing the data into groups based on some characteristic, like gender. Sequential hot-deck sorts the column with missing data based on an auxiliary column and then fills in the data with the value from the next available data point. K-Nearest Neighbors can also be used to identify similar data points.

The last option is to flag the data as missing. This retains the information from missing data and removes the missing data (by replacing it). For categorical data, simply replace the data with a new category. For numerical data, we can fill the missing data with 0, or some value that makes sense, and add an indicator variable for missing data. This allows the algorithm to estimate the constant for missing data instead of just using the mean.

```
## Replace missing data
import numpy as np
```

```
# Add an indicator column based on missing Marriage_Len
>>> df['missing_ML'] =df['Marriage_Len'].isna()
# Fill in all missing data with 0
>>> df['Marriage_Len'] = df['Marriage_Len'].fillna(0)
# Change all other NaNs to missing
>>> df = df.fillna('missing')
# Change Not Applicable row to NaNs
>>> df = df.replace('Not Applicable',np.nan)
# Drop rows will NaNs
>>> df = df.dropna()
>>> df
          Name
                 Age
                             DOB Marital_Status
0
      JOHN DOE
                  30
                     01/01/2010
                                        divorcee
1
      JANE DOE
                  29
                     12/02/1990
                                        divorced
2
    JILL SMITH
                  40
                      03/04/1980
                                         married
3
    JACK SMITH
                  40
                        4/4/1980
                                         married
   JENNY SMITH
                   5
                     05/05/2015
                                         missing
                                      Spouse missing_ML
   Height
           Weight Marriage_Len
0
     72.0
               175
                              5
                                    missing
                                                   False
                              5
1
     68.0
               125
                                    John Doe
                                                   False
2
     64.0
               120
                             10
                                 Jack Smith
                                                   False
3
     71.0
               220
                                 jill smith
                                                   False
                             10
4
     41.0
               40
                              0
                                    missing
                                                    True
```

Nonnumerical Values Misencoded as Numbers

More dangerous, in many ways, than numerical errors, are entries that are recorded as a numerical value (float or int) when they should be recorded as nonnumerical data, that is, in a format that cannot be summed, multiplied, or averaged. One example is missing data recorded as 0. Missing data should always be stored in a form that cannot accidentally be incorporated into the model. Typically this is done by storing NaN as the value. However, the above method of using missing as the value is more valuable since some algorithms will not run on data with NaN. Unfortunately, many datasets have recorded missing values with a 0 or some other number. You should verify that this does not occur in your dataset. Similarly, a survey with a scale from 1 to 5 will sometimes have the additional choice of "N/A" (meaning "not applicable"), which could be coded as 6, not because the value 6 is meaningful, but just because that is the next thing after 5. Again, this should be fixed so that the "N/A" choice cannot accidentally be used for any computations.

Categorical data are also often encoded as numerical values. These values should not be left as numbers that can be computed with. For example, postal codes are shorthand for locations, and there is no numerical meaning to the code. It makes no sense to add, subtract, or multiply postal codes, so it is important not to let those accidentally be added, subtracted, or multiplied, for example by inadvertently including them in the design matrix (unless they are one-hot encoded or given some other meaningful numerical value). It is good practice to convert postal codes, area codes, ID numbers, and other non-numeric data into strings or other data types that cannot be computed with.).

Ordinal Data

Ordinal data is data that has a meaningful order, but the differences between the values aren't consistent, or maybe aren't even meaningful at all. For example, a survey question might ask about your level of education, with 1 being high-school graduate, 2 bachelor's degree, 3 master's degree, and 4 doctoral degree. These values are called ordinal data because it is meaningful to talk about an answer of 1 being less than an answer of 2. However, the difference between 1 and 2 is not necessarily the same as the difference between 3 and 4, and it would not make sense to compute an average answer—the average of a high school diploma and a masters degree is not a bachelor's degree, despite the fact that the average of 1 and 3 is 2. Treating these like categorical data loses the information of the ordering, but treating it like regular numerical data implies that a difference of 2 has the same meaning whether it comes as 3-1 or 4-2. If that last assumption is approximately true, then it may be ok to treat these data as numerical in your model, but if that assumption is not correct, it may be better to treat the variable as categorical.

Problem 2. imdb.csv contains a small set of information about 99 movies. Clean the data set by doing the following in order:

- 1. Remove duplicate rows by dropping the first or last. Print the shape of the dataframe after removing the rows.
- 2. Drop all rows that contain missing data. Print the shape of the dataframe after removing the rows.
- 3. Remove rows that have data outside valid data ranges and explain briefly how you determined your ranges for each column.
- 4. Identify and drop columns with three or fewer different values. Print a tuple with the names of the columns dropped.
- 5. Convert the titles to all lower case.

Print the first five rows of your dataframe.

Feature Engineering

One often needs to construct new columns, commonly referred to as **features** in the context of machines learning, for a dataset, because the dependent variable is not necessarily a linear function of the features in the original dataset. Constructing new features is called *feature engineering*. Once new features are created, we can analyze how much a model depends on each feature. Features with low importance probably do not contributed much and could potentially be removed.

Fognets are fine mesh nets that collect water that condenses on the netting. These are used in some desert cities in Morocco to produce drinking water. Consider a dataset measuring the amount of water Y collected from fognets, where one of the features WindDir is the wind direction, measured in degrees. This feature is not likely to contribute meaningfully in a linear model because the direction 359 is almost the same as the direction 0, but no nonzero linear multiple of WindDir will reflect this relation. One way to improve the situation is to replace the WindDir with two new (engineered) features: $\sin\left(\frac{\pi}{180}\text{WindDir}\right)$ and $\cos\left(\frac{\pi}{180}\text{WindDir}\right)$.

Discrete Fourier transforms and wavelet decomposition often reveal important properties of data collected over time (*called time-series*), like sound, video, economic indicators, etc. In many such settings it is useful to engineer new features from a wavelet decomposition, the DFT, or some other function of the data.

Problem 3. basketball.csv contains data for all NBA players between 2001 and 2018. Each row represents a player's stats for a year. The features in this data set are

- player (str): the player's name
- age (int): the player's age
- team id (cat): the player's team
- per (float): player efficiency rating, how much a player produced in one minute of play
- ws (float): win shares, an estimate of how much the player contributed to
- bpm (float): box plus/minus is the estimated number of points a player contributed to over 100 possessions
- year (int): the year

(float):

Create two new features:

- career length (int): number of years player has been playing (start at 0).
- target (str): The target team if the player is leaving. If the player is retiring, the target should be 'retires'. A player is retiring if their name doesn't exist the next year. (Set the players in 2019 to NaN).

Remove all duplicates of a player in each year. Remove all rows except those where a player changes team, that is, target is not null nor 'retires'. Drop the player, year, and team_id columns.

Return the first ten lines of the dataframe.

Engineering for Categorical Variables

Categorical features are those that take only a finite number of values, and usually no categorical value has a numerical meaning, even if it happens to be number. For example in an election dataset, the names of the candidates in the race are categorical, and there is no numerical meaning (neither ordering nor size) to numbers assigned to candidates based soley on their names.

Consider the following election data.

Ballot number	For Governor	For President
001	Herbert	Romney
002	Cooke	Romney
003	Cooke	Obama
004	Herbert	Romney
005	Herbert	Romney
006	Cooke	Stein

A common mistake occurs when someone assigns a number to each categorical entry (say 1 for Cooke, 2 for Herbert, 3 for Romney, etc.). While this assignment is not, in itself, inherently incorrect, it is incorrect to use the value of this number in a statistical model. Any such model would be fundamentally wrong because a vote for Cooke cannot, in any reasonable way, be considered half of a vote for Herbert or a third of a vote for Romney. Many researchers have accidentally used categorical data in this way (and some have been very publicly embarrassed) because their categorical data was encoded numerically, which made it hard to recognize as categorical data.

Whenever you encounter categorical data that is encoded numerically like this, immediately change it either to non-numerical form ("Cooke," "Herbert," "Romney,"...) or apply a one-hot encoding as described below.

In order to construct a meaningful model with categorical data, one normally applies a *one-hot encoding* or *dummy variable encoding*. ¹ To do this construct a new feature for every possible value of the categorical variable, and assign the value 1 to that feature if the variable takes that value and zero otherwise. Pandas makes one-hot encoding simple:

```
# one-hot encoding
df = pd.get_dummies(df, columns=['For President']])
```

The previous dataset, when the presidential race is one-hot encoded, becomes

Ballot number	Governor	Romney	Obama	Stein
001	Herbert	1	0	0
002	Cooke	1	0	0
003	Cooke	0	1	0
004	Herbert	1	0	0
005	Herbert	1	0	0
006	Cooke	0	0	1

Note that the sum of the terms of the one-hot encoding in each row is 1, corresponding to the fact that every ballot had exactly one presidential candidate.

When the gubernatorial race is also one-hot encoded, this becomes

¹Yes, these are silly names, but they are the most common names for it. Unfortunately, it is probably too late to change these now.

Ballot number	Cooke	Herbert	Romney	Obama	Stein
001	0	1	1	0	0
002	1	0	1	0	0
003	1	0	0	1	0
004	0	1	1	0	0
005	0	1	1	0	0
006	1	0	0	0	1

Now the sum of the terms of the one-hot encodings in each row is 2, corresponding to the fact that every ballot had two names—one gubernatorial candidate and one presidential candidate.

Summing the columns of the one-hot-encoded data gives the total number of votes for the candidate of that column. So the numerical values in the one-hot encodings are actually numerically meaningful, and summing the entries gives meaningful information. One-hot encoding also avoids the pitfalls of incorrectly using numerical proxies for categorical data.

The main disadvantage of one-hot encoding is that it is an inefficient representation of the data. If there are C categories and n datapoints, a one-hot encoding takes an $n \times 1$ -dimensional feature and turns it into an $n \times C$ sparse matrix. But there are ways to store these data efficiently and still maintain the benefits of the one-hot encoding.

ACHTUNG!

When performing linear regression, it is good practice to add a constant column to your dataset and to remove one column of the one-hot encoding of each categorical variable. (Adding a constant column should only be done in linear regression).

To see why, notice that summing terms in one row corresponding to the one-hot encoding of a specific categorical variable (for example the presidential candidate) always gives 1. If the dataset already has a constant column (which you really always should add if it isn't there already), then the constant column is a linear combination of the one-hot encoded columns. This cause the matrix to fail to be invertible and can cause identifiability problems.

The standard way to deal with this is to remove one column of the one-hot embedding for each categorical variable. For example, with the elections dataset above, we could remove the Cooke and Romney columns. Doing that means that in the new dataset a row sum of 0 corresponds to a ballot with a vote for Cooke and a vote for Romney, while a 1 in any column indicates how the ballot differed from the base choice of Cooke and Romney.

When using pandas, you can drop the first column of a one-hot encoding by passing in drop_first=True.

Problem 4. Load housing.csv into a dataframe with index=0. Descriptions of the features are in housing_data_description.txt. The goal is to construct a regression model that predicts SalePrice using the other features of the dataset. Do this as follows:

1. Identify and handle the missing data. Hint: Dropping every row with some missing data is not a good choice because it gives you an empty dataframe. What can you do instead?

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2. Identify the variable with nonnumerical values that are misencoded as numbers. One-hot encode it. Hint: don't forget to remove one of the encoded columns to prevent collinearity with the constant column).

- 3. Add a constant column to the dataframe.
- 4. Save a copy of the dataframe.
- 5. Choose four categorical features that seem very important in predicting SalePrice. One-hot encode these features, and remove all other categorical features.
- 6. Run an OLS regression on your model.

Print the ten features that have the highest coef in your model and the summary. To run an OLS model in python, use the following code.

```
import statsmodels.api as sm

>>> results = sm.OLS(y, X).fit()

# Print the summary
>>> results.summary()

# Convert the summary table to a dataframe
>>> results_as_html = a.tables[1].as_html()
>>> result_df = pd.read_html(results_as_html, header=0, index_col=0)[0]
```

Problem 5. Using the copy of the dataframe you created in Problem 4, one-hot encode all the categorical variables. Print the shape of you database, and Run OLS.

Print the ten features that have the highest coef in your model and the summary. Write a couple of sentences discussing which model is better and why.

MongoDB

Lab Objective: Relational databases, including those managed with SQL or pandas, require data to be organized into tables. However, many data sets have an inherently dynamic structure that cannot be efficiently represented as tables. MongoDB is a non-relational database management system that is well-suited to large, fast-changing datasets. In this lab we introduce the Python interface to MongoDB, including common commands and practices.

Database Initialization

Suppose the manager of a general store has all sorts of inventory: food, clothing, tools, toys, etc. There are some common attributes shared by all items: name, price, and producer. However, other attributes are unique to certain items: sale price, number of wheels, or whether or not the product is gluten-free. A relational database housing this data would be full of mostly-blank rows, which is extremely inefficient. In addition, adding new items to the inventory requires adding new columns, causing the size of the database to rapidly increase. To efficiently store the data, the whole database would have to be restructured and rebuilt often.

To avoid this problem, NoSQL databases like MongoDB avoid using relational tables. Instead, each item is a JSON-like object, and thus can contain whatever attributes are relevant to the specific item, without including any meaningless attribute columns.

Note

MongoDB is a database management system (DBMS) that runs on a server, which should be running in its own dedicated terminal. Refer to the Additional Material section for installation instructions.

The Python interface to MongoDB is called pymongo. After installing pymongo and with the MongoDB server running, use the following code to connect to the server.

```
>>> from pymongo import MongoClient
# Create an instance of a client connected to a database running
# at the default host IP and port of the MongoDB service on your machine.
>>> client = MongoClient()
```

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Creating Collections and Documents

A MongoDB database stores *collections*, and a collection stores *documents*. The syntax for creating databases and collections is a little unorthodox, as it is done through attributes instead of methods.

```
# Create a new database.
>>> db = client.db1

# Create a new collection in the db database.
>>> col = db.collection1
```

Documents in MongoDB are represented as JSON-like objects, and therefore do not adhere to a set schema. Each document can have its own *fields*, which are completely independent of the fields in other documents.

NOTE

Once information has been added to the database it will remain there, even if the python environment you are working with is shut down. It can be accessed anytime using the same commands as before.

```
>>> client = MongoClient()
>>> db = client.db1
>>> col = db.collection1
```

To delete a collection, use the database's drop_collection() method. To delete a database, use the client's drop_database() method.

Problem 1. The file trump.json, located in trump.json.zip, contains posts from http://www.twitter.com (tweets) over the course of an hour that have the key word "trump". Each line in the file is a single JSON message that can be loaded with json.loads().

Create a MongoDB database and initialize a collection in the database. Use the collection's delete_many() method with an empty set as input to clear existing contents of the collection, then fill the collection one line at a time with the data from trump.json. Check that your collection has 67,859 entries with its estimated_document_count() method.

Querying a Collection

MongoDB uses a *query by example* pattern for querying. This means that to query a database, an example must be provided for the database to use in matching other documents.

```
# Find all the documents that have a 'name' field containing the value 'Jack'.
>>> data = col.find({'name': 'Jack'})

# Count how many documents have a 'name' field containing the value 'Jack'.
>>> count = col.count_documents({'name': 'Jack'})

# Find the FIRST document with a 'name' field containing the value 'Jack'.
>>> data = col.find_one({'name': 'Jack'})
```

The find_one() method returns the first matching document as a dictionary. The find() query may find any number of objects, so it will return a Cursor, a Python object that is used to iterate over the query results. There are many useful functions that can be called on a Cursor; for more information see https://pymongo.readthedocs.io/en/stable/api/pymongo/cursor.html.

```
# Search for documents containing True in the 'student' field.
>>> students = col.find({'student': True})
>>> col.count_documents({'student': True})  # There are 2 matching documents.
2

# List the first student's data.
# Notice that each document is automatically assigned an ID number as '_id'.
>>> students[0]
{'_id': ObjectId('59260028617410748cc7b8c7'),
    'age': 22,
    'classes': ['Math', 'Geography', 'English'],
    'name': 'Jack',
    'student': True}

# Get the age of the first student.
>>> students[0]['age']
22
```

^aSee the Additional Materials section for an example of using the Twitter API.

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```
# List the data for every student.
>>> list(students)
[{'_id': ObjectId('59260028617410748cc7b8c7'),
    'age': 22,
    'classes': ['Math', 'Geography', 'English'],
    'name': 'Jack',
    'student': True},
{'_id': ObjectId('59260028617410748cc7b8ca'),
    'name': 'Jeremy',
    'occupation': 'waiter',
    'student': True}]
```

The logical operators listed in the following table can be used to do more complex queries.

Operator	Description
\$1t, \$gt	<,>
\$lte,\$gte	<=, >=
\$eq, \$ne	==, !=
\$in, \$nin	in, not in
<pre>\$or, \$and, \$not</pre>	or, and, not
\$exists	Match documents with a specific field
\$type	Match documents with values of a specific type
\$all	Match arrays that contain all queried elements
\$size	Match arrays with a specified number of elements
\$regex	Search documents with a regular expression

Table 14.1: MongoDB Query Operators

```
# Query for everyone that is either above the age of 23 or a soldier.
>>> results = col.find({'$or':[{'age':{'$gt': 23}},{'soldier': True}]})

# Query for everyone that is a student (those that have a 'student' attribute
# and haven't been expelled).
>>> results = col.find({'student': {'$not': {'$in': [False, 'Expelled']}}})

# Query for everyone that has a student attribute.
>>> results = col.find({'student': {'$exists': True}})

# Query for people whose name contains a the letter 'e'.
>>> import re
>>> results = col.find({'name': {'$regex': re.compile('e')}})
```

It is likely that a database will hold more complex JSON entries than these, with many nested attributes and arrays. For example, an entry in a database for a school might look like this:

```
{'name': 'Jason', 'age': 16,
  'student': {'year':'senior', 'grades': ['A','C','A','B'],'flunking': False},
  'jobs':['waiter', 'custodian']}
```

To query the nested attributes and arrays, use a dot, as in the following examples:

```
# Query for student that are seniors
>>> results = col.find({'student.year': 'senior'})

# Query for students that have an A in their first class.
>>> results = col.find({'student.grades.0': 'A'})
```

The Twitter JSON files are large and complex. To see what they look like, either look at the JSON file used to populate the collection or print any tweet from the database. The following website also contains useful information about the fields in the JSON file: https://dev.twitter.com/overview/api/tweets.

The distinct() function is also useful in seeing what the possible values are for a given field.

```
# Find all the values in the names field.
>>> col.distinct("name")
['Jack', 'Jill', 'John', 'Jeremy']
```

Problem 2. Query the Twitter collection from Problem 1 for the following information.

- How many tweets include the word Russia? Use re.IGNORECASE.
- How many tweets came from one of the main continental US time zones? These are listed as "Central Time (US & Canada)", "Pacific Time (US & Canada)", "Eastern Time (US & Canada)", and "Mountain Time (US & Canada)".
- How often did each language occur? Construct a dictionary with each language and its frequency count.

(Hint: use distinct() to get the language options.)

Deleting and Sorting Documents

Items can be deleted from a database using the same syntax that is used to find them. Use delete_one to delete just the first item that matches your search, or delete_many to delete all items that match your search. Note that using an empty dictionary {} as the query causes it to match all documents in the collection.

```
# Delete the first person from the database whose name is Jack.
>>> col.delete_one({'name':'Jack'})

# Delete everyone from the database whose name is Jack.
>>> col.delete_many({'name':'Jack'})

# Clear the entire collection.
>>> col.delete_many({})
```

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Another useful function is the **sort** function, which can sort the data by some attribute. It takes in the attribute by which the data will be sorted, and then the direction (1 for ascending and -1 for descending). Ascending is the default. The following code is an example of sorting:

```
# Sort the students by name in alphabetic order.
>>> results = col.find({}).sort('name', 1)
>>> for person in results:
        print(person['name'])
. . .
Jack
Jack
Jeremy
Jill
John
# Sort the students oldest to youngest, ignoring those whose age is not listed.
>>> results = col.find({'age': {'$exists': True}}).sort('age', -1)
>>> for person in results:
       print(person['name'])
. . .
Jill
Jack
Jack
```

Problem 3. Query the Twitter collection from Problem 1 for the following information.

- What are the usernames of the 5 most popular (defined as having the most followers) tweeters? Don't include repeats.
- Of the tweets containing at least 5 hashtags, sort the tweets by how early the 5th hashtag appears in the text. What is the earliest spot (character count) it appears?
- What are the coordinates of the tweet that came from the northernmost location? Use the latitude and longitude point in "coordinates".

Updating Documents

Another useful attribute of MongoDB is that data in the database can be updated. It is possible to change values in existing fields, rename fields, delete fields, or create new fields with new values. This gives much more flexibility than a relational database, in which the structure of the database must stay the same. To update a database, use either update_one or update_many, depending on whether one or more documents should be changed (the same as with delete). Both of these take two parameters; a find query, which finds documents to change, and the update parameters, telling these things what to update. The syntax is update_many({find query}, {update parameters}).

The update parameters must contain update operators. Each update operator is followed by the field it is changing and the value to change it. The syntax is the same as with query operators. The operators are shown in the table below.

Operator	Description
<pre>\$inc , \$mul</pre>	+=, *=
<pre>\$min, \$max</pre>	min(), max()
\$rename	Rename a specified field to the given new name
\$set	Assign a value to a specified field (creating the field if necessary)
<pre>\$unset</pre>	Remove a specified field
\$currentDate	Set the value of the field to the current date.
	With "\$type": "date", use a datetime format;
	with "\$type": "timestamp:, use a timestamp.

Table 14.2: MongoDB Update Operators

```
# Update the first person from the database whose name is Jack to include a
# new field 'lastModified' containing the current date.
>>> col.update_one({'name':'Jack'},
... {'$currentDate': {'lastModified': {'$type': 'date'}}})

# Increment everyones age by 1, if they already have an age field.
>>> col.update_many({'age': {'$exists': True}}, {'$inc': {'age': 1}})

# Give the first John a new field 'best_friend' that is set to True.
>>> col.update_one({'name':'John'}, {'$set': {'best_friend': True}})
```

Problem 4. Clean the twitter collection in the following ways.

- Get rid of the "retweeted_status" field in each tweet.
- Update every tweet from someone with at least 1000 followers to include a popular field whose value is True. Report the number of popular tweets.
- (OPTIONAL) The geographical coordinates used before in coordinates.coordinates are turned off for most tweets. But many more have a bounding box around the coordinates in the place field. Update every tweet without coordinates that contains a bounding box so that the coordinates contains the average value of the points that form the bounding box. Make the structure of coordinates the same as the others, so it contains coordinates with a longitude, latitude array and a type, the value of which should be 'Point'.

(Hint: Iterate through each tweet in with a bounding box but no coordinates. Then for each tweet, grab it's id and the bounding box coordinates. Find the average, and then update the tweet. To update it search for it's id and then give the needed update parameters. First unset coordinates, and then set coordinates and coordinates and coordinates.type to the needed values.)

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Additional Material

Installation of MongoDB

MongoDB runs as an isolated program with a path directed to its database storage. To run a practice MongoDB server on your machine, complete the following steps:

Create Database Directory

To begin, navigate to an appropriate directory on your machine and create a folder called data. Within that folder, create another folder called db. Make sure that you have read, write, and execute permissions for both folders.

Retrieve Shell Files

To run a server on your machine, you will need the proper executable files from MongoDB. The following instructions are individualized by operating system. For all of them, download your binary files from https://www.mongodb.com/download-center?jmp=nav#community.

1. For Linux/Mac:

Extract the necessary files from the downloaded package. In the terminal, navigate into the bin directory of the extracted folder. You may then start a Mongo server by running in a terminal: ./mongod --dbpath /pathtoyourdatafolder.

2. For Windows:

Go into your Downloads folder and run the Mongo .msi file. Follow the installation instructions. You may install the program at any location on your machine, but do not forget where you have installed it. You may then start a Mongo server by running in command prompt: $C:\$ docation of mongo program \mongo d.exe -dbpath $C:\$ pathtodata folder \data \db.

MongoDB servers are set by default to run at address:port 127.0.0.1:27107 on your machine. You can also run Mongo commands through a mongo terminal shell. More information on this can be found at https://docs.mongodb.com/getting-started/shell/introduction/.

Twitter API

Pulling information from the Twitter API is simple. First you must get a Twitter account and register your app with them on apps.twitter.com. This will enable you to have a consumer key, consumer secret, access token, and access secret, all required by the Twitter API.

You will also need to install tweepy, an open source library that allows python to easily work with the Twitter API. This can be installed with pip by running from the command line

```
$pip install tweepy
```

The data for this lab was then pulled using the following code on May 26, 2017.

```
import tweepy
from tweepy import OAuthHandler
from tweepy import Stream
```

```
from tweepy.streaming import StreamListener
from pymongo import MongoClient
import json
#Set up the databse
client = MongoClient()
mydb = client.db1
twitter = mydb.collection1
f = open('trump.txt','w') #If you want to write to a file
consumer_key = #Your Consumer Key
consumer_secret = #Your Consumer Secret
access_token = #Your Access Token
access_secret = #Your Access Secret
my_auth = OAuthHandler(consumer_key, consumer_secret)
my_auth.set_access_token(access_token, access_secret)
class StreamListener(tweepy.StreamListener):
    def on_status(self, status):
        print(status.text)
    def on_data(self, data):
        try:
            twitter.insert_one(json.loads(data)) #Puts the data into your ←
            f.write(str(data)) #Writes the data to an output file
            return True
        except BaseException as e:
            print(str(e))
            print("Error")
        return True
    def on_error(self, status):
        print(status)
        if status_code == 420: #This means twitter has blocked us temporarily, ←
            so we want to stop or they will get mad. Wait 30 minutes or so and \leftarrow
            try again. Running this code often in a short period of time will \hookleftarrow
            cause twitter to block you. But you can stream tweets for as long \hookleftarrow
            as you want without any problems.
            return False
        else:
            return True
stream_listener = StreamListener()
stream = tweepy.Stream(auth=my_auth, listener=stream_listener)
stream.filter(track=["trump"]) #This pulls all tweets that include the keyword ←
    "trump". Any number of keywords can be searched for.
```

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Introduction to Parallel Computing

Lab Objective: Many modern problems involve so many computations that running them on a single processor is impractical or even impossible. There has been a consistent push in the past few decades to solve such problems with parallel computing, meaning computations are distributed to multiple processors. In this lab, we explore the basic principles of parallel computing by introducing the cluster setup, standard parallel commands, and code designs that fully utilize available resources.

Parallel Architectures

Imagine that you are in charge of constructing a very large building. You could, in theory, do all of the work yourself, but that would take so long that it simply would be impractical. Instead, you hire workers, who collectively can work on many parts of the building at once. Managing who does what task takes some effort, but the overall effect is that the building will be constructed many times faster than if only one person was working on it. This is the essential idea behind parallel computing.

A serial program is executed one line at a time in a single process. This is analogous to a single person creating a building. Since modern computers have multiple processor cores, serial programs only use a fraction of the computer's available resources. This is beneficial for smooth multitasking on a personal computer because multiple programs can run at once without interrupting each other.

For smaller computations, running serially is fine. However, some tasks are large enough that running serially could take days, months, or in some cases years. In these cases it is beneficial to devote all of a computer's resources (or the resources of many computers) to a single program by running it in parallel. Each processor can run part of the program on some of the inputs, and the results can be combined together afterwards. In theory, using N processors at once can allow the computation to run N times faster. Even though communication and coordination overhead prevents the improvement from being quite that good, the difference is still substantial.

A computer cluster or supercomputer is essentially a group of regular computers that share their processors and memory. There are several common architectures that are used for parallel computing, and each architecture has a different protocol for sharing memory, processors, and tasks between computing nodes, the different simultaneous processing areas. Each architecture offers unique advantages and disadvantages, but the general commands used with each are very similar.

In this lab, we will explore the usage and capabilities of parallel computing using Python's iPyParallel package. iPyParallel can be installed with either pip or conda:

```
$ pip install ipyparallel
```

\$ conda install ipyparallel

The iPyParallel Architecture

There are three main parts of the iPyParallel architecture:

- Client: The main program that is being run.
- Controller: Receives directions from the client and distributes instructions and data to the computing nodes. Consists of a hub to manage communications and schedulers to assign processes to the engines.
- Engines: The individual processors. Each engine is like a separate Python terminal, each with its own namespace and computing resources.

Essentially, a Python program using iPyParallel creates a Client object connected to the cluster that allows it to send tasks to the cluster and retreive their results. The engines run the tasks, and the controller manages which engines run which tasks.

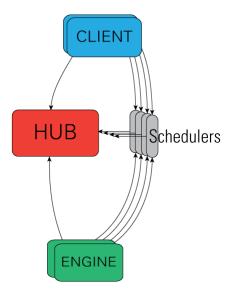


Figure 15.1: An outline of the iPyParallel architecture.

Setting up an iPyParallel Cluster

Before being able to use iPyParallel in a script or interpreter, it is necessarty to start an iPyParallel cluster. We demonstrate here how to use a single machine with multiple processor cores as a cluster. Establishing a cluster on multiple machines requires additional setup, which is detailed in the Additional Material section. The following commands initialize parts or all of a cluster when run in a terminal window:

Command	Description
ipcontroller start	Initialize a controller process.
ipengine start	Initialize an engine process.
ipcluster start	Initialize a controller process and several engines simultaneously.

Each of these processes can be stopped with a keyboard interrupt (Ctrl+C). By default, the controller uses JSON files in UserDirectory/.ipython/profile-default/security/ to determine its settings. Once a controller is running, it acts like a server, listening connections from clients and engines. Engines will connect automatically to the controller when they start running. There is no limit to the number of engines that can be started in their own terminal windows and connected to the controller, but it is recommended to only use as many engines as there are cores to maximize efficiency.

ACHTUNG!

The directory that the controller and engines are started from matters. To facilitate connections, navigate to the same folder as your source code before using ipcontroller, ipengine, or ipcluster. Otherwise, the engines may not connect to the controller or may not be able to find auxiliary code as directed by the client.

Starting a controller and engines in individual terminal windows with ipcontroller and ipengine is a little inconvenient, but having separate terminal windows for the engines allows the user to see individual errors in detail. It is also actually more convenient when starting a cluster of multiple computers. For now, we use ipcluster to get the entire cluster started quickly.

Note

Jupyter notebooks also have a **Clusters** tab in which clusters can be initialized using an interactive GUI. To enable the tab, run the following command. This operation may require root permissions.

```
$ ipcluster nbextension enable
```

The iPyParallel Interface

Once a controller and its engines have been started and are connected, a cluster has successfully been established. The controller will then be able to distribute messages to each of the engines, which will compute with their own processor and memory space and return their results to the controller. The client uses the ipyparallel module to send instructions to the controller via a Client object.

```
>>> from ipyparallel import Client
```

```
>>> client = Client()  # Only works if a cluster is running.
>>> client.ids
[0, 1, 2, 3]  # Indicates that there are four engines running.
```

Once the client object has been created, it can be used to create one of two classes: a DirectView or a LoadBalancedView. These views allow for messages to be sent to collections of engines simultaneously. A DirectView allows for total control of task distribution while a LoadBalancedView automatically tries to spread out the tasks equally on all engines. The remainder of the lab will be focused on the DirectView class.

```
>>> dview = client[:] # Group all engines into a DirectView.
>>> dview2 = client[:2] # Group engines 0,1, and 2 into a DirectView.
>>> dview2.targets # See which engines are connected.
[0, 1, 2]
```

Since each engine has its own namespace, modules must be imported in every engine. There is more than one way to do this, but the easiest way is to use the DirectView object's execute() method, which accepts a string of code and executes it in each engine.

```
# Import NumPy in each engine.
>>> dview.execute("import numpy as np")
```

Problem 1. Write a function that initializes a Client object, creates a DirectView with all available engines, and imports scipy.sparse as sparse on all engines. Return the DirectView.

Managing Engine Namespaces

Before continuing, set the DirectView you are using to use blocking:

```
>>> dview.block = True
```

This affects the way that functions called using the DirectView return their values. Using blocking makes the process simpler, so we will use it initially. What blocking is will be explained later.

Push and Pull

The push() and pull() methods of a DirectView object manage variable values in the engines. Use push() to set variable values and pull() to get variables. Each method also has a shortcut via indexing.

```
# Initialize the variables 'a' and 'b' on each engine.
>>> dview.push({'a':10, 'b':5})  # OR dview['a'] = 10; dview['b'] = 5
[None, None, None, None]  # Output from each engine
# Check the value of 'a' on each engine.
```

Problem 2. Write a function variables(dx) that accepts a dictionary of variables. Create a Client object and a DirectView and distribute the variables. Pull the variables back and make sure they haven't changed.

Scatter and Gather

Parallelization almost always involves splitting up collections and sending different pieces to each engine for processing. The process is called *scattering* and is usually used for dividing up arrays or lists. The inverse process of pasting a collection back together is called *gathering* and is usually used on the results of processing. This method of distributing a dataset and collecting the results is common for processing large data sets using parallelization.

```
>>> import numpy as np

# Send parts of an array of 8 elements to each of the 4 engines.
>>> x = np.arange(1, 9)
>>> dview.scatter("nums", x)
>>> dview["nums"]
[array([1, 2]), array([3, 4]), array([5, 6]), array([7, 8])]

# Scatter the array to only the first two engines.
>>> dview.scatter("nums_big", x, targets=[0,1])
>>> dview.pull("nums_big", targets=[0,1])
[array([1, 2, 3, 4]), array([5, 6, 7, 8])]

# Gather the array again.
>>> dview.gather("nums")
array([1, 2, 3, 4, 5, 6, 7, 8])
>>> dview.gather("nums_big", targets=[0,1])
array([1, 2, 3, 4, 5, 6, 7, 8])
```

Executing Code on Engines

Execute

The execute() method is the simplest way to run commands on parallel engines. It accepts a string of code (with exact syntax) to be executed. Though simple, this method works well for small tasks.

```
# 'nums' is the scattered version of np.arange(1, 9).
>>> dview.execute("c = np.sum(nums)")  # Sum each scattered component.
<AsyncResult: execute:finished>
>>> dview['c']
[3, 7, 11, 15]
```

Apply

The apply() method accepts a function and arguments to plug into it, and distributes them to the engines. Unlike execute(), apply() returns the output from the engines directly.

```
>>> dview.apply(lambda x: x**2, 3)
[9, 9, 9, 9]
>>> dview.apply(lambda x,y: 2*x + 3*y, 5, 2)
[16, 16, 16, 16]
```

Note that the engines can access their local variables in either of the execution methods.

Мар

The built-in map() function applies a function to each element of an iterable. The iPyParallel equivalent, the map() method of the DirectView class, combines apply() with scatter() and gather(). Simply put, it accepts a dataset, splits it between the engines, executes a function on the given elements, returns the results, and combines them into one object.

Blocking vs. Non-Blocking

Parallel commands can be implemented two ways. The difference is subtle but extremely important.

- Blocking: The main program sends tasks to the controller, and then waits for all of the engines to finish their tasks before continuing (the controller "blocks" the program's execution). This mode is usually best for problems in which each node is performing the same task.
- Non-Blocking: The main program sends tasks to the controller, and then continues without waiting for responses. Instead of the results, functions return an AsyncResult object that can be used to check the execution status and eventually retrieve the actual result.

Whether a function uses blocking is determined by default by the block attribute of the DirectView The execution methods execute(), apply(), and map(), as well as push(), pull(), scatter(), and gather(), each have a keyword argument block that can instead be used to specify whether or not to using blocking. Alternatively, the methods apply_sync() and map_sync() always use blocking, and apply_async() and map_async() always use non-blocking.

```
>>> f = lambda n: np.sum(np.random.random(n))
# Evaluate f(n) for n=0,1,\ldots,999 with blocking.
>>> %time block_results = [dview.apply_sync(f, n) for n in range(1000)]
CPU times: user 9.64 s, sys: 879 ms, total: 10.5 s
Wall time: 13.9 s
# Evaluate f(n) for n=0,1,\ldots,999 with non-blocking.
>>> %time responses = [dview.apply_async(f, n) for n in range(1000)]
CPU times: user 4.19 s, sys: 294 ms, total: 4.48 s
Wall time: 7.08 s
# The non-blocking method is faster, but we still need to get its results.
# Both methods produced a list, although the contents are different
>>> block_results[10] # This list holds actual result values from each engine.
[3.833061790352166,
4.8943956129713335,
4.268791758626886,
4.73533677711277]
>>> responses[10]
                            # This list holds AsyncResult objects.
<AsyncResult: <lambda>:finished>
# We can get the actual results by using the get() method of each AsyncResult
>>> %time nonblock_results = [r.get() for r in responses]
CPU times: user 3.52 ms, sys: 11 mms, total: 3.53 ms
Wall time: 3.54 ms
                           # Getting the responses takes little time.
>>> nonblock_results[10]
                         # This list also holds actual result values
[5.652608204341693,
4.984164642641558,
4.686288406810953,
5.275735658763963]
```

When non-blocking is used, commands can be continuously sent to engines before they have finished their previous task. This allows them to begin their next task without waiting to send their calculated answer and receive a new command. However, this requires a design that incorporates checkpoints to retrieve answers and enough memory to store response objects.

Class Method	Description
wait(timeout)	Wait until the result is available or until timeout seconds pass.
ready()	Return whether the call has completed.
successful()	Return whether the call completed without raising an exception.
	Will raise AssertionError if the result is not ready.
<pre>get(timeout)</pre>	Return the result when it arrives. If timeout is not None and the result does not arrive within timeout seconds then TimeoutError
	is raised.

Table 15.1: All information from https://ipyparallel.readthedocs.io/en/latest/details.html#AsyncResult.

Table 15.1 details the methods of the AsyncResult object.

There are additional magic methods supplied by iPyParallel that make some of these operations easier. These methods are explained in the Additional Material section. More information on iPyParallel architecture, interface, and methods can also be found at https://ipyparallel.readthedocs.io/en/latest/index.html.

Problem 3. Write a function that accepts an integer n. Instruct each engine to make n draws from the standard normal distribution, then hand back the mean, minimum, and maximum draws to the client. Return the results in three lists.

If you have four engines running, your results should resemble the following:

```
>>> means, mins, maxs = problem3(1000000)
>>> means
[0.0031776784, -0.0058112042, 0.0012574772, -0.0059655951]
>>> mins
[-4.1508589, -4.3848019, -4.1313324, -4.2826519]
>>> maxs
[4.0388107, 4.3664958, 4.2060184, 4.3391623]
```

Problem 4. Use your function from Problem 3 to compare serial and parallel execution times. For n = 1000000, 5000000, 10000000, 15000000,

- 1. Time how long it takes to run your function.
- 2. Time how long it takes to do the same process serially. Make n draws and then calculate and record the statistics, but use a for loop with N iterations, where N is the number of engines running.

Plot the execution times against n. You should notice an increase in efficiency in the parallel version as the problem size increases.

Applications

Parallel computing, when used correctly, is one of the best ways to speed up the run time of an algorithm. As a result, it is very commonly used today and has many applications, such as the following:

- Graphic rendering
- Facial recognition with large databases
- Numerical integration
- Calculating discrete Fourier transforms
- Simulation of various natural processes (weather, genetics, etc.)
- Natural language processing

In fact, there are many problems that are only feasible to solve through parallel computing because solving them serially would take too long. With some of these problems, even the parallel solution could take years. Some brute-force algorithms, like those used to crack simple encryptions, are examples of this type of problem.

The problems mentioned above are well suited to parallel computing because they can be manipulated in such a way that running them on multiple processors results in a significant run time improvement. Manipulating an algorithm to be run with parallel computing is called *parallelizing* the algorithm. When a problem only requires very minor manipulations to parallelize, it is often called *embarrassingly parallel*. Typically, an algorithm is embarrassingly parallel when there is little to no dependency between results. Algorithms that do not meet this criteria can still be parallelized, but there is not always a significant enough improvement in run time to make it worthwhile. For example, calculating the Fibonacci sequence using the usual formula, F(n) = F(n-1) + F(n-2), is poorly suited to parallel computing because each element of the sequence is dependent on the previous two elements.

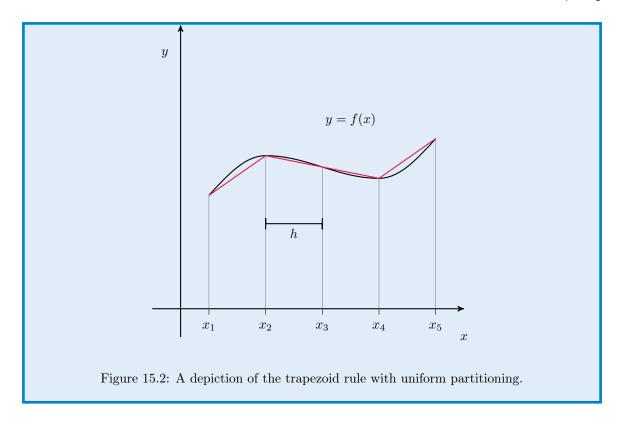
Problem 5. The *trapeziod rule* is a simple technique for numerical integration:

$$\int_{a}^{b} f(x)dx \approx \frac{h}{2} \sum_{k=1}^{N} (f(x_{k}) + f(x_{k+1})),$$

where $a = x_1 < x_2 < \ldots < x_N = b$ and $h = x_{n+1} - x_n$ for each n. See Figure 15.2.

Note that estimation of the area of each interval is independent of all other intervals. As a result, this problem is considered embarrassingly parallel.

Write a function that accepts a function handle to integrate, bounds of integration, and the number of points to use for the approximation. Parallelize the trapezoid rule in order to estimate the integral of f. That is, evenly divide the points among all available processors and run the trapezoid rule on each portion simultaneously. The sum of the results of all the processors will be the estimation of the integral over the entire interval of integration. Return this sum.



Intercommunication

The phrase parallel computing refers to designing an architecture and code that makes the best use of computing resources for a problem. Occasionally, this will require nodes to be interdependent on each other for previous results. This contributes to a slower result because it requires a great deal of communication latency, but is sometimes the only method to parallelize a function. Although important, the ability to effectively communicate between engines has not been added to iPyParallel. It is, however, possible in an MPI framework and will be covered in the MPI lab.

Additional Material

Clusters of Multiple Machines

Though setting up a computing cluster with iPyParallel on multiple machines is similar to a cluster on a single computer, there are a couple of extra considerations to make. The majority of these considerations have to do with the network setup of your machines, which is unique to each situation. However, some basic steps have been taken from https://ipyparallel.readthedocs.io/en/latest/process.html and are outlined below.

SSH Connection

When using engines and controllers that are on separate machines, their communication will most likely be using an SSH tunnel. This Secure Shell allows messages to be passed over the network.

In order to enable this, an SSH user and IP address must be established when starting the controller. An example of this follows.

```
\ ipcontroller --ip=<controller IP> --user=<user of controller> --enginessh=<\leftarrowuser of controller>@<controller IP>
```

Engines started on remote machines then follow a similar format.

```
\ ipengine --location=<controller IP> --ssh=<user of controller>@<controller IP\leftrightarrow >
```

Another way of affecting this is to alter the configuration file in UserDirectory/.ipython/profile-default/security/ipcontroller-engine.json. This can be modified to contain the controller IP address and SSH information.

All of this is dependent on the network feasibility of SSH connections. If there are a great deal of remote engines, this method will also require the SSH password to be entered many times. In order to avoid this, the use of SSH Keys from computer to computer is recommended.

Magic Methods & Decorators

To be more easily usable, the iPyParallel module has incorporated a few magic methods and decorators for use in an interactive iPython or Python terminal.

Magic Methods

The iPyParallel module has a few magic methods that are very useful for quick commands in iPython or in a Jupyter Notebook. The most important are as follows. Additional methods are found at https://ipyparallel.readthedocs.io/en/latest/magics.html.

%px - This magic method runs the corresponding Python command on the engines specified in dview.targets.

%autopx - This magic method enables a boolean that runs any code run on every engine until %autopx is run again.

Examples of these magic methods with a client and four engines are as follows.

```
# %px
In [4]: with dview.sync_imports():
           import numpy
  . . . :
importing numpy on engine(s)
In [5]: \%px a = numpy.random.random(2)
In [6]: dview['a']
Out[6]:
[array([ 0.30390162, 0.14667075]),
 array([ 0.95797678, 0.59487915]),
 array([ 0.20123566,  0.57919846]),
 array([ 0.87991814, 0.31579495])]
 # %autopx
In [7]: %autopx
%autopx enabled
In [8]: max_draw = numpy.max(a)
In [9]: print('Max_Draw: {}'.format(max_draw))
[stdout:0] Max_Draw: 0.30390161663280246
[stdout:1] Max_Draw: 0.957976784975849
[stdout:2] Max_Draw: 0.5791984571339429
[stdout:3] Max_Draw: 0.8799181411958089
In [10]: %autopx
%autopx disabled
```

Decorators

The iPyParallel module also has a few decorators that are very useful for quick commands. The two most important are as follows:

@remote - This decorator creates methods on the remote engines.

@parallel - This decorator creates methods on remote engines that break up element wise operations and recombine results.

Examples of these decorators are as follows.

```
# Remote decorator
>>> @dview.remote(block=True)
>>> def plusone():
...     return a+1
>>> dview['a'] = 5
>>> plusone()
    [6, 6, 6, 6,]
```

Parallel Programming with MPI

Lab Objective: In the world of parallel computing, MPI is the most widespread and standardized message passing library. As such, it is used in the majority of parallel computing programs. In this lab, we explore and practice the basic principles and commands of MPI to further recognize when and how parallelization can occur.

MPI: the Message Passing Interface

At its most basic, the Message Passing Interface (MPI) provides functions for sending and receiving messages between different processes. MPI was developed to provide a standard framework for parallel computing in any language. It specifies a library of functions — the syntax and semantics of message passing routines — that can be called from programming languages such as Fortran and C.

MPI can be thought of as "the assembly language of parallel computing," because of this generality. MPI is important because it was the first portable and universally available standard for programming parallel systems and continues to be the de facto standard today.

For more information on how MPI works and how to get it installed on your machine, see the additional material for this lab.

Note

Most modern personal computers now have multicore processors. Programs that are designed for these multicore processors are "parallel" programs and are typically written using OpenMP or POSIX threads. MPI, on the other hand, is designed for any general architecture.

¹ Parallel Programming with MPI, by Peter S. Pacheco, pg. 7.

Why MPI for Python?

In general, programming in parallel is more difficult than programming in serial because it requires managing multiple processors and their interactions. Python, however, is an excellent language for simplifying algorithm design because it allows for problem solving without too much detail. Unfortunately, Python is not designed for high performance computing and is a notably slower scripted language. It is best practice to prototype in Python and then to write production code in fast compiled languages such as C or Fortran.

In this lab, we will explore the Python library mpi4py which retains most of the functionality of C implementations of MPI and is a good learning tool. If you do not have the MPI library and mpi4py installed on your machine, please refer to the Additional Material at the end of this lab. There are three main differences to keep in mind between mpi4py and MPI in C:

- Python is array-based while C is not.
- mpi4py is object oriented but MPI in C is not.
- mpi4py supports two methods of communication to implement each of the basic MPI commands. They are the upper and lower case commands (e.g. Bcast(...) and bcast(...)). The uppercase implementations use traditional MPI datatypes while the lower case use Python's pickling method. Pickling offers extra convenience to using mpi4py, but the traditional method is faster. In these labs, we will only use the uppercase functions.

Using MPI

We will start with a Hello World program.

```
#hello.py
from mpi4py import MPI

COMM = MPI.COMM_WORLD
RANK = COMM.Get_rank()

print("Hello world! I'm process number {}.".format(RANK))
```

hello.py

Save this program as hello.py and execute it from the command line as follows:

```
$ mpiexec -n 5 python hello.py
```

The program should output something like this:

```
Hello world! I'm process number 3.
Hello world! I'm process number 2.
Hello world! I'm process number 0.
Hello world! I'm process number 4.
Hello world! I'm process number 1.
```

Notice that when you try this on your own, the lines will not necessarily print in order. This is because there will be five separate processes running autonomously, and we cannot know beforehand which one will execute its print() statement first.

ACHTUNG!

It is usually bad practice to perform I/O (e.g., call **print()**) from any process besides the root process (rank 0), though it can be a useful tool for debugging.

How does this program work? First, the mpiexec program is launched. This is the program which starts MPI, a wrapper around whatever program you to pass into it. The -n 5 option specifies the desired number of processes. In our case, 5 processes are run, with each one being an instance of the program "python". To each of the 5 instances of python, we pass the argument hello.py which is the name of our program's text file, located in the current directory. Each of the five instances of python then opens the hello.py file and runs the same program. The difference in each process's execution environment is that the processes are given different ranks in the communicator. Because of this, each process prints a different number when it executes.

MPI and Python combine to make succinct source code. In the above program, the line from mpi4py import MPI loads the MPI module from the mpi4py package. The line COMM = MPI .COMM_WORLD accesses a static communicator object, which represents a group of processes which can communicate with each other via MPI commands. The next line, RANK = COMM.Get_rank(), accesses the processes rank number. A rank is the process's unique ID within a communicator, and they are essential to learning about other processes. When the program mpiexec is first executed, it creates a global communicator and stores it in the variable MPI.COMM_WORLD. One of the main purposes of this communicator is to give each of the five processes a unique identifier, or rank. When each process calls COMM.Get_rank(), the communicator returns the rank of that process. RANK points to a local variable, which is unique for every calling process because each process has its own separate copy of local variables. This gives us a way to distinguish different processes while writing all of the source code for the five processes in a single file.

Here is the syntax for Get_size() and Get_rank(), where Comm is a communicator object:

Comm.Get_size() Returns the number of processes in the communicator. It will return the same number to every process. Parameters:

Return value - the number of processes in the communicator

Return type - integer

Example:

```
#Get_size_example.py
from mpi4py import MPI
SIZE = MPI.COMM_WORLD.Get_size()
print("The number of processes is {}.".format(SIZE))
```

 $Get_size_example.py$

Comm.Get rank() Determines the rank of the calling process in the communicator. Parameters:

Return value - rank of the calling process in the communicator

Return type - integer

Example:

```
#Get_rank_example.py
from mpi4py import MPI
RANK = MPI.COMM_WORLD.Get_rank()
print("My rank is {}.".format(RANK))
```

Get rank example.py

The Communicator

A communicator is a logical unit that defines which processes are allowed to send and receive messages. In most of our programs we will only deal with the MPI.COMM_WORLD communicator, which contains all of the running processes. In more advanced MPI programs, you can create custom communicators to group only a small subset of the processes together. This allows processes to be part of multiple communicators at any given time. By organizing processes this way, MPI can physically rearrange which processes are assigned to which CPUs and optimize your program for speed. Note that within two different communicators, the same process will most likely have a different rank.

Note that one of the main differences between mpi4py and MPI in C or Fortran, besides being array-based, is that mpi4py is largely object oriented. Because of this, there are some minor changes between the mpi4py implementation of MPI and the official MPI specification.

For instance, the MPI Communicator in mpi4py is a Python class and MPI functions like Get_size() or Get_rank() are instance methods of the communicator class. Throughout these MPI labs, you will see functions like Get_rank() presented as Comm.Get_rank() where it is implied that Comm is a communicator object.

Separate Codes in One File

When an MPI program is run, each process receives the same code. However, each process is assigned a different rank, allowing us to specify separate behaviors for each process. In the following code, the three processes perform different operations on the same pair of numbers.

```
#separateCode.py
from mpi4py import MPI
RANK = MPI.COMM_WORLD.Get_rank()

a = 2
b = 3
if RANK == 0:
print a + b
elif RANK == 1:
print a*b
elif RANK == 2:
print max(a, b)
```

separateCode.py

Problem 1. Write a program in which processes with an even rank print "Hello" and process with an odd rank print "Goodbye." Print the process number along with the "Hello" or "Goodbye" (for example, "Goodbye from process 3").

Message Passing between Processes

Let us begin by demonstrating a program designed for two processes. One will draw a random number and then send it to the other. We will do this using the routines Comm.Send() and Comm.Recv().

```
#passValue.py
  import numpy as np
  from mpi4py import MPI
  COMM = MPI.COMM_WORLD
  RANK = COMM.Get_rank()
  if RANK == 1: # This process chooses and sends a random value
      num_buffer = np.random.rand(1)
      print("Process 1: Sending: {} to process 0.".format(num_buffer))
      COMM.Send(num_buffer, dest=0)
      print("Process 1: Message sent.")
  if RANK == 0: # This process recieves a value from process 1
      num_buffer = np.zeros(1)
14
      print("Process 0: Waiting for the message... current num_buffer={}.".format ←
          (num_buffer))
      COMM.Recv(num_buffer, source=1)
16
      print("Process 0: Message recieved! num_buffer={}.".format(num_buffer))
```

passValue.py

To illustrate simple message passing, we have one process choose a random number and then pass it to the other. Inside the receiving process, we have it print out the value of the variable num_buffer before it calls Recv() to prove that it really is receiving the variable through the message passing interface.

Here is the syntax for Send() and Recv(), where Comm is a communicator object:

Comm.Send(buf, dest=0, tag=0) Performs a basic send from one process to another. Parameters:

```
buf (array-like) : data to send
dest (integer) : rank of destination
tag (integer) : message tag
```

The buf object is not as simple as it appears. It must contain a pointer to a Numpy array. It cannot, for example, simply pass a string. The string would have to be packaged inside an array first.

Comm.Recv(buf, source=0, tag=0, Status status=None) Basic point-to-point receive of data.

Parameters:

```
buf (array-like) : initial address of receive buffer (choose receipt location)
source (integer) : rank of source
tag (integer) : message tag
status (Status) : status of object
```

Example:

```
#Send_example.py
from mpi4py import MPI
import numpy as np

RANK = MPI.COMM_WORLD.Get_rank()

a = np.zeros(1, dtype=int) # This must be an array.
if RANK == 0:
    a[0] = 10110100
    MPI.COMM_WORLD.Send(a, dest=1)
elif RANK == 1:
    MPI.COMM_WORLD.Recv(a, source=0)
    print(a[0])
```

Send example.py

Problem 2. Write a script that runs on two processes and passes an n by 1 vector of random values from one process to the other. Write it so that the user passes the value of n in as a command-line argument. The following code demonstrates how to access command-line arguments.

```
from sys import argv

# Pass in the first command line argument as n.
n = int(argv[1])
```

Note

Send() and Recv() are referred to as *blocking* functions. That is, if a process calls Recv(), it will sit idle until it has received a message from a corresponding Send() before it will proceed. (However, in Python the process that calls Comm.Send will *not* necessarily block until the message is received, though in C, MPI_Send does block) There are corresponding *non-blocking* functions Isend() and Irecv() (The *I* stands for immediate). In essence, Irecv() will return immediately. If a process calls Irecv() and doesn't find a message ready to be picked up, it will indicate to the system that it is expecting a message, proceed beyond the Irecv() to do other useful work, and then check back later to see if the message has arrived. This can be used to dramatically improve performance.

Problem 3. Write a script in which the process with rank i sends a random value to the process with rank i+1 in the global communicator. The process with the highest rank will send its random value to the root process. Notice that we are communicating in a ring. For communication, only use Send() and Recv(). The program should work for any number of processes. Does the order in which Send() and Recv() are called matter?

Note

When calling Comm.Recv, you can allow the calling process to accept a message from any process that happened to be sending to the receiving process. This is done by setting source to a predefined MPI constant, source=ANY_SOURCE (note that you would first need to import this with from mpi4py.MPI import ANY_SOURCE or use the syntax source=MPI.ANY_SOURCE).

Application: Monte Carlo Integration

Monte Carlo integration uses random sampling to approximate volumes (whereas most numerical integration methods employ some sort of regular grid). It is a useful technique, especially when working with higher-dimensional integrals. It is also well-suited to parallelization because it involves a large number of independent operations. In fact, Monte Carlo algorithms can be made "embarassingly parallel" — the processes don't need to communicate with one another during execution, simply reporting results to the root process upon completion.

In a simple example, the following code calculates the value of π by sampling random points inside the square $[-1,1] \times [-1,1]$. Since the volume of the unit circle is π and the volume of the square is 4, the probability of a given point landing inside the unit circle is $\pi/4$, so the proportion of samples that fall within the unit circle should also be $\pi/4$. The program samples N=2000 points, determines which samples are within the unit circle (say M are), and estimates $\pi \approx 4M/N$.

```
# pi.py
import numpy as np
from scipy import linalg as la

# Get 2000 random points in the 2-D domain [-1,1]x[-1,1].
```

```
points = np.random.uniform(-1, 1, (2,2000))

# Determine how many points are within the unit circle.
lengths = la.norm(points, axis=0)
num_within = np.count_nonzero(lengths < 1)

# Estimate the circle's area.
print(4 * (num_within / 2000))</pre>
```

pi.py

```
$ python pi.py
3.166
```

Problem 4. The *n*-dimensional open unit ball is the set $U_n = \{\mathbf{x} \in \mathbb{R}^n \mid ||\mathbf{x}||_2 < 1\}$. Write a script that accepts integers n and N on the command line. Estimate the volume of U_n by drawing N points over the n-dimensional domain $[-1,1] \times [-1,1] \times \cdots \times [-1,1]$ on each available process except the root process (for a total of (r-1)N draws, where r is the number of processes). Have the root process print the volume estimate. (Hint: the volume of $[-1,1] \times [-1,1] \times \cdots \times [-1,1]$ is 2^n .)

When n=2, this is the same experiment outlined above so your function should return an approximation of π . The volume of the U_3 is $\frac{4}{3}\pi \approx 4.18879$, and the volume of U_4 is $\frac{\pi^2}{2} \approx 4.9348$. Try increasing the number of sample points N or processes r to see if your estimates improve.

Note

Good parallel code should pass as little data as possible between processes. Sending large or frequent messages requires a level of synchronization and causes some processes to pause as they wait to receive or send messages, negating the advantages of parallelism. It is also important to divide work evenly between simultaneous processes, as a program can only be as fast as its slowest process. This is called load balancing, and can be difficult in more complex algorithms.

Additional Material

Installation of MPI

MPI is a library of functions that interface with your computer's hardware to provide optimal parallel computing performance. In order to use mpi4py, we need to have an MPI Library on installed on the computer as well as the mpi4py package. When you invoke mpi4py in your python code, mpi4py takes what you have written in python and applies it using an MPI Library, so only installing mpi4py is not enough to use MPI.

Installing MPI Library

- 1. For Linux/Mac: We recommend using OpenMPI for your MPI Library installation, though it is not the only library available.
 - Download the binary files from https://www-lb.open-mpi.org/software/ompi/v4.0/.
 - Extract the files from their compressed form and navigate into the new folder titled "openmpi-X.X.X".
 - Configure the files so that they will install correctly on your machine.
 - Compile OpenMPI and install it.

The following is a bash script written for Linux that will install OpenMPI version 4.0.2. It will take about 15 minutes to complete.

```
#!/bin/bash

# download openMPI

wget https://download.open-mpi.org/release/open-mpi/v4.0/openmpi ←

-4.0.2.tar.gz

# extract the files

tar -zxf openmpi-4.0.2.tar.gz

cd openmpi-4.0.2

# configure the files

./configure --prefix=/usr/local/openmpi

# compile openMPI

make all

# install openMPI

sudo make install
```

Finally, you must add OpenMPI to your PATH variable. This is so your computer knows where to look when it wants to execute a certain MPI command. Here is a link that describes how to edit the PATH variable https://gist.github.com/nex3/c395b2f8fd4b02068be37c961301caa7.

On linux you will open a file called .bashrc, on Mac the file is called .bash_profile, both are in the home directory. Add the following line, save the file, and restart your terminal.

```
export PATH=/usr/local/openmpi/bin: $PATH
```

2. For Windows: There is only one free MPI library available for Windows at https://msdn.microsoft.com/en-us/library/bb524831(v=vs.85).aspx. Download the appropriate .exe or .msi file to install on your machine.

Installing mpi4py

1. For All Systems: The easiest installation is using conda install mpi4py. You may also run pip install mpi4py

Ethics in Machine Learning

Lab Objective: Machine learning algorithms can be extremely useful and convenient, but they can also have negative consequences. In this lab, we'll explore the impact people have on machine learning algorithms and some of the unintended effects of machine learning that can result.

Introduction

Machine learning can be an extremely powerful tool in helping us interpret large datasets and then making decisions based on our data. A well-designed algorithm can use a dataset to train a model and identify patterns as well as make decisions with minimal human contact. As machine learning continues to advance and gain power and validity in the world, more and more datasets are being compiled to be trained on and then implemented into some kind of model. This implementation can be anything from predicting the next word when you are texting on your phone to typing at your computer to extremely powerful and accurate facial recognition software. Even though machine learning can be and is exceptionally useful, it has already demonstrated some drawbacks. These drawbacks have negative impacts that often outweigh the power and helpfulness of a well-designed machine learning model. In this lab we will be looking at a few of these drawbacks, as well as some ethical repercussions to help us understand how to be aware of and avoid them in our future endeavors.

Understanding Bias

To begin, we need to make a quick distinction about the term bias. Bias has many different meanings depending on the circumstance and field of study. From a mathematical perspective, bias is defined simply as a measure of the average error of an estimator, a statistical estimate of some quantity. In mathematical terms,

$$bias(\hat{\theta}) = \mathbb{E}[\hat{\theta}] - \hat{\theta}$$

where \mathbb{E} is the expected value, θ is the term we are estimating, and $\hat{\theta}$ is the estimator. In machine learning, one of the goals is often to minimize this type of bias, which we will refer to as statistical bias.

This idea of minimizing bias also applies to other types of biases, including cognitive and data bias. These kinds of biases often result in predictions from our machine learning model being partial to a certain subset of the data. In this lab, we will investigate problems that involve several types of biases.

ACHTUNG!

Not every type of bias has a clear or standard definition. Some types of biases even have different names. For instance, Wikipedia defines statistical bias more broadly,as "a systematic tendency in the process of data collection, which results in lopsided, misleading results". In this lab we have used common terms and definitions specific in the machine learning field but note that they are not universal. With sensitive topics like bias, it is important to be clear about the definition and meaning so that misunderstanding do not occur.

See https://en.wikipedia.org/wiki/Bias#Statistical_biases for Wikipedia's definitions of different biases.

Statistical Bias and Variance

In machine learning there is a constant battle between statistical bias and variance. Often, the goal of a specific machine learning algorithm is to minimize error. Since the error of an algorithm can be described as the sum of irreducible error and reducible error (the sum of statistical bias squared and variance), this equates to minimizing statistical bias and variance.

$$Error = Bias^2 + Var + Irreducible Error$$

where if q(x) is the function the model predicted and f(x) is the actual target function,

$$Var(x) = \mathbb{E}[(q(x) - \mathbb{E}[q(x)])^2]$$

$$Bias(x) = \mathbb{E}[g(x)] - f(x).$$

By definition, a model with high variance means that small changes in the training set will result in large changes of the target function, so the model is overfitted. Low variance is just the opposite; changes in the training set will hardly affect the target function. Statistical bias, on the other hand, deals more specifically with the general form of the target function. High statistical bias implies that we are making large assumptions about the form of the target function, and small bias implies that we are making small assumptions about the form of the target function. Models with high bias are often classified as being underfitted, meaning it will not generalize well to any other data. Simply put, high bias assumes a model and tries to fit the data to that model, and low bias tries to fit a model to the data. Making the statistical bias smaller often makes the variance of the model go up and a smaller variance will result in a larger bias. The relationship between statistical bias and variance, or overfitting and underfitting, is inescapable in machine learning. In the end, the best algorithm is achieved by finding the middle ground.

Algorithm	Bias	Variance
Linear Regression	High	Low
Logistic Regression	High	Low
Decision Trees	Low	High
k-Nearest Neighbors	Low	High
Support Vector Machine	Low	High

Table 17.1: List of common machine learning algorithms whether they have low or high Bias and Variance.

A common example for evaluating this relationship is that of fitting a dataset to a polynomial. Based on our definitions of statistical bias and variance, we can conclude that as the degree of polynomial gets larger, the statistical bias decreases because the end result begins to depend more and more on the specific data points given to the training set.

We will be using the mean square error to calculate the error. The mean square error is defined as

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2$$
 (17.1)

Here Y_i is the given value and \hat{Y}_i is the predicted value.

Consider the following example using numpy in fitting a third-degree polynomial to cos(x).

```
>>> import numpy as np
>>> from sklearn.metrics import mean_squared_error as mse
>>> x = np.linspace(-1,1,25)
>>> degree = 3 # polynomial degree
# generate data to fit on
>>> y = np.cos(x)
# fit the polynomial
>>>poly_fit = np.polyfit(x, y, degree)
# evaluate the polynomial
>>> y_predicted = np.polyval(poly_fit, x)
# calculate the mean square error of the fit
>>> mse(y_predicted, y)
1.2075486783458322e-05
# plot the original and fitted data
>>> plt.plot(x,y,'r')
>>> plt.plot(x,y_predicted,'b')
```

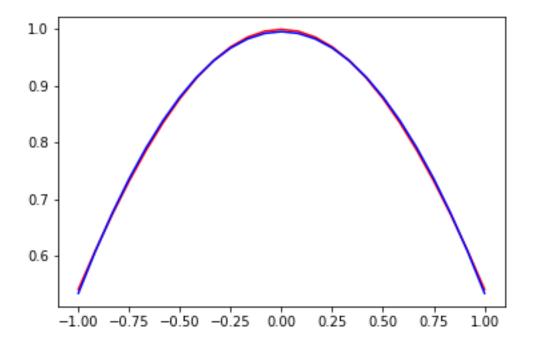


Figure 17.1: Plot of cos(x) (red) and a third-degree polynomial approximation (blue).

To simulate the idea of generalization, we will generate 100 datasets. The better the algorithm performs across all the sets, the more we can assume that it will fit well on different datasets that were not in the training data.

Problem 1. Approximate $sin(\pi x)$ with polynomials. To do this, write a function that accepts as parameters \min_{degree} and \max_{degree} . Inside it, generate data using the provided generate_sets() function. x_test and x_train are 1-d arrays with the x-values needed to test and train. y_test and y_train are 100-d arrays, each subarray contains the y-values for one dataset.

For each dataset in y_train,

- 1. Fit a polynomial of each degree $d \in \{\min \text{ degree}, \dots, \max \text{ degree}\}$, inclusive.
- 2. Use np.polyeval() to predict the values of x_{train} and x_{test} .
- 3. Calculate the mean squared error of the training and testing data.

Return the mean squared error of both the training and testing data for each dataset, as well as an array containing the predicted values for x_test for each degree and dataset, and the generated x_test values (needed to calculate the bias).

Plot the mean test error and the mean train error for each degree with the corresponding polynomial degree as the horizontal axis and compare with Figure 17.2.

Hint: The ndarrays outputted by your function should have the following shapes:

```
(100,9)(100,9)(100,9,7)(7,)
```

Now that we have the predictions and the error values, we can also evaluate the variance and bias. Recall that variance is calculated solely using the prediction values. In this case, the estimator q is the function generated when we used numpy.polyfit().

Bias, on the other hand, is calculated using the estimator and the desired target function, which in this case is $\sin(\pi x)$. Using the equation for bias given above

$$Bias = (mean(y pred) - sin(\pi x))^2$$

. For the returned x_{test} and results_list from $\text{test_polyfits}()$, we can calculate the mean variance across all the datasets on degree i using the method given below.

Problem 2. Use the results of 1 to calculate the mean of the bias, variance, test error, and train error of each polynomial degree in range $\{0, \ldots, 8\}$. Plot the mean test error, variance, and bias with the corresponding polynomial degree as the horizontal axis. Make sure to include axis labels, a title, and plot legends for readability. Your plot should look like the right plot in Figure 17.2.

Create a single sample dataset with 500 samples using generate_sets with num_datasets=1 and num_samples=500. Choose the polynomial of degree n that showed the smallest mean test error in the previous problems and fit your training set to that model.

Evaluate your results by plotting $sin(\pi x)$, the sample points, and the best fit polynomial. Include plot legends, display the mean squared error of the test set in the title of the plot, and display the degree of the polynomial as the label on the horizontal axis.

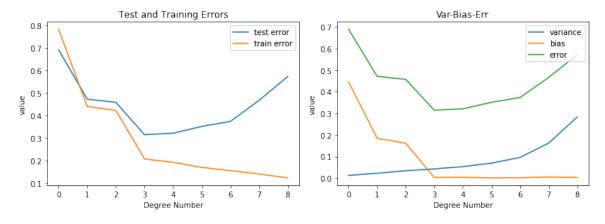


Figure 17.2

The way that you evaluated and chose the best algorithm for the given datasets is common in evaluating and choosing models to use in machine learning. If you continue to decrease the bias the training error will often continue to decrease, but there will be a point where the testing error starts to increase.

In Problem 1 we generated our own dataset, but if we are given a dataset from which we wanted to create a model, we can use *cross validation*, which is similar to what we did in the previous problem, to evaluate and choose the best model. *Cross validation* takes the given data and splits it into multiple training and testing sets. Using these new splits, we can then train and test on every one of these train-test-splits and evaluate the results. The model that showed the best performance across all of these splits is the one you will probably want to use, because it will perform better on datasets that were not in the training test. Computational complexity and size are other factors that could also influence your choice.

Though this kind of model evaluation can be both tedious and time consuming, but it is often the key to choosing the best model for a specific machine learning task as well as future model development. Even the smallest change in your model can result in a significant change in accuracy. Faulty data might look good initially but will not transfer over to different datasets very well. Evaluating the statistical bias and variance in conjuction with the error of your model will help you avoid these issues.

Measurement Bias

Measurement bias occurs when some of the data used as a variable is inaccurate. This could be because the equipment measuring the data can't detect small changes or the device measuring changes the data. One example is taking pictures on a camera that increases the brightness of the photo or has a spot on the lens.

Cancer detection is well-known machine learning problem. A model will train on images of cells, some of which are cancerous, and then predict whether new samples are cancerous. Some melanoma classification algorithms have been shown to predict melanoma better than trained physicians. This success has led to developers releasing software that allows a user to take picture and then the software will use a previously trained algorithm to predict the presence of melanoma. While this can be extremely useful and helpful, if there is a measurement error, such as a damaged camera lens, there can be issues in correct classification.

We will examine a model created to predict whether a specific skin lesion is melanomic. The files melanoma_test.pkl and melanoma_modified.pkl contain pandas DataFrames that will be used for testing the trained model which will be trained on melanoma_train.pkl. The file melan oma.pkl is a flattened array of a black and white image of a skin lesion. The other testing file melanoma_modified.pkl contains the same data, with an added black square to the image to simulate a faulty camera or damaged machine.

Problem 3. In this problem we will compare the differences between good data and faulty data in predicting if a person has melanoma. First, use <code>get_melanoma_data()</code> to get the relevant training and testing data. Notice that there are two different testing datasets, the *test* and *modified* datasets as explained above. Next, train a Random Forest model using SkLearn's RandomForestClassifier with <code>random_state=15</code>. After the model is trained, use the model to predict the <code>test</code> and <code>modified</code> datasets.

Compute the accuracy and the percentage of false positive results for both datasets. Display all four of these numbers in a plt.bar graph so that the reader can understand which ones are from the modified test data and which one is from the original image.

Write a few sentences explaining the results of the graph and how this can affect the usefulness of the model.

Sampling Bias

Sampling bias is a type of bias that results from the way the data, or a sample, is collected. More specifically, sampling bias is when the sample is collected in a way that results in some members of the intended population having a smaller sampling probability than others. This can happen when a sample is taken in a specific area that is not representative of the entire population. Sampling bias will result in many issues for prediction algorithms. In these next couple of sections and problems we will be focusing on only a few of them.

The Judicial System

Minority groups have a history of facing discrimination in many forms, including legal discrimination. Because of the power and usefulness of machine learning, predictive algorithms have already made their way into the judicial system as recidivism tools. One example is a machine learning algorithm that uses facial recognition with other factors, such as whether a defendant has a job and their education level, to produce a score called a risk assessment. The risk assessment score is then used to help determine things like sentence length, bond amount, and parole.

An analysis¹ showed that the algorithm had a 20% false positive rate for violent crime and of those predicted to commit another crime, about 61% did. It also showed that black defendants were 77% more likely to receive a higher risk for future violent crime and 45% more likely to receive a higher risk score for future crime of any kind. Many of these algorithms have not been independently evaluated for accuracy and racial bias, and the defendants are not allowed to see how their scores are calculated.

 $^{^{}m l}$ https://www.propublica.org/article/machine-bias-risk-assessments-in-criminal-sentencing

For Problems 4 and 5, we will be using sentence_labeled.csv and sentence_unlabeled.csv. The first will be used for training and testing the algorithm and the second will be used for prediction and analysis of the results. Each of these files contain a large sample of an even larger dataset containing information of incarcerated persons. The files have columns titled AGE, RACE, OFFENSE, and FACILITY. In addition, sentence_labeled.csv contains a column titled SENTENCE YEARS. This is the label that we will be training our model to predict, and it represents the sentence length in years. For simplicity, all sentences that were above 50 years were removed from the data.

We will be using sklearn's RandomForestRegressor, which is the continuous variable version of the RandomForestClassifier. To analyze the regressor we will be using the R-squared score. This scoring metric is a little more complicated, but it is used to help us determine the effectiveness of a specific regressor. If you wish to know more about it look at, https://en.wikipedia.org/wiki/Coefficient_of_determination. R-squared score is part of the sklearn metrics and takes two parameters, the actual labels and the predicted labels.

```
>>> from sklearn.metrics import r2_score

# compute R-squared score between actual (y_test) and predicted (y_hat)
>>> accuracy = r2_score(y_test,y_hat)
```

Problem 4. Identify the importance of the RACE, FACILITY, AGE, and OFFENSE features in sentence_labeled.csv in predicting SENTENCE YEARS. To do this, implement the following steps:

- Load the sentence_labeled.csv. Create the labels and split into test and training data, (use SkLearn's test_train_split()) with a 70/30 train/test split and random_state=21.
- Train the model using the RandomForestRegressor with random_state=13.
- Using the model, predict the labels for the test data. Calculate and print the R-squared score of the predicted test labels. It should be around 0.8 1.0.
- Compute the feature importance (model.feature_importances_ and create a descriptive bar plot with a column for each feature. Your results should look similar to Figure 17.3.
- Remove RACE from the features. Retrain the model, predict the labels, compute the R-squared score and feature importance, and create a new bar plot.

Write a few sentences about your results.

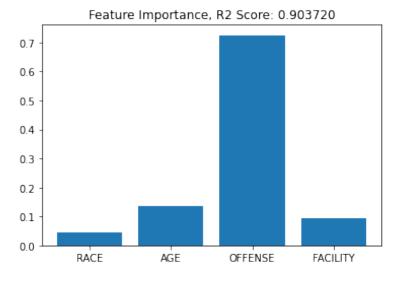


Figure 17.3

In this case, removing the RACE feature will not eliminate prejudice because of the FACILITY feature. The facilities that generally have longer sentences are those that are used to incarcerate the individuals of racial minority communities in the United States. More information on the facilities can be found in the facility_map.p file. It is common, that other less obvious features can also include sample bias in them. In other words, a column such as FACILITY, which does not necessarily indicate race, will also help to propagate negative prejudice into our machine learning models because it may disguise underlying characteristics. For example, since neighborhoods can be segregated, using zip codes in these areas can support a racial bias. It is extremely important to look at feature importance and compare results across demographics to prevent prejudice and discrimination.

Problem 5. Using the model with all four features, make predictions on the unlabeled data, sentence_unlabeled.p. Create histograms for the SENTENCE YEARS of black convicts for the following OFFENSE numbers: 27,42,95,64. Overlay the SENTENCE YEARS of the same OFFENSE for white convicts. Include plot legends and use 51 bins, each representing a single year from 0-50. Use the OFFENSE number as a key to get its description using offense_map.p and use it as the title of the plot. See Figure 17.4 for an example.

Hint: Set the hist parameter alpha to a value which allows for you to see both plots, even if they overlap.

Note: These offenses have been chosen because the sample size was significant and almost equivalent for both black and white convicts.

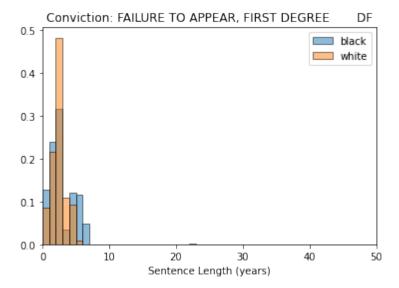


Figure 17.4: The percent of whites and blacks sentenced to lengths of time (in year).

Recognizing and Reducing Sampling Bias

Another example of sampling bias is found in resume learning. In 2014, Amazon's machine learning specialists started working on an algorithm that sorted through resumes and helped choose the applicants who would qualify for an interview. Given the large number of application Amazon receives and the time needed to sort through resumes, this seemed like a great idea. However, the next year, the company discovered that the algorithm was prejudiced against women². So a woman was significantly less likely to be given an interview than a man, even though both applicants had more or less the same qualifications.

This is an additional example of sampling bias, because the data Amazon used to train their model on was data from previously hired employees over the previous ten years. Because the tech industry is a male dominated industry, the alogrithm favored patterns found on male resumes. This sample, based on imbalanced data, resulted in a machine learning algorithm that often chose men over women with the same relevant qualifications.

The typical machine learning algorithm for resume sorting goes as follows: The first part uses natural language processing techniques to pick keywords off each resume to make sorting easier. A model is trained on the keywords to determine which keywords are most important in determining whether a candidate successfully gets hired. Going back to the Amazon example, their model learned keywords and phrases that are were common on male applicants' resumes, such as executed and captured, and counted them as important, even though the words and phrases were irrelevant to the actual job.

For the next problem we will be considering a similar scenario. A group of veterans with special programming and development skills came together and formed a software engineering company. They decided that their platform would be structured around fairness for all. Because of their specific advertising and present demographic, they received almost exclusively veteran applicants. Accommodations for disabled veterans were in place and posed no problems for those wanting to apply.

²https://reuters.com/article/us-amazon-com-jobs-automation-insight

The company grew and began receiving more skilled applicants outside of their specific veteran demographic. To reduce the time it took to sort through the growing stack of resumes, they decided to create a model that could do the preliminary sorting for them. Using previous hiring data, they created an algorithm that selected keywords that were common on applicants and simplified all the previous and current applicants based on those key words. After this, they created the model to make the prediction that they wanted.

The data is located in three files; skills.txt, resumes_train.csv, and resumes_test.csv. The first file, skills.txt contains the key words the algorithm identified as important on the resumes. The second file, resumes_train.csv, contains the training data. It is a pandas DataFrame and contains a list of resumes in csv form, where each column is labeled with a keyword from the resume with corresponding value 0 (keyword was not on resume) or 1 (keyword was on resume). The first column is Interview, which indicates if the resume owner received an interview. resumes_test.csv is the new batch of resumes, so it is similar to resumes_train.csv but without a column to indicate whether a person received an interview or not.

Problem 6. Analyze the algorithm that the company created. The first steps of identifying key words, simplifying the resumes and model creation have all been done for you. To get the accuracy and results of the model call,

```
# get the accuracy and the results of the algorithm
>>> accuracy, results = resume_model("skills.txt")
```

This function will return a cross validation mean accuracy score called accuracy, and a pandas DataFrame, called results. results contains the training data. Each row represents an applicant and the columns represent a keyword that could appear on the applicant's resume. The last column, 'Interview', is the model's prediction of whether that applicant received an interview.

Create a function called get_percentages() that accepts the results and calculates and returns the following.

- The percentage of applicants the model predicted to receive an interview.
- The percentage of women applicants predicted to receive an interview.
- The percentage of veteran, women applicants predicted to receive an interview.
- The percentage of non-veteran, women applicants predicted to receive an interview.

Finally, use a plt.bar graph to display the cross validation accuracy score, the percentage of people who received an interview, the percentage of women that received an interview, the percentage of women who were veterans that received an interview, and the percentage of women who are not veterans that received an interview. Compare your graph with Figure 17.5.

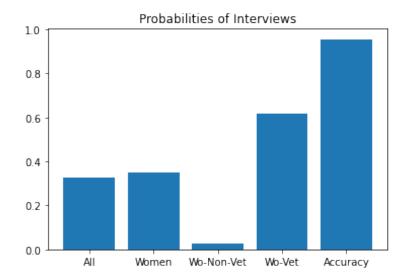


Figure 17.5: Probability different demographics would receive an interview.

If we only looked at three of the results: the percentage of applicants that received an interview, the percentage of women that received an interview, and the accuracy, we would think that the model performed well. The percentage of women who received an interview was similar to the percentage of total people who got an interview. However, if you look at more specific results, like the percentage of women veterans that got the interview versus the percentage of non-veteran women that received an interview, the algorithm shows some intense favoritism to veterans.

As discussed previously, the model to select keywords was trained on the company's previous data. This data was gathered from a time when they previously received applications from and hired exclusively veterans. Some of these key words in *skills.txt* are not relevant for a software engineer, but the algorithm deemed them important because of the frequency of their appearance in the training data. The training data did not always represent what the employers were actually looking for.

Discussion on Ethics

In this lab, we discussed many important techniques for examining and determining multiple types of bias in machine learning algorithms. Statistical bias and variance can be optimized and measurement error can be avoided, but other kinds of cognitive and social bias are more nuanced. Being aware of these issues is important as machine learning becomes ingrained in how the world and its machines function. We will mention three ethical concerns regarding machine learning that were more or less a part of this lab. Be aware that this list of three does not contain all possible ethical questions when it comes to machine learning.

The first concern is of the fairness of the model. We examined this idea in both the resume and the incarceration problems. Data based on previous prejudice or sampling bias may be replicated in your algorithm, propagating error and resulting in unintentional discrimination. Avoiding this problem requires conscious effort and a proper understanding of the sources of your data and the impact of the model.

The second concern is dehumanization. Machine learning can take humans out of many important decision-making processes, which can be a good thing if the algorithms are extremely well designed, but it also poses a significant risk if the model contains any amount of accidental bias or discrimination, as in the incarceration problem.

The final idea is consent. It is important to consider what data the model uses, whose data it is, and if it was gathered appropriately. Privacy and permission must be respected. This is an important concern to consider before beginning a project and while considering potential effects of the analysis.

There is not a single answer to any of these questions that will please everyone, such is the nature of ethics, but before implementing a machine learning algorithm, consider what you are doing and how it might affect those around you. As this issue gains awareness, people are starting to create tools to identify and mitigate bias and discrimination.

- AI Fairness 360³: Created by IBM, it is a well-known open-source package that not only identifies and mitigates discrimination and bias.
- Skater⁴: Developed by Oracle, Skater can be used on complex algorithms and black-box models to detect bias.
- Audit-AI⁵: A python library that can integrate with Pandas an SkLearn to measure and mitigate discriminatory patterns.

Other python packages for identifying bias include FairML, aequitas, fairNN, and parity-fairness. For more information on fairness, accountability, transparency, and ethics in machine learning, visit https://www.microsoft.com/en-us/research/theme/fate/.

³https://aif360.mybluemix.net/

⁴https://pypi.org/project/skater/

 $^{^5 {}m https://github.com/pymetrics/audit-ai}$

18 Apache Spark

Lab Objective: Dealing with massive amounts of data often requires parallelization and cluster computing; Apache Spark is an industry standard for doing just that. In this lab we introduce the basics of PySpark, Spark's Python API, including data structures, syntax, and use cases. Finally, we conclude with a brief introduction to the Spark Machine Learning Package.

Apache Spark

Apache Spark is an open-source, general-purpose distributed computing system used for big data analytics. Spark is able to complete jobs substantially faster than previous big data tools (i.e. Apache Hadoop) because of its in-memory caching, and optimized query execution. Spark provides development APIs in Python, Java, Scala, and R. On top of the main computing framework, Spark provides machine learning, SQL, graph analysis, and streaming libraries.

Spark's Python API can be accessed through the PySpark package. You must install Spark, along with the supporting tools like Java, on your local machine for PySpark to work. This will include ensuring that both Java and Spark are included in the environment variable PATH. ¹ Installation of PySpark for local execution or remote connection to an existing cluster can be done with conda or pip commands.²

```
# install Java
$ sudo apt-get install openjdk-8-jdk
# check the version, it may not be exactly the same
$ java -version
openjdk version "1.8.0_242"
OpenJDK Runtime Environment (build 1.8.0_242-b09)
OpenJDK 64-Bit Server VM (build 25.242-b09, mixed mode)

# Install Spark by following instructions in the footnote
# Following these steps, you must configure your PATH environment variable
# CHOOSE ONE
```

¹See the Apache Spark configuration instructions for detailed installation instructions

²You may also use the script provided with the spec file that will completely install Spark and its requirements. Note however that this script is provided AS IS and is not the recommended method.

```
# PySpark installation with conda
$ conda install -c conda-forge pyspark

# PySpark installation with pip
$ pip install pyspark
```

If you use python3 in your terminal, you will need to set the PYSPARK_PYTHON environment variable to python3. When using an IDE, you must call it from the terminal or set the variables inside the editor so that PySpark can be found.

PySpark

One major benefit of using PySpark is the ability to run it in an interactive environment. One such option is the interactive Spark shell that comes prepackaged with PySpark. To use the shell, simply run pyspark in the terminal. In the Spark shell you can run code one line at a time without the need to have a fully written program. This is a great way to get a feel for Spark. To get help with a function use help(function); to exit the shell simply run quit().

In the interactive shell, the SparkSession object - the main entrypoint to all Spark functionality - is available by default as spark. When running Spark in a standard Python script (or in IPython) you need to define this object explicitly. The code box below outlines how to do this. It is standard practice to name your SparkSession object spark.

It is important to note that when you are finished with a SparkSession you should end it by calling spark.stop().

Note

While the interactive shell is very robust, it may be easier to learn Spark in an environment that you are more familiar with (like IPython). To do so, just use the code given below. Help can be accessed in the usual way for your environment. Just remember to stop() the SparkSession!

```
NOTE
The syntax
```

```
>>> spark = SparkSession\
... .builder\
... .appName("app_name")\
... .getOrCreate()
```

is somewhat unusual. While this code can be written on a single line, it is often more readable to break it up when dealing with many chained operations; this is standard styling for Spark. Note that you *cannot* write a comment after a line continuation character '\'.

Resilient Distributed Datasets

The most fundamental data structure used in Apache Spark is the Resilient Distributed Dataset (RDD). RDDs are immutable distributed collections of objects. They are *resilient* because performing an operation on one RDD produces a *new* RDD without altering the original; if something goes wrong, you can always go back to your original RDD and restart. They are *distributed* because the data resides in logical partitions across multiple machines. While RDDs can be difficult to work with, they offer the most granular control of all the Spark data structures.

There are two main ways of creating RDDs. The first is reading a file directly into Spark and the second is parallelizing an existing collection (list, numpy array, pandas dataframe, etc.). We will use the Titanic dataset³ in most of the examples throughout this lab. The example below shows various ways to load the Titanic dataset as an RDD.

```
# SparkSession available as spark
# load the data directly into an RDD
>>> titanic = spark.sparkContext.textFile('titanic.csv')
# the file is of the format
#Pclass,Survived,Name,Sex,Age,Sibsp,Parch,Ticket,Fare
# Survived | Class | Name | Sex | Age | Siblings/Spouses Aboard | Parents/\leftarrow
   Children Aboard | Fare
>>> titanic.take(2)
['0,3,Mr. Owen Harris Braund,male,22,1,0,7.25',
 '1,1,Mrs. John Bradley (Florence Briggs Thayer) Cumings,female,38,1,0,71.283']
# note that each element is a single string - not particularly useful
# one option is to first load the data into a numpy array
>>> np_titanic = np.loadtxt('titanic.csv', delimiter=',', dtype=list)
# use sparkContext to parallelize the data into 4 partitions
>>> titanic_parallelize = spark.sparkContext.parallelize(np_titanic, 4)
>>> titanic_parallelize.take(2)
[array(['0', '3', ..., 'male', '22', '1', '0', '7.25'], dtype=object),
```

 $^{^3} https://web.stanford.edu/class/archive/cs/cs109/cs109.1166/problem12.html$

```
array(['1', '1', ..., 'female', '38', '1', '0', '71.2833'], dtype=object)]
```

ACHTUNG!

Because Apache Spark partitions and distributes data, calling for the first n objects using the same code (such as take(n)) may yield different results on different computers (or even each time you run it on one computer). This is not something you should worry about; it is the result of variation in partitioning and will not affect data analysis.

RDD Operations

Transformations

There are two types of operations you can perform on RDDs: transformations and actions. Transformations are functions that produce new RDDs from existing ones. Transformations are also lazy; they are not executed until an action is performed. This allows Spark to boost performance by optimizing how a sequence of transformations is executed at runtime.

One of the most commonly used transformations is the map(func), which creates a new RDD by applying func to each element of the current RDD. This function, func, can be any callable python function, though it is often implemented as a lambda function. Similarly, flatMap(func) creates an RDD with the flattened results of map(func).

The filter(func) transformation returns a new RDD containing only the elements that satisfy func. In this case, func should be a callable python function that returns a Boolean. The elements of the RDD that evaluate to True are included in the new RDD while those that evaluate to False are excluded.

```
# create a new RDD containing only the female passengers
>>> titanic = titanic.map(lambda row: row.split(','))
>>> titanic_f = titanic.filter(lambda row: row[3] == 'female')
```

```
>>> titanic_f.take(3)
[['1', '1', ..., 'female', '38', '1', '0', '71.2833'],
['1', '3', ..., 'female', '26', '0', '0', '7.925'],
['1', '1', ..., 'female', '35', '1', '0', '53.1']]
```

Note

A great transformation to help validate or explore your dataset is distinct(). This will return a new RDD containing only the distinct elements of the original. In the case of the Titanic dataset, if you did not know how many classes there were, you could do the following:

Spark Command	Transformation		
map(f)	Returns a new RDD by applying f to each element of this RDD		
flatmap(f)	Same as map(f), except the results are flattened		
filter(f)	Returns a new RDD containing only the elements that satisfy f		
distinct()	Returns a new RDD containing the distinct elements of the		
	original		
reduceByKey(f)	Takes an RDD of (key, val) pairs and merges the values for		
reduceBykey(1)	each key using an associative and commutative reduce function f		
sortBy(f)	Sorts this RDD by the given function f		
sortByKey(f)	Sorts an RDD assumed to consist of (key, val) pairs by the		
Sol cbykey (1)	given function f		
groupBy(f)	Returns a new RDD of groups of items based on f		
groupByKey()	Takes an RDD of (key, val) pairs and returns a new RDD		
	with (key, (val1, val2,)) pairs		

```
# the following counts the number of passengers in each class
# note that this isn't necessarily the best way to do this

# create a new RDD of (pclass, 1) elements to count occurances
>>> pclass = titanic.map(lambda row: (row[1], 1))
>>> pclass.take(5)
[('3', 1), ('1', 1), ('3', 1), ('1', 1), ('3', 1)]

# count the members of each class
>>> pclass = pclass.reduceByKey(lambda x, y: x + y)
>>> pclass.collect()
[('3', 487), ('1', 216), ('2', 184)]
```

```
# sort by number of passengers in each class, ascending order
>>> pclass.sortBy(lambda row: row[1]).collect()
[('2', 184), ('1', 216), ('3', 487)]
```

Problem 1. Write a function that accepts the name of a text file with default filename=huck_finn.txt.^a Load the file as a PySpark RDD, and count the number of occurrences of each word. Sort the words by count, in descending order, and return a list of the (word, count) pairs for the 20 most used words. The data does not need to be cleaned.

Actions

Actions are operations that return non-RDD objects. Two of the most common actions, take(n) and collect(), have already been seen above. The key difference between the two is that take(n) returns the first n elements from one (or more) partition(s) while collect() returns the contents of the entire RDD. When working with small datasets this may not be an issue, but for larger datasets running collect() can be very expensive.

Another important action is reduce(func). Generally, reduce() combines (reduces) the data in each row of the RDD using func to produce some useful output. Note that func *must* be an associative and commutative binary operation; otherwise the results will vary depending on partitioning.

```
# create an RDD with the first million integers in 4 partitions
>>> ints = spark.sparkContext.parallelize(range(1, 1000001), 4)
# [1, 2, 3, 4, 5, ..., 1000000]
# sum the first one million integers
>>> ints.reduce(lambda x, y: x + y)
500000500000

# create a new RDD containing only survival data
>>> survived = titanic.map(lambda row: int(row[0]))
>>> survived.take(5)
[0, 1, 1, 1, 0]

# find total number of survivors
>>> survived.reduce(lambda x, y: x + y)
5000
```

 $[^]a$ https://www.gutenberg.org/files/76/76-0.txt

Spark Command	Action		
take(n)	returns the first n elements of an RDD		
collect()	returns the entire contents of an RDD		
reduce(f)	merges the values of an RDD using an associative and		
	commutative operator f		
count()	returns the number of elements in the RDD		
min(): man(): mann()	returns the minimum, maximum, or mean of the RDD,		
min(); max(); mean()	respectively		
sum()	adds the elements in the RDD and returns the result		
saveAsTextFile(path)	saves the RDD as a collection of text files (one for each		
saveAsiextrile(path)	partition) in the directory specified		
	immediately applies f to each element of the RDD; not to be		
foreach(f)	confused with map(), foreach() is useful for saving data		
	somewhere not natively supported by PySpark		

Problem 2. Since the area of a circle of radius r is $A = \pi r^2$, one way to estimate π is to estimate the area of the unit circle. A Monte Carlo approach to this problem is to uniformly sample points in the square $[-1,1] \times [-1,1]$ and then count the percentage of points that land within the unit circle. The percentage of points within the circle approximates the percentage of the area occupied by the circle. Multiplying this percentage by 4 (the area of the square $[-1,1] \times [-1,1]$) gives an estimate for the area of the circle. ^a

Write a function that uses Monte Carlo methods to estimate the value of π . Your function should accept two keyword arguments: n=10**5 and parts=6. Use n*parts sample points and partition your RDD with parts partitions. Return your estimate.

DataFrames

While RDDs offer granular control, they can be slower than their Scala and Java counterparts when implemented in Python. The solution to this was the creation of a new data structure: Spark DataFrames. Just like RDDs, DataFrames are immutable distributed collections of objects; however, unlike RDDs, DataFrames are organized into named (and typed) columns. In this way they are conceptually similar to a relational database (or a pandas DataFrame).

The most important difference between a relational database and Spark DataFrames is in the execution of transformations and actions. When working with DataFrames, Spark's Catalyst Optimizer creates and optimizes a logical execution plan before sending any instructions to the drivers. After the logical plan has been formed, an optimal physical plan is created and executed. This provides significant performance boosts, especially when working with massive amounts of data. Since the Catalyst Optimizer functions the same across all language APIs, DataFrames bring performance parity to all of Spark's APIs.

^aSee Example 7.1.1 in the Volume 2 textbook

Spark SQL and DataFrames

Creating a DataFrame from an existing text, csv, or JSON file is generally easier than creating an RDD. The DataFrame API also has arguments to deal with file headers or to automatically infer the schema.

```
# load the titanic dataset using default settings
>>> titanic = spark.read.csv('titanic.csv')
>>> titanic.show(2)
+---+---+
                  _c2| _c3|_c4|_c5|_c6|
|_c0|_c1|
+---+---+
| 0| 3|Mr. Owen Harris B...| male| 22| 1| 0| 7.25|
| 1| 1|Mrs. John Bradley...|female| 38| 1| 0|71.2833|
+---+---+
only showing top 2 rows
# spark.read.csv('titanic.csv', inferSchema=True) will try to infer
# data types for each column
# load the titanic dataset specifying the schema
>>> schema = ('survived INT, pclass INT, name STRING, sex STRING, '
          'age FLOAT, sibsp INT, parch INT, fare FLOAT'
>>> titanic = spark.read.csv('titanic.csv', schema=schema)
>>> titanic.show(2)
+-----+----+----+-----+
|survived|pclass|
                      name| sex|age|sibsp|parch| fare|
+----+
          3|Mr. Owen Harris B... | male | 22 | 1 | 0 | 7.25 |
          1|Mrs. John Bradley...|female| 38| 1| 0|71.2833|
     1|
only showing top 2 rows
# for files with headers, the following is convenient
spark.read.csv('my_file.csv', header=True, inferSchema=True)
```

Note

To convert a DataFrame to an RDD use my_df.rdd; to convert an RDD to a DataFrame use spark.createDataFrame(my_rdd). You can also use spark.createDataFrame() on numpy arrays and pandas DataFrames.

DataFrames can be easily updated, queried, and analyzed using SQL operations. Spark allows you to run queries directly on DataFrames similar to how you perform transformations on RDDs. Additionally, the pyspark.sql.functions module contains many additional functions to further analysis. Below are many examples of basic DataFrame operations; further examples involving the pyspark.sql.functions module can be found in the additional materials section. Full documentation can be found at https://spark.apache.org/docs/latest/api/python/pyspark.sql.html.

```
# select data from the survived column
>>> titanic.select(titanic.survived).show(3) # or titanic.select("survived")
+----+
|survived|
+----+
      0|
      11
      11
only showing top 3 rows
# find all distinct ages of passengers (great for data exploration)
>>> titanic.select("age")\
         .distinct()\
         .show(3)
. . .
+---+
| age|
+---+
|18.0|
[64.0]
10.421
+---+
only showing top 3 rows
# filter the DataFrame for passengers between 20-30 years old (inclusive)
>>> titanic.filter(titanic.age.between(20, 30)).show(3)
+----+
                          name | sex | age | sibsp | parch | fare |
|survived|pclass|
+----+
            3|Mr. Owen Harris B...| male|22.0|
                                            1|
                                                 0| 7.25|
      1|
            3|Miss. Laina Heikk...|female|26.0| 0|
                                                 0 | 7.925 |
                Mr. James Moran | male | 27.0 | 0 |
                                                 0|8.4583|
+----+---+----+----+----+
only showing top 3 rows
# find total fare by pclass (or use .avg('fare') for an average)
>>> titanic.groupBy('pclass')\
       .sum('fare')\
        .show()
+----+
|pclass|sum(fare)|
+----+
```

228

```
1 | 18177.41 |
   3| 6675.65|
   2| 3801.84|
+----+
# group and count by age and survival; order age/survival descending
>>> titanic.groupBy("age", "survived").count()\
      .sort("age", "survived", ascending=False)\
       .show(2)
+---+
|age|survived|count|
+---+
| 80 | 1 | 1 |
| 74|
       0|
+---+
only showing top 2 rows
# join two DataFrames on a specified column (or list of columns)
>>> titanic_cabins.show(3)
+----+
           name| cabin|
+----+
|Miss. Elisabeth W...| B5|
|Master. Hudsen Tr... | C22 C26 |
|Miss. Helen Lorai... | C22 C26 |
+----+
only showing top 3 rows
>>> titanic.join(titanic_cabins, on='name').show(3)
+----+
           name|survived|pclass| sex| age|sibsp|parch| fare| cabin|
+-----+
|Miss. Elisabeth W...| 0| 3| male|22.0| 1| 0| 7.25| B5| |Master. Hudsen Tr...| 1| 3|female|26.0| 0| 0| 7.925|C22 C26|
|Miss. Helen Lorai...| 0| 3| male|27.0| 0| 0|8.4583|C22 C26|
+----+
only showing top 3 rows
```

Note

If you prefer to use traditional SQL syntax you can use spark.sql("SQL QUERY"). Note that this requires you to first create a temporary view of the DataFrame.

```
# create the temporary view so we can access the table through SQL
>>> titanic.createOrReplaceTempView("titanic")
```

SQLite Command	
SELECT	
GROUP BY	
ORDER BY	
WHERE	
WHEN	
BETWEEN	
DROP	
JOIN (join type specified by how)	
COUNT()	
SUM()	
AVG()	
fetchall()	

Problem 3. Write a function with keyword argument filename='titanic.csv'. Load the file into a PySpark DataFrame and find (1) the number of women on-board, (2) the number of men on-board, (3) the survival rate of women, and (4) the survival rate of men. Return these four values in the order given.

Problem 4. In this problem, you will be using the london_income_by_borough.csv and the london_crime_by_lsoa.csv files to visualize the relationship between income and the frequency of crime.^a The former contains estimated mean and median income data for each London borough, averaged over 2008-2016; the first line of the file is a header with columns borough, mean-08-16, and median-08-16. The latter contains over 13 million lines of crime data, organized by borough and LSOA (Lower Super Output Area) code, for London between 2008 and 2016; the first line of the file is a header, containing the following seven columns:

```
1soa_code: LSOA code (think area code) where the crime was committed
     borough: London borough were the crime was committed
     major_category: major (read: general) category of the crime
    minor_category: minor (read: specific) category of the crime
     value: number of occurrences of this crime in the given lsoa_code, month, and year
     year: year the crime was committed
    month: month the crime was committed
     Write a function that accepts three keyword arguments: crimefile='london_crime_by_lsoa
.csv', incomefile='london_income_by_borough.csv', and major_cat='Robbery'. Load
the two files as PySpark DataFrames. Use them to create a new DataFrame containing, for each
borough, the total number of crimes for the given major category (major_cat) and the median
income. Order the DataFrame by the average crime rate, descending. The final DataFrame
should have three columns: borough, average_crime_rate, median-08-16 (column names
may be different).
     Convert the DataFrame to a numpy array using np.array(df.collect()), and create
a scatter plot of the number of murders by the median income for each borough. Return the
numpy array.
  adata.london.gov.uk
```

Machine Learning with Apache Spark

Apache Spark includes a vast and expanding ecosystem to perform machine learning. PySpark's primary machine learning API, pyspark.ml, is DataFrame-based.

Here we give a start to finish example using Spark ML to tackle the classic Titanic classification problem.

```
# prepare data
# convert the 'sex' column to binary categorical variable
>>> from pyspark.ml.feature import StringIndexer, OneHotEncoder
>>> sex_binary = StringIndexer(inputCol='sex', outputCol='sex_binary')
# one-hot-encode pclass (Spark automatically drops a column)
>>> onehot = OneHotEncoder(inputCols=['pclass'],
                                    outputCols=['pclass_onehot'])
. . .
# create single features column
from pyspark.ml.feature import VectorAssembler
features = ['sex_binary', 'pclass_onehot', 'age', 'sibsp', 'parch', 'fare']
features_col = VectorAssembler(inputCols=features, outputCol='features')
# now we create a transformation pipeline to apply the operations above
# this is very similar to the pipeline ecosystem in sklearn
>>> from pyspark.ml import Pipeline
>>> pipeline = Pipeline(stages=[sex_binary, onehot, features_col])
>>> titanic = pipeline.fit(titanic).transform(titanic)
```

```
# drop unnecessary columns for cleaner display (note the new columns)
>>> titanic = titanic.drop('pclass', 'name', 'sex')
>>> titanic.show(2)
+-----+
|survived| age|sibsp|parch|fare|sex_binary|pclass_onehot| features|
+----+
      0|22.0| 1| 0|7.25| 0.0| (3,[],[])|(8,[4,5...|
      1|38.0| 1|
                    0|71.3|
                                1.0| (3,[1],...|[0.0,1....|
+-----+
# split into train/test sets (75/25)
>>> train, test = titanic.randomSplit([0.75, 0.25], seed=11)
# initialize logistic regression
>>> from pyspark.ml.classification import LogisticRegression
>>> lr = LogisticRegression(labelCol='survived', featuresCol='features')
# run a train-validation-split to fit best elastic net param
# ParamGridBuilder constructs a grid of parameters to search over.
>>> from pyspark.ml.tuning import ParamGridBuilder, TrainValidationSplit
>>> from pyspark.ml.evaluation import MulticlassClassificationEvaluator as MCE
>>> paramGrid = ParamGridBuilder()\
                 .addGrid(lr.elasticNetParam, [0, 0.5, 1]).build()
# TrainValidationSplit will try all combinations and determine best model using
# the evaluator (see also CrossValidator)
>>> tvs = TrainValidationSplit(estimator=lr,
                           estimatorParamMaps=paramGrid,
                           evaluator=MCE(labelCol='survived'),
. . .
                           trainRatio=0.75,
                           seed=11)
# we train the classifier by fitting our tvs object to the training data
>>> clf = tvs.fit(train)
# use the best fit model to evaluate the test data
>>> results = clf.bestModel.evaluate(test)
>>> results.predictions.select(['survived', 'prediction']).show(5)
+----+
|survived|prediction|
+----+
      01
              1.01
      01
             1.0|
      0|
              1.0
      01
              1.0|
       01
              0.01
# performance information is stored in various attributes of "results"
>>> results.accuracy
```

```
0.7527272727272727
>>> results.weightedRecall
0.7527272727272727
>>> results.weightedPrecision
0.751035147726004
# many classifiers do not have this object-oriented interface (yet)
# it isn't much more effort to generate the same statistics for a \hookleftarrow
   DecisionTreeClassifier, for example
>>> dt_clf = dt_tvs.fit(train) # same process, except for a different paramGrid
# generate predictions - this returns a new DataFrame
>>> preds = clf.bestModel.transform(test)
>>> preds.select('survived', 'probability', 'prediction').show(5)
+----+
|survived|probability|prediction|
+----+
       0| [1.0,0.0]|
                          0.01
       0| [1.0,0.0]|
                         0.0
       0| [1.0,0.0]|
                          0.01
       0| [0.0,1.0]|
                         1.0
+----+
# initialize evaluator object
>>> dt_eval = MCE(labelCol='survived')
>>> dt_eval.evaluate(preds, {dt_eval.metricName: 'accuracy'})
0.8433179723502304
```

Below is a broad overview of the pyspark.ml ecosystem. It should help give you a starting point when looking for a specific functionality.

PySpark ML Module	Module Purpose
pyspark.ml.feature	provides functions to transform data into feature vectors
pyspark.ml.tuning	grid search, cross validation, and train/validation split functions
pyspark.ml.evaluation	tools to compute prediction metrics (accuracy, f1, etc.)
pyspark.ml.classification	classification models (logistic regression, SVM, etc.)
pyspark.ml.clustering	clustering models (k-means, Gaussian mixture, etc.)
pyspark.ml.regression	regression models (linear regression, decision tree regressor, etc.)

Problem 5. Write a function with keyword argument filename='titanic.csv'. Load the file into a PySpark DataFrame, and use the pyspark.ml package to train a classifier that outperforms the logistic regression each of the three metrics from the example above (accuracy, weightedRecall, weightedPrecision).

Some of Spark's available classifiers are listed below. For complete documentation, visit https://spark.apache.org/docs/latest/api/python/pyspark.ml.html.

```
# from pyspark.ml.classification import LinearSVC
# DecisionTreeClassifier
# GBTClassifier
# MultilayerPerceptronClassifier
# NaiveBayes
# RandomForestClassifier
```

Use randomSplit([0.75, 0.25], seed=11) to split your data into train and test sets before fitting the model. Return the accuracy, weightedRecall, and weightedPrecision for your model, in the given order.

Hint: to calculate the accuracy of a classifer in PySpark, use accuracy = MCE(labelCol ='survived',metricName='accuracy').evaluate(predictions).

Additional Material

Further DataFrame Operations

There are a few other functions built directly on top of DataFrames to further analysis. Additionally, the pyspark.sql.functions module expands the available functions significantly.⁴

```
# some immediately accessible functions
# covariance between pclass and fare
>>> titanic.cov('pclass', 'fare')
-22.86289824115662
# summary of statistics for selected columns
>>> titanic.select("pclass", "age", "fare")\
... .summary().show()
pclass
                               agel
+----+
         887|
| count|
                               887|
  mean | 2.305524239007892 | 29.471443066501564 | 32.305420253026846 |
| stddev|0.8366620036697728|14.121908405492908| 49.78204096767521|
                         20.0|
                  1|
                                          7.925|
                  2|
   25% |
                             28.0|
                                         14.4542|
 50%|
                 31
                             38.0|
  75%|
                  3|
                                           31.275
                  3|
                             80.0|
| max|
                                         512.3292
+----+
# additional functions from the functions module
>>> from pyspark.sql import functions as sqlf
# finding the mean of a column without grouping requires sqlf.avg()
# alias(new_name) allows us to rename the column on the fly
>>> titanic.select(sqlf.avg("age").alias("Average Age")).show()
+----+
| Average Age|
+----+
|29.471443066516347|
+----+
# use .agg([dict]) on GroupedData to specify [multiple] aggregate
# functions, including those from pyspark.sql.functions
>>> titanic.groupBy('pclass')\
     .agg({'fare': 'var_samp', 'age': 'stddev'})\
       .show(3)
+----+
|pclass| var_samp(fare)| stddev(age)|
+----+
```

 $^{^4} https://spark.apache.org/docs/latest/api/python/pyspark.sql.html \\$

```
| 1| 6143.483042924841|14.183632587264817|
| 3|139.64879027298073|12.095083834183779|
| 2|180.02658999396826|13.756191206499766|
+----+

# perform multiple aggregate actions on the same column
>>> titanic.groupBy('pclass')\
... agg(sqlf.sum('fare'), sqlf.stddev('fare'))\
... show()
+----+
|pclass| sum(fare)| stddev_samp(fare)|
+----+
| 1|18177.412506103516| 78.38037409278448|
| 3| 6675.653553009033| 11.81730892686574|
| 2|3801.8417053222656|13.417398778972332|
+-----+
```

pyspark.sql.functions	Operation		
ceil(col)	computes the ceiling of each element in col		
floor(col)	computes the floor of each element in col		
min(col), max(col)	returns the minimum/maximum value of col		
mean(col)	returns the average of the values of col		
stddev(col)	returns the unbiased sample standard deviation of col		
<pre>var_samp(col)</pre>	returns the unbiased variance of the values in col		
rand(seed=None)	generates a random column with i.i.d. samples from $[0,1]$		
randn(seed=None)	generates a random column with i.i.d. samples from the		
	standard normal distribution		
exp(col)	computes the exponential of col		
log(arg1, arg2=None)	returns arg1-based logarithm of arg2; if there is only one		
	argument, then it returns the natural logarithm		
cos(col), sin(col), etc.	computes the given trigonometric or inverse trigonometric		
	(asin(col), etc.) function of col		

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Part II Appendices

A

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
- $\bullet \ \, GitHub \ git \ cheat \ sheet: \ \verb|services.github.com/.../github-git-cheat-sheet.pdf| \\$
- 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
$ 1s *.md
                      # ls means 'list files'.
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>".

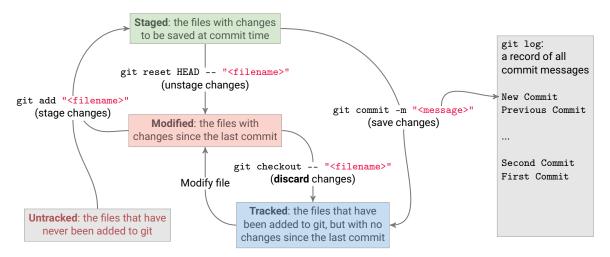


Figure A.1: Git commands to stage, unstage, save, or discard changes. Commit messages are recorded in the log.

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.

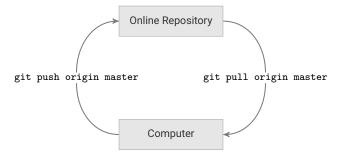


Figure A.2: Exchanging git commits between the repository and a local clone.

Command	Explanation
git status	Display the staging area and untracked changes.
git pull origin master	Pull changes from the online repository.
git push origin master	Push changes to the online repository.
<pre>git add <filename(s)></filename(s)></pre>	Add a file or files to the staging area.
git add -u	Add all modified, tracked files to the staging area.
git commit -m " <message>"</message>	Save the changes in the staging area with a given message.
git checkout <filename></filename>	Revert changes to an unstaged file since the last commit.
git reset HEAD <filename></filename>	Remove a file from the staging area.
git diff <filename></filename>	See the changes to an unstaged file since the last commit.
git diffcached <filename></filename>	See the changes to a staged file since the last commit.
git configlocal <option></option>	Record your credentials (user.name, user.email, etc.).

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.

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 IATEX, 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.

$$A = \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}$$

$$B = \begin{bmatrix} * & * & * \\ * & * & * \end{bmatrix}$$

$$np.hstack((A,B,A)) = \begin{bmatrix} \times & \times & \times & * & * & \times & \times \\ \times & \times & * & * & * & \times & \times \\ \times & \times & \times & * & * & * & \times & \times \end{bmatrix}$$

$$np.vstack((A,B,A)) = \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ * & * & * \\ * & * & * \\ * & * & * \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}$$

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().

$$\text{np.vstack((x,y,x))} = \begin{bmatrix} \times & \times & \times & \times \\ * & * & * & * \\ \times & \times & \times & \times \end{bmatrix} \quad \text{np.column_stack((x,y,x))} = \begin{bmatrix} \times & * & \times \\ \times & * & \times \\ \times & * & \times \end{bmatrix}$$

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.

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \\ 1 & 2 & 3 \end{bmatrix} \qquad \mathbf{x} = \begin{bmatrix} 10 & 20 & 30 \end{bmatrix}$$

$$\mathbf{A} + \mathbf{x} = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \\ 1 & 2 & 3 \end{bmatrix} \\ + \\ \begin{bmatrix} 10 & 20 & 30 \end{bmatrix}$$
 =
$$\begin{bmatrix} 11 & 22 & 33 \\ 11 & 22 & 33 \\ 11 & 22 & 33 \end{bmatrix}$$

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.

$$A = \left[\begin{array}{cccc} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{array} \right]$$

A.sum(axis=0) =
$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{bmatrix} = \begin{bmatrix} 4 & 8 & 12 & 16 \end{bmatrix}$$

A.sum(axis=1) =
$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ \hline 1 & 2 & 3 & 4 \\ \hline 1 & 2 & 3 & 4 \end{bmatrix} = \begin{bmatrix} 10 & 10 & 10 & 10 \end{bmatrix}$$

D

Introduction to Scikit-Learn

Lab Objective: Scikit-learn is the one of the fundamental tools in Python for machine learning. In this appendix we highlight and give examples of some popular scikit-learn tools for classification and regression, training and testing, data normalization, and constructing complex models.

Note

This guide corresponds to scikit-learn version 0.20, which has a few significant differences from previous releases. See http://scikit-learn.org/stable/whats_new.html for current release notes. Install scikit-learn (the sklearn module) with conda install scikit-learn.

Base Classes and API

Many machine learning problems center on constructing a function $f: X \to Y$, called a *model* or *estimator*, that accurately represents properties of given data. The domain X is usually \mathbb{R}^D , and the range Y is typically either \mathbb{R} (regression) or a subset of \mathbb{Z} (classification). The model is trained on N samples $(\mathbf{x}_i)_{i=1}^N \subset X$ that usually (but not always) have N accompanying labels $(y_i)_{i=1}^N \subset Y$.

Scikit-learn [PVG⁺11, BLB⁺13] takes a highly object-oriented approach to machine learning models. Every major scikit-learn class inherits from sklearn.base.BaseEstimator and conforms to the following conventions:

- 1. The constructor <code>__init__()</code> receives hyperparameters for the classifier, which are parameters for the model f that are **not dependent on data**. Each hyperparameter must have a default value (i.e., every argument of <code>__init__()</code> is a keyword argument), and each argument must be saved as an instance variable of the **same name** as the parameter.
- 2. The fit() method constructs the model f. It receives an $N \times D$ matrix X and, optionally, a vector \mathbf{y} with N entries. Each row \mathbf{x}_i of X is one sample with corresponding label y_i . By convention, fit() always returns self.

Along with the BaseEstimator class, there are several other "mix in" base classes in sklearn.base that define specific kinds of models. The three listed below are the most common.¹

See http://scikit-learn.org/stable/modules/classes.html#base-classes for the complete list.

- ClassifierMixin: for *classifiers*, estimators that take on discrete values.
- RegressorMixin: for regressors, estimators that take on continuous values.
- TransformerMixin: for preprocessing data before estimation.

Classifiers and Regressors

The ClassifierMixin and RegressorMixin both require a predict() method that acts as the actual model f. That is, predict() receives an $N \times D$ matrix X and returns N predicted labels $(y_i)_{i=1}^N$, where y_i is the label corresponding to the ith row of X. Both of these base class have a predefined score() method that uses predict() to test the accuracy of the model. It accepts $N \times D$ test data and a vector of N corresponding labels, then reports either the classification accuracy (for classifiers) or the R^2 value of the regression (for regressors).

For example, a KNeighborsClassifier from sklearn.neighbors inherits from BaseEstimator and ClassifierMixin. This classifier uses a simple strategy: to classify a new piece of data \mathbf{z} , find the k training samples that are "nearest" to \mathbf{z} , then take the most common label corresponding to those nearest neighbors to be the label for \mathbf{z} . Its constructor accepts hyperparameters such as n_n eighbors, for determining the number of neighbors k to search for, algorithm, which speficies the strategy to find the neighbors, and n_j obs, the number of parallel jobs to run during the neighbors search. Again, these hyperparameters are independent of any data, which is why they are set in the constructor (before fitting the model). Calling fit() organizes the data X into a data structure for efficient nearest neighbor searches (determined by algorithm). Calling predict() executes the search, determines the most common label of the neighbors, and returns that label.

```
>>> from sklearn.datasets import load_breast_cancer
>>> from sklearn.neighbors import KNeighborsClassifier
>>> from sklearn.model_selection import train_test_split
# Load the breast cancer dataset and split it into training and testing groups.
>>> cancer = load_breast_cancer()
>>> X_train, X_test, y_train, y_test = train_test_split(cancer.data,
                                                         cancer.target)
>>> print(X_train.shape, y_train.shape)
                        # There are 426 training points, each with 30 features.
(426, 30) (426,)
# Train a KNeighborsClassifier object on the training data.
# fit() returns the object, so we can instantiate and train in a single line.
>>> knn = KNeighborsClassifier(n_neighbors=2).fit(X_train, y_train)
# The hyperparameter 'n_neighbors' is saved as an attribute of the same name.
>>> knn.n_neighbors
2
# Test the classifier on the testing data.
>>> knn.predict(X_test[:6])
array([0, 1, 0, 1, 1, 0])
                                # Predicted labels for the first 6 test points.
>>> knn.score(X_test, y_test)
0.8951048951048951
                                # predict() chooses 89.51% of the labels right.
```

The KNeighborsClassifier object could easily be replaced with a different classifier, such as a GaussianNB object from sklearn.naive_bayes. Since GaussianNB also inherits from BaseEstimator and ClassifierMixin, it has fit(), predict(), and score() methods that take in the same kinds of inputs as the corresponding methods for the KNeighborsClassifier. The only difference, from an external perspective, is the hyperparameters that the constructor accepts.

```
>>> from sklearn.naive_bayes import GaussianNB
>>> gnb = GaussianNB().fit(X_train, y_train)
>>> gnb.predict(X_test[:6])
array([1, 1, 0, 1, 1, 0])
>>> gnb.score(X_test, y_test)
0.9440559440559441
```

Roughly speaking, the GaussianNB classifier assumes all features in the data are independent and normally distributed, then uses Bayes' rule to compute the likelihood of a new point belonging to a label for each of the possible labels. To do this, the fit() method computes the mean and variance of each feature, grouped by label. These quantities are saved as the attributes theta_ (the means) and sigma_ (the variances), then used in predict(). Parameters like these that are dependent on data are only defined in fit(), not the constructor, and they are always named with a trailing underscore. These "non-hyper" parameters are often simply called model parameters.

The fit() method should do all of the "heavy lifting" by calculating the model parameters. The predict() method should then use these parameters to choose a label for test data.

	Hyperparameters	Model Parameters
Data dependence	No	Yes
Initialization location	init()	fit()
Naming convention	Same as argument name	Ends with an underscore
Examples	n_neighbors, algorithm, n_jobs	classes_, theta_, sigma_

Table D.1: Naming and initialization conventions for scikit-learn model parameters.

Building Custom Estimators

The consistent conventions in the various scikit-learn classes makes it easy to use a wide variety of estimators with near-identical syntax. These conventions also makes it possible to write custom estimators that behave like native scikit-learn objects. This usually only involves writing fit() and predict() methods and inheriting from the appropriate base classes. As a simple (though poorly performing) example, consider an estimator that either always predicts the same user-provided label, or that always predicts the most common label in the training data. Which strategy to use is independent of the data, so we encode that behavior with hyperparameters; the most common label must be calculated from the data, so that is a model parameter.

```
>>> import numpy as np
>>> from collections import Counter
>>> from sklearn.base import BaseEstimator, ClassifierMixin
>>> class PopularClassifier(BaseEstimator, ClassifierMixin):
        """Classifier that always guesses the most common training label."""
        def __init__(self, strategy="most_frequent", constant=None):
            self.strategy = strategy # Store the hyperparameters, using
            self.constant = constant # the same names as the arguments.
        def fit(self, X, y):
            """Find and store the most common label."""
            self.popular_label_ = Counter(y).most_common(1)[0][0]
            return self
                                       # fit() always returns 'self'.
        def predict(self, X):
            """Always guess the most popular training label."""
            M = X.shape[0]
           if self.strategy == "most_frequent":
                return np.full(M, self.popular_label_)
           elif self.strategy == "constant":
               return np.full(M, self.constant)
           else:
                raise ValueError("invalid value for 'strategy' param")
. . .
# Train a PopularClassifier on the breast cancer training data.
>>> pc = PopularClassifier().fit(X_train, y_train)
>>> pc.popular_label_
# Score the model on the testing data.
>>> pc.score(X_test, y_test)
0.6573426573426573
                                   # 65.73% of the testing data is labeled 1.
# Change the strategy to always guess 0 by changing the hyperparameters.
>>> pc.strategy = "constant"
>>> pc.constant = 0
>>> pc.score(X_test, y_test)
0.34265734265734266
                                     # 34.27% of the testing data is labeled 0.
```

This is a terrible classifier, but it is actually implemented as sklearn.dummy.DummyClassifier because any legitimate machine learning algorithm should be able to beat it, so it is useful as a baseline comparison.

Note that score() was inherited from ClassifierMixin (it isn't defined explicitly), so it returns a classification rate. In the next example, a slight simplification of the equally unintelligent sklearn.dummy.DummyRegressor, the score() method is inherited from RegressorMixin, so it returns an R^2 value.

```
>>> from sklearn.base import RegressorMixin
>>> class ConstRegressor(BaseEstimator, RegressorMixin):
        """Regressor that always predicts a mean or median of training data."""
        def __init__(self, strategy="mean", constant=None):
            self.strategy = strategy # Store the hyperparameters, using
            self.constant = constant
                                      # the same names as the arguments.
        def fit(self, X, y):
            self.mean_, self.median_ = np.mean(y), np.median(y)
           return self
                                        # fit() always returns 'self'.
        def predict(self, X):
            """Always predict the middle of the training data."""
            M = X.shape[0]
           if self.strategy == "mean":
                return np.full(M, self.mean_)
            elif self.strategy == "median":
                return np.full(M, self.median_)
            elif self.strategy == "constant":
                return np.full(M, self.constant)
            else:
                raise ValueError("invalid value for 'strategy' param")
. . .
# Train on the breast cancer data (treating it as a regression problem).
>>> cr = ConstRegressor(strategy="mean").fit(X_train, y_train)
>>> print("mean:", cr.mean_, " median:", cr.median_)
mean: 0.6173708920187794 median: 1.0
# Get the R^2 score of the regression on the testing data.
>>> cr.score(X_train, y_train)
                            # Unsurprisingly, no correlation.
```

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Both PopularClassifier and ConstRegressor wait until predict() to validate the strategy hyperparameter. The check could easily be done in the constructor, but that goes against scikit-learn conventions: in order to cooperate with automated validation tools, the constructor of any class inheriting from BaseEstimator must store the arguments of __init__() as attributes—with the same names as the arguments—and do nothing else.

Note

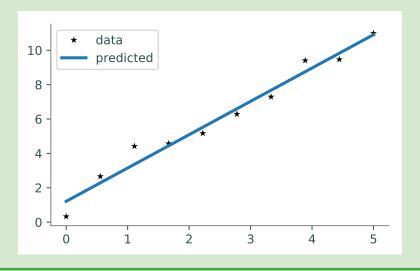
The first input to $\mathtt{fit}()$ and $\mathtt{predict}()$ are always two-dimensional $N \times D$ NumPy arrays, where N is the number of observations and D is the number of features. To fit or predict on one-dimensional data (D=1), reshape the input array into a "column vector" before feeding it into the estimator. One-dimensional problems are somewhat rare in machine learning, but the following example shows how to do a simple one-dimensional linear regression.

```
>>> from matplotlib import pyplot as plt
>>> from sklearn.linear_model import LinearRegression

# Generate data for a 1-dimensional regression problem.
>>> X = np.linspace(0, 5, 10)
>>> Y = 2*X + 1 + np.random.normal(size=10)

# Reshape the training data into a column vector.
>>> lr = LinearRegression().fit(X.reshape((-1,1)), Y)

# Define another set of points to do predictions on.
>>> x = np.linspace(0, 5, 20)
>>> y = lr.predict(x.reshape((-1,1))) # Reshape before predicting.
>>> plt.plot(X, Y, 'k*', label="data")
>>> plt.plot(x, y, label="predicted")
>>> plt.legend(loc="upper left")
>>> plt.show()
```



Transformers

A scikit-learn *transformer* processes data to make it better suited for estimation. This may involve shifting and scaling data, dropping columns, replacing missing values, and so on.

Classes that inherit from the TransformerMixin base class have a fit() method that accepts an $N \times D$ matrix X (like an estimator) and an optional set of labels. The labels are not needed—in fact the fit() method should do nothing with them—but the parameter for the labels remains as a keyword argument to be consistent with the fit(X,y) syntax of estimators. Instead of a predict() method, the transform() method accepts data, modifies it (usually via a copy), and returns the result. The new data may or may not have the same number of columns as the original data.

One common transformation is shifting and scaling the features (columns) so that they each have a mean of 0 and a standard deviation of 1. The following example implements a basic version of this transformer.

```
>>> from sklearn.base import TransformerMixin
>>> class NormalizingTransformer(BaseEstimator, TransformerMixin):
        def fit(self, X, y=None):
            """Calculate the mean and standard deviation of each column."""
            self.mu_ = np.mean(X, axis=0)
            self.sig_ = np.std(X, axis=0)
            return self
        def transform(self, X):
            """Center each column at zero and normalize it."""
            return (X - self.mu_) / self.sig_
# Fit the transformer and transform the cancer data (both train and test).
>>> nt = NormalizingTransformer()
>>> Z_train = nt.fit_transform(X_train) # Or nt.fit(X_train).transform(X_train)
>>> Z_test = nt.transform(X_test)
                                   # Transform test data (without fitting)
>>> np.mean(Z_train, axis=0)[:3]
                                       # The columns of Z_train have mean 0...
array([-8.08951237e-16, -1.72006384e-17, 1.78678147e-15])
>>> np.std(Z_train, axis=0)[:3]
                                   # ...and have unit variance.
array([1., 1., 1.])
>>> np.mean(Z_test, axis=0)[:3]
                                      # The columns of Z_test each have mean
array([-0.02355067, 0.11665332, -0.03996177])
                                                                # close to 0...
>>> np.std(Z_test, axis=0)[:3]
                                       # ...and have close to unit deviation.
array([0.9263711 , 1.18461151, 0.91548103])
# Check to see if the classification improved.
>>> knn.fit(X_train, y_train).score(X_test, y_test)
                                                                # Old score.
0.8951048951048951
>>> knn.fit(Z_train, y_train).score(Z_test, y_test)
                                                                # New score.
0.958041958041958
```

This particular transformer is implemented as sklearn.preprocessing.StandardScaler. A close cousin is sklearn.preprocessing.RobustScaler, which ignores outliers when choosing the scaling and shifting factors.

Like estimators, transformers may have both hyperparameters (provided to the constructor) and model parameters (determined by fit()). Thus a transformer looks and acts like an estimator, with the exception of the predict() and transform() methods.

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The transform() method should only rely on model parameters derived from the training data in fit(), not on the data that is worked on in transform(). For example, if the NormalizingTransformer is fit with the input \widehat{X} , then transform() should shift and scale any input X by the mean and standard deviation of \widehat{X} , not by the mean and standard deviation of X. Otherwise, the transformation is different for each input X.

Scikit-learn Module	Classifier Name	Notable Hyperparameters
discriminant_analysis	LinearDiscriminantAnalysis	solver, shrinkage, n_components
${ t discriminant_analysis}$	QuadraticDiscriminantAnalysis	reg_param
ensemble	AdaBoostClassifier	n_estimators, learning_rate
ensemble	RandomForestClassifier	n_estimators, max_depth
linear_model	LogisticRegression	penalty, C
linear_model	SGDClassifier	loss, penalty, alpha
naive_bayes	GaussianNB	priors
naive_bayes	MultinomialNB	alpha
neighbors	KNeighborsClassifier	n_neighbors, weights
neighbors	RadiusNeighborsClassifier	radius, weights
neural_network	MLPClassifier	hidden_layer_size, activation
svm	SVC	C, kernel
tree	DecisionTreeClassifier	max_depth
Scikit-learn Module	Regressor Name	Notable Hyperparameters
ensemble	AdaBoostRegressor	n_estimators, learning_rate
ensemble	ExtraTreesRegressor	n_estimators, max_depth
ensemble	GradientBoostingRegressor	n_estimators, max_depth
ensemble	RandomForestRegressor	n_estimators, max_depth
isotonic	IsotonicRegression	y_min, y_max
kernel_ridge	KernelRidge	alpha, kernel
linear_model	LinearRegression	fit_intercept
neural_network	MLPRegressor	hidden_layer_size, activation
svm	SVR	C, kernel
tree	DecisionTreeRegressor	max_depth
Module	Transformer Name	Notable Hyperparameters
decomposition	PCA	n_components
preprocessing	Imputer	missing_values, strategy
preprocessing	MinMaxScaler	feature_range
preprocessing	OneHotEncoder	categorical_features
preprocessing	QuantileTransformer	n_quantiles, output_distribution
preprocessing	RobustScaler	with_centering, with_scaling
preprocessing	StandardScaler	with_mean, with_std

Table D.2: Common scikit-learn classifiers, regressors, and transformers. For full documentation on these classes, see http://scikit-learn.org/stable/modules/classes.html.

Validation Tools

Knowing how to determine whether or not an estimator performs well is an essential part of machine learning. This often turns out to be a surprisingly sophisticated issue that largely depends on the type of problem being solved and the kind of data that is available for training. Scikit-learn has validation tools for many situations; for brevity, we restrict our attention to the simple (but important) case of binary classification, where the range of the desired model is $Y = \{0, 1\}$.

Evaluation Metrics

The score() method of a scikit-learn estimator representing the model $f: X \to \{0, 1\}$ returns the accuracy of the model, which is the percent of labels that are predicted correctly. However, accuracy isn't always the best measure of success. Consider the confusion matrix for a classifier, the matrix where the (i, j)th entry is the number of observations with actual label i but that are classified as label j. In binary classification, calling the class with label 0 the negatives and the class with label 1 the positives, this becomes the following.

With this terminology, we define the following metrics.

- Accuracy: $\frac{TN+TP}{TN+FN+FP+TP}$, the percent of labels predicted correctly.
- Precision: $\frac{TP}{TP+FP}$, the percent of predicted positives that are actually correct.
- Recall: $\frac{TP}{TP+FN}$, the percent of actual positives that are predicted correctly.

Precision is useful in situations where false positives are dangerous or costly, while recall is important when avoiding false negatives takes priority. For example, an email spam filter should avoid filtering out an email that isn't actually spam, so precision is a valuable metric for the filter. On the other hand, recall is more important in disease detection: it is better to test positive and not have the disease than to test negative when the disease is actually present. Focusing on a single metric often leads to skewed results (for example, always predicting the same label), so the following metric is also common.

•
$$F_{\beta}$$
 Score: $(1 + \beta^2) \frac{\text{precision} \cdot \text{recall}}{(\beta^2 \cdot \text{precision}) + \text{recall}} = \frac{(1 + \beta^2)TP}{(1 + \beta^2)TP + FP + \beta^2 FN}$.

Choosing $\beta < 1$ weighs precision more than recall, while $\beta > 1$ prioritizes recall over precision. The choice of $\beta = 1$ yields the common F_1 score, which weighs precision and recall equally. This is an important alternative to accuracy when, for example, the training set is heavily unbalanced with respect to the class labels.

Scikit-learn implements these metrics in sklearn.metrics, as well as functions for evaluating regression, non-binary classification, and clustering models. The general syntax for such functions is some_score(actual_labels, predicted_labels). For the complete list and further discussion, see http://scikit-learn.org/stable/modules/model_evaluation.html.

```
>>> from sklearn.metrics import (confusion_matrix, classification_report,
                                 accuracy_score, precision_score,
                                 recall_score, f1_score)
. . .
# Fit the esimator to training data and predict the test labels.
>>> knn.fit(X_train, y_train)
>>> knn_predicted = knn.predict(X_test)
# Compute the confusion matrix by comparing actual labels to predicted labels.
>>> CM = confusion_matrix(y_test, knn_predicted)
>>> CM
array([[44, 5],
       [10, 84]])
# Get accuracy (the "usual" score), precision, recall, and f1 scores.
>>> accuracy_score(y_test, knn_predicted) # (CM[0,0] + CM[1,1]) / CM.sum()
0.8951048951048951
>>> precision_score(y_test, knn_predicted) # CM[1,1] / CM[:,1].sum()
0.9438202247191011
>>> recall_score(y_test, knn_predicted) # CM[1,1] / CM[1,:].sum()
0.8936170212765957
>>> f1_score(y_test, knn_predicted)
0.9180327868852459
# Get all of these scores at once with classification_report().
>>> print(classification_report(y_test, knn_predicted))
            precision
                       recall f1-score
                                            support
           0
                   0.81
                             0.90
                                       0.85
                                                   49
           1
                   0.94
                             0.89
                                       0.92
                                                   94
                   0.90
                             0.90
                                       0.90
                                                  143
  micro avg
                   0.88
                             0.90
                                       0.89
                                                  143
   macro avg
                   0.90
                             0.90
                                       0.90
                                                  143
weighted avg
```

Cross Validation

The sklearn.model_selection module has utilities to streamline and improve model evaluation.

- train_test_split() randomly splits data into training and testing sets (we already used this).
- cross_val_score() randomly splits the data and trains and scores the model a set number of times. Each trial uses different training data and results in a different model. The function returns the score of each trial.
- cross_validate() does the same thing as cross_val_score(), but it also reports the time it took to fit, the time it took to score, and the scores for the test set as well as the training set.

Doing multiple evaluations with different testing and training sets is extremely important. If the scores on a cross validation test vary wildly, the model is likely overfitting to the training data.

```
>>> from sklearn.model_selection import cross_val_score, cross_validate

# Make (but do not train) a classifier to test.
>>> knn = KNeighborsClassifier(n_neighbors=3)

# Test the classifier on the training data 4 times.
>>> cross_val_score(knn, X_train, y_train, cv=4)
array([0.88811189, 0.92957746, 0.96478873, 0.92253521])

# Get more details on the train/test procedure.
>>> cross_validate(knn, X_train, y_train, cv=4,
... return_train_score=False)
{'fit_time': array([0.00064683, 0.00042295, 0.00040913, 0.00040436]),
    'score_time': array([0.00115728, 0.00109601, 0.00105286, 0.00102782]),
    'test_score': array([0.88811189, 0.92957746, 0.96478873, 0.92253521])}

# Do the scoring with an alternative metric.
>>> cross_val_score(knn, X_train, y_train, scoring="f1", cv=4)
array([0.93048128, 0.95652174, 0.96629213, 0.93103448])
```

Note

Any estimator, even a user-defined class, can be evaluated with the scikit-learn tools presented in this section as long as that class conforms to the scikit-learn API discussed previously (i.e., inheriting from the correct base classes, having fit() and predict() methods, managing hyperparameters and parameters correctly, and so on). Any time you define a custom estimator, following the scikit-learn API gives you instant access to tools such as cross_val_score().

Grid Search

Recall that the *hyperparameters* of a machine learning model are user-provided parameters that do not depend on the training data. Finding the optimal hyperparameters for a given model is a challenging and active area of research.² However, brute-force searching over a small hyperparameter space is simple in scikit-learn: a sklearn.model_selection.GridSearchCV object is initialized with an estimator, a dictionary of hyperparameters, and cross validation parameters (such as cv and scoring). When its fit() method is called, it does a cross validation test on the given estimator with every possible hyperparameter combination.

For example, a k-neighbors classifier has a few important hyperparameters that can have a significant impact on the speed and accuracy of the model: n_neighbors, the number of nearest neighbors allowed to vote; and weights, which specifies a strategy for weighting the distances between points. The following code tests various combinations of these hyperparameters.

²Intelligent hyperparameter selection is sometimes called *metalearning*. See, for example, [SGCP⁺18].

```
>>> from sklearn.model_selection import GridSearchCV

>>> knn = KNeighborsClassifier()
# Specify the hyperparameters to vary and the possible values they should take.
>>> param_grid = {"n_neighbors": [2, 3, 4, 5, 6],
... "weights": ["uniform", "distance"]}
>>> knn_gs = GridSearchCV(knn, param_grid, cv=4, scoring="f1", verbose=1)
>>> knn_gs.fit(X_train, y_train)
Fitting 4 folds for each of 5 candidates, totalling 20 fits
[Parallel(n_jobs=1)]: Using backend SequentialBackend with 1 concurrent worker.
[Parallel(n_jobs=1)]: Done 20 out of 20 | elapsed: 0.1s finished

# After fitting, the gridsearch object has data about the results.
>>> print(knn_gs.best_params_, knn_gs.best_score_)
{'n_neighbors': 5, 'weights': 'uniform'} 0.9532526583188765
```

The cost of a grid search rapidly increases as the hyperparameter space grows. However, the outcomes of each trial are completely independent of each other, so the problem of training each classifier is *embarassingly parallel*. To parallelize the grid search over n cores, set the n_{jobs} parameter to n, or set it to -1 to divide the labor between as many cores as are available.

In some circumstances, the parameter grid can be also organized in a way that eliminates redundancy. Consider an SVC classifier from sklearn.svm, an estimator that works by lifting the data into a high-dimensional space, then constructing a hyperplane to separate the classes. The SVC has a hyperparameter, kernel, that determines how the lifting into higher dimensions is done, and for each choice of kernel there are additional corresponding hyperparameters. To search the total hyperparameter space without redundancies, enter the parameter grid as a list of dictionaries, each of which defines a different section of the hyperparameter space. In the following code, doing so reduces the number of trials from $3 \times 2 \times 3 \times 4 = 72$ to only $1 + (1 \times 1 \times 3) + (1 \times 4) = 11$.

```
>>> from sklearn.svm import SVC
>>> svc = SVC(C=0.01, max_iter=100)
>>> param_grid = [
        {"kernel": ["linear"]},
. . .
        {"kernel": ["poly"], "degree": [2,3], "coef0": [0,1,5]},
        {"kernel": ["rbf"], "gamma": [.01, .1, 1, 100]}]
>>> svc_gs = GridSearchCV(svc, param_grid,
                          cv=4, scoring="f1",
                          verbose=1, n_jobs=-1).fit(X_train, y_train)
Fitting 4 folds for each of 11 candidates, totalling 44 fits
[Parallel(n_jobs=-1)]: Using backend LokyBackend with 8 concurrent workers.
[Parallel(n_jobs=-1)]: Done 44 out of 44 | elapsed:
                                                         2.4s finished
>>> print(svc_gs.best_params_, svc_gs.best_score_)
{'gamma': 0.01, 'kernel': 'rbf'} 0.8909310239174055
```

See https://scikit-learn.org/stable/modules/grid_search.html for more details about GridSearchCV and its relatives.

Pipelines

Most machine learning problems require at least a little data preprocessing before estimation in order to get good results. A scikit-learn pipeline (sklearn.pipeline.Pipeline) chains together one or more transformers and one estimator into a single object, complete with fit() and predict() methods. For example, it is often a good idea to shift and scale data before feeding it into a classifier. The StandardScaler transformer can be combined with a classifier with a pipeline. Calling fit() on the resulting object calls fit_transform() on each successive transformer, then fit() on the estimator at the end. Likewise, calling predict() on the Pipeline object calls transform() on each transformer, then predict() on the estimator.

Since Pipeline objects behaves like estimators (following the fit() and predict() conventions), they can be used with tools like cross_val_score() and GridSearchCV. To specify which hyperparameters belong to which steps of the pipeline, precede each hyperparameter name with < stepname>__. For example, knn__n_neighbors corresponds to the n_neighbors hyperparameter of the part of the pipeline that is labeled knn.

```
# Specify the possible hyperparameters for each step.
>>> pipe_param_grid = {"scaler__with_mean": [True, False],
                       "scaler__with_std": [True, False],
                       "knn__n_neighbors": [2,3,4,5,6],
. . .
                       "knn__weights": ["uniform", "distance"]}
# Pass the Pipeline object to the GridSearchCV and fit it to the data.
>>> pipe = Pipeline([("scaler", StandardScaler()),
                     ("knn", KNeighborsClassifier())])
>>> pipe_gs = GridSearchCV(pipe, pipe_param_grid,
                           cv=4, n_jobs=-1, verbose=1).fit(X_train, y_train)
Fitting 4 folds for each of 40 candidates, totalling 160 fits
[Parallel(n_jobs=-1)]: Using backend LokyBackend with 8 concurrent workers.
[Parallel(n_jobs=-1)]: Done 160 out of 160 | elapsed:
                                                         0.3s finished
>>> print(pipe_gs.best_params_, pipe_gs.best_score_, sep='\n')
{'knn_n_neighbors': 6, 'knn_weights': 'distance',
 'scaler__with_mean': True, 'scaler__with_std': True}
0.971830985915493
```

Pipelines can also be used to compare different transformations or estimators. For example, a pipeline could end in either a KNeighborsClassier() or an SVC(), even though they have different hyperparameters. Like before, use a list of dictionaries to specify the hyperparameter space.

```
>>> pipe = Pipeline([("scaler", StandardScaler()),
                     ("classifier", KNeighborsClassifier())])
>>> pipe_param_grid = [
        {"classifier": [KNeighborsClassifier()],
                                                   # Try a KNN classifier...
        "classifier__n_neighbors": [2,3,4,5],
        "classifier__weights": ["uniform", "distance"]},
        {"classifier": [SVC(kernel="rbf")],
                                                   # ...and an SVM classifier.
        "classifier__C": [.001, .01, .1, 1, 10, 100],
. . .
         "classifier__gamma": [.001, .01, .1, 1, 10, 100]}]
>>> pipe_gs = GridSearchCV(pipe, pipe_param_grid,
                           cv=5, scoring="f1",
. . .
                           verbose = 1, n_jobs=-1).fit(X_train, y_train)
. . .
Fitting 5 folds for each of 44 candidates, totalling 220 fits
[Parallel(n_jobs=-1)]: Using backend LokyBackend with 8 concurrent workers.
[Parallel(n_jobs=-1)]: Done 220 out of 220 | elapsed: 0.6s finished
>>> params = pipe_gs.best_params_
>>> print("Best classifier:", params["classifier"])
Best classifier: SVC(C=10, cache_size=200, class_weight=None, coef0=0.0,
 decision_function_shape='ovr', degree=3, gamma=0.01, kernel='rbf',
 max_iter=-1, probability=False, random_state=None, shrinking=True,
 tol=0.001, verbose=False)
# Check the best classifier against the test data.
>>> confusion_matrix(y_test, pipe_gs.predict(X_test))
array([[48, 1],
                                        # Near perfect!
       [ 1, 93]])
```

Additional Material

Exercises

Problem 1. Writing custom scikit-learn transformers is a convenient way to organize the data cleaning process. Consider the data in titanic.csv, which contains information about passengers on the maiden voyage of the *RMS Titanic* in 1912. Write a custom transformer class to clean this data, implementing the transform() method as follows:

- 1. Extract a copy of data frame with just the "Pclass", "Sex", and "Age" columns.
- 2. Replace NaN values in the "Age" column (of the copied data frame) with the mean age. The mean age of the training data should be calculated in fit() and used in transform() (compare this step to using sklearn.preprocessing.Imputer).
- 3. Convert the "Pclass" column datatype to pandas categoricals (pd.CategoricalIndex).
- 4. Use pd.get_dummies() to convert the categorical columns to multiple binary columns (compare this step to using sklearn.preprocessing.OneHotEncoder).
- 5. Cast the result as a NumPy array and return it.

Ensure that your transformer matches scikit-learn conventions (it inherits from the correct base classes, fit() returns self, etc.).

Problem 2. Read the data from titanic.csv with pd.read_csv(). The "Survived" column indicates which passengers survived, so the entries of the column are the labels that we would like to predict. Drop any rows in the raw data that have NaN values in the "Survived" column, then separate the column from the rest of the data. Split the data and labels into training and testing sets. Use the training data to fit a transformer from Problem 1, then use that transformer to clean the training set, then the testing set. Finally, train a LogisticRegressionClassifier and a RandomForestClassifier on the cleaned training data, and score them using the cleaned test set.

Problem 3. Use classification_report() to score your classifiers from Problem 2. Next, do a grid search for each classifier (using only the cleaned training data), varying at least two hyperparameters for each kind of model. Use classification_report() to score the resulting best estimators with the cleaned test data. Try changing the hyperparameter spaces or scoring metrics so that each grid search yields a better estimator.

Problem 4. Make a pipeline with at least two transformers to further process the Titanic dataset. Do a gridsearch on the pipeline and report the hyperparameters of the best estimator.

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