

A Python programming primer for biologists

**(Named after *Monty Python's Flying Circus* &
designed to be fun to use)**

**Systems Biology/Bioinformatics
Edward Marcotte, Univ of Texas at Austin**

In bioinformatics, you often want to do completely new analyses. Having the ability to program a computer opens all sorts of research opportunities. Plus, it's fun!

Most bioinformatics researchers use a scripting language, such as Python, Perl, or R, rather than a compiled language like C++

These languages are not the fastest, not the slowest, nor best, nor worst languages, but they're easy to learn and write, and for many reasons, are well-suited to bioinformatics.

We'll spend the next 2 lectures introducing Python to give you a sense for the language and help introduce the basics of algorithms.

Python documentation: <http://www.python.org/doc/>
& tips: <http://www.tutorialspoint.com/python>

Good introductory Python books:

- *Learning Python*, Mark Lutz & David Ascher, O'Reilly Media
- *Bioinformatics Programming Using Python: Practical Programming for Biological Data*, Mitchell Model, O'Reilly

Good intro video (from a 2 day intro class at Google):

- <https://www.youtube.com/playlist?list=PLC8825D0450647509>

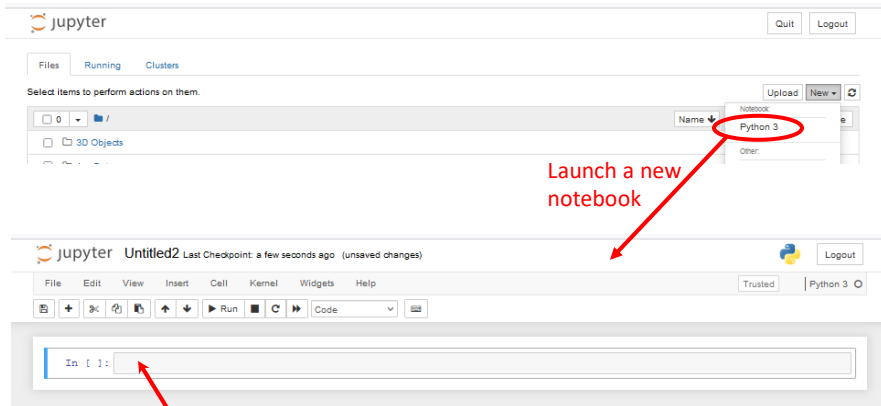
Practical Python, a self-paced online intro course:

- <https://dabeaz-course.github.io/practical-python/>

An online Python tutor with a nice interactive code viewer:

- <http://www.pythontutor.com/>

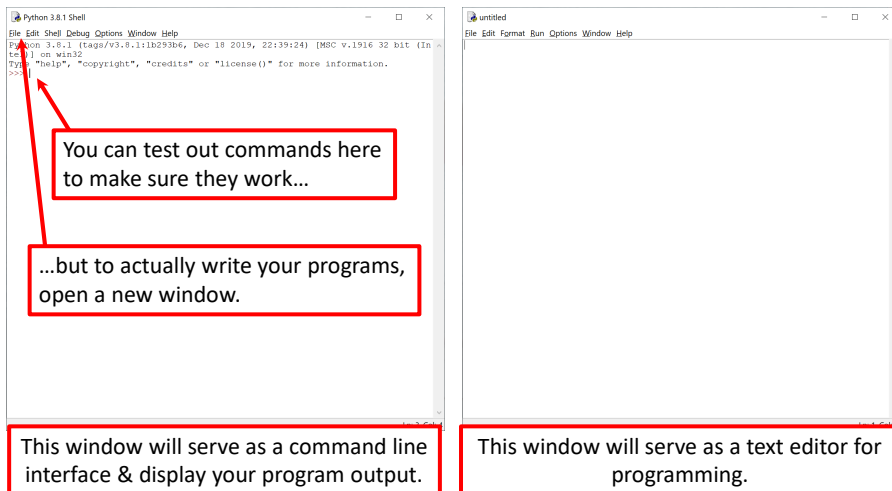
**By now, you should have installed Python on your computer.
If you're using Anaconda/Jupyter, it runs in a web browser:**



You can write your commands and programs here and they will be evaluated when you press Shift-Enter (or other options from the Cell pulldown menu)

Or if you installed IDLE by following the instructions in Rosalind Homework problem #1:

Launch IDLE:



This window will serve as a command line interface & display your program output.

This window will serve as a text editor for programming.

Let's start with some simple programs in Python:

A very simple example is:

```
print("Hello, future bioinformatician!")    # print out the greeting
```

Run the program. In Jupyter, you can just type Shift-Enter & the output will appear below this cell of the notebook.

The output looks like this:

Hello, future bioinformatician!

FYI: This is version agnostic. Python 3 takes `print("X")`. Python 2 also takes `print "X"` as in Rosalind

A slightly more sophisticated version:

```
name = input("What is your name? ")        # asks a question and saves the answer
                                           # in the variable "name"
print("Hello, future bioinformatician " + name + "!") # print out the greeting
```

When you run it this time, the output looks like:

What is your name?

If you type in your name, followed by the enter key, the program will print:

Hello, future bioinformatician Alice!

FYI: Python 2.x uses `raw_input()` instead of `input()`


GENERAL CONCEPTS

Names, numbers, words, etc. are stored as ***variables***.

Variables in Python can be named essentially anything except words Python uses as command.

For example:

```
BobsSocialSecurityNumber = 456249685  
mole = 6.022e-23  
password = "7 infinite fields of blue"
```



Note that strings of letters and/or numbers are in quotes, unlike numerical values.

LISTS

Groups of variables can be stored as lists.

A list is a numbered series of values,
like a vector, an array, or a matrix.

Lists are variables, so you can name them just as you would name any other variable.

Individual elements of the list can be referred to using [] notation:

```
The list nucleotides might contain the elements  
nucleotides[0] = "A"  
nucleotides[1] = "C"  
nucleotides[2] = "G"  
nucleotides[3] = "T"
```

(Notice the numbering starts from zero. This is standard in Python.)

DICTIONARIES

A VERY useful variation on lists is called a **dictionary** or *dict* (sometimes also called a *hash*).

→ Groups of values indexed not with numbers (although they could be) but with other values.

Individual hash elements are accessed like array elements:

For example, we could store the genetic code in a hash named *codons*, which might contain 64 entries, one for each codon, e.g.

```
codons["ATG"] = "Methionine"  
codons["TAG"] = "Stop codon"  
etc...
```

Now, for some control over what happens in programs.

There are two very important ways to control the logical flow of your programs:

if statements


and

for loops

There are some other ways too, but this will get you going for now.

if statements


```
if dnaTriplet == "ATG":  
    # Start translating here. We're not going to write this part  
    # since we're really just learning about IF statements  
else:  
    # Read another codon
```



Python cares about the white space (tabs & spaces) you use!
This is how it knows where the conditional actions that follow
begin and end. **These conditional steps must *always* be
indented by the same number of spaces (e.g., 4).**

Pick one (e.g. a tab or 4 spaces) and *always* be consistent.

**Note: in the sense of performing a
comparison, not as in setting a value.**



==	equals
!=	is not equal to
<	is less than
>	is greater than
<=	is less than or equal to
>=	is greater than or equal to

**Can nest these using parentheses and Boolean operations, such as
and, *not*, or *or*, e.g.:**

```
if dnaTriplet == "TAA" or dnaTriplet == "TAG" or dnaTriplet == "TGA":  
    print("Reached stop codon")
```

for loops

Often, we'd like to perform the same command repeatedly or with slight variations.

For example, to calculate the mean value of the number in an array, we might try:

Take each value in the array in turn.
Add each value to a running sum.
Divide the total by the number of values.

In Python, you could write this as:

```
grades = [93, 95, 87, 63, 75] # create a list of grades
sum = 0.0                     # variable to store the sum

for grade in grades:         # iterate over each grade
    sum = sum + grade         # add grade to sum

mean = sum / 5               # now calculate the average grade

print ("The average grade is ",mean) # print the results
```

In general, Python cares whether numbers are integers or floating point (also long integers and complex numbers).
You can tell Python you want floating point by defining your variables accordingly (e.g., $X = 1.0$ versus $X = 1$)

Python 2.x: `print ("The average grade is ",mean)`

Python 2	Python 3
<code>>>> 2 / 3</code> 0	<code>>>> 2 / 3</code> 0.666666

In general, Python will perform most mathematical operations, e.g.

multiplication	(A * B)
division	(A / B)
exponentiation	(A ** B)
etc.	

There are lots of advanced mathematical capabilities you can explore later on.

READING FILES

You can use a *for* loop to read text files line by line:

```
count = 0                # Declare a variable to count lines
file = open("mygenomefile", "r")  # Open a file for reading (r)
for raw_line in file:          # Loop through each line in the file
    line = raw_line.rstrip("\r\n")  # \r = carriage return, \n = newline
    words = line.split(" ")        # split into a list of words

    # Print the appropriate word:
    print ("The first word of line {0} of the file is {1}".format(count, words[0]))
    count += 1                # shorthand for count = count + 1

file.close()               # Increment counter by 1, close the file.
print ("Read in {0} lines\n".format(count))
```

Placeholders (e.g., {0}) in the print statement indicate variables listed at the end of the line after the format command

Note: Python expects the file to be in your working directory or that you give it a full path.

WRITING FILES

Same as reading files, but use "w" for 'write':

```
file = open("test_file", "w")  
file.write("Hello!\n")  
file.write("Goodbye!\n")  
file.close() # close the file as you did before
```

Unless you specify otherwise, you can find the new text file you created (test_file) in the default Python directory on your computer. In Jupyter, you should see now it appear in the Jupyter home page directory.

PUTTING IT ALL TOGETHER

```
1 seq_filename = "EcoliGenome.txt"  
2 total_length = 0  
3 nucleotide = {} # create an empty dictionary  
4  
5 seq_file = open(seq_filename, "r")  
6 for raw_line in seq_file:  
7     line = raw_line.rstrip("\r\n")  
8     length = len(line) # Python function to calculate the length of a string  
9     for nuc in line:  
10         if nuc not in nucleotide:  
11             nucleotide[nuc] = 1  
12         else:  
13             nucleotide[nuc] += 1  
14     total_length += length  
15  
16 seq_file.close()  
17  
18 for n in nucleotide.keys():  
19     fraction = 100.0 * nucleotide[n] / total_length  
20     print ("The nucleotide {0} occurs {1} times, or {2:.2f} %".format(n, nucleotide[n], fraction))  
21
```

Let's choose the input DNA sequence in the file to be the genome of *E. coli*, available the class web site (& originally from the **Entrez genomes** web site)

The format of the file is ~66,000 lines of A's, C's, G's and T's:
AGCTTTTCATTCTGACTGCAACGGGCAATATGTCTCTGTGTGGATTAAAAAAGAGTGC
TGATAGCAGCTTCTGAACCTGGTTACCTGCCGTGAGTAAATTTAAATTTTATTGACTTAGG
TCACTAAATACTTTAACCAATATAGGCATAGCGCACAGACAGATAAAAATTACAGAGTAC
ACAACATCCATGAAACGCATTAGCACCACCATTACCACCACCATTACCATTACCACAGGT
etc...

Running the program produces the output:

The nucleotide A occurs 1142742 times, or 24.62 %
The nucleotide G occurs 1177437 times, or 25.37 %
The nucleotide C occurs 1180091 times, or 25.42 %
The nucleotide T occurs 1141382 times, or 24.59 %

So, now we know that the four nucleotides are present in roughly equal numbers in the *E. coli* genome.

One really important aspect of Python is that there are literally *thousands* of existing libraries of pre-written functions that you can use to make life easier

Some examples you might use at some point are:

Numpy for numerical analyses (<https://numpy.org/>)
Scipy for scientific computation (<https://scipy.org/>)
BioPython for biological data analysis (<https://biopython.org/>)
Matplotlib for data visualization (<https://matplotlib.org/>)
Scikit-image for image processing (<https://scikit-image.org/>)

Many are preinstalled with Python (like numpy and scipy), but if not, open the Anaconda Powershell Prompt & type:

pip install biopython

That's it! Now you should have access to BioPython

Let's use BioPython to rewrite our last program:

```
1 from Bio import SeqIO # This imports the BioPython library into our program
2 nucleotide = {'A': 0, 'C': 0, 'T': 0, 'G': 0} # Doing it a bit differently here by pre-specifying the nuc's
3
4
5 seq_file = open("NewEcoli_genome.fasta", "r") # Open a fasta format sequence file
6 for seq_record in SeqIO.parse(seq_file, "fasta"): # then parse the file using BioPython to
7 # assign each consecutive record inside the file, i.e. each full
8 # sequence that appears after a line starting with a ">" symbol,
9 # to a new BioPython "sequence"-style variable named seq_record
10     sequence = seq_record.seq # BioPython sequence variables have a few special functions, such as
11     total_length = len(sequence) # using variablename.seq to get the amino acid or nucleotide sequence
12
13     for n in nucleotide.keys():
14         count = sequence.count(n) # Python strings have a nice .count command to count characters, i.e. nucleotides here
15         fraction = 100.0 * count / total_length
16         print(f"The nucleotide {n} occurs {count} times, or {fraction:.2f} %")
17
18 seq_file.close()

The nucleotide A occurs 1142742 times, or 24.62 %
The nucleotide C occurs 1180091 times, or 25.42 %
The nucleotide T occurs 1141382 times, or 24.59 %
The nucleotide G occurs 1177437 times, or 25.37 %
```

We get the same answer, but without having to worry about parsing lines, newlines, etc., & this will make life a *lot* easier for dealing with files with 1000's of protein or DNA sequences

Finally, let's give you a new programming super-power with ChatGPT

ChatGPT (& other AI chatbots like Claude, etc) is (1) truly amazing and powerful, and (2) a pathological liar. Caveat emptor.

Try it out, but don't trust it implicitly. It will give you an astonishing leg up with your programming, with the caveat that ***you have to check every single piece of code or fact supplied by it.*** It's like getting programming help from a gifted psychopath.

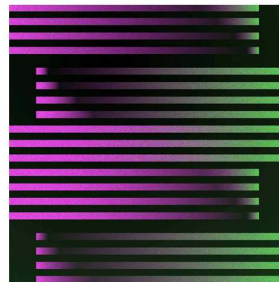


API RESEARCH BLOG ABOUT

ChatGPT: Optimizing Language Models for Dialogue

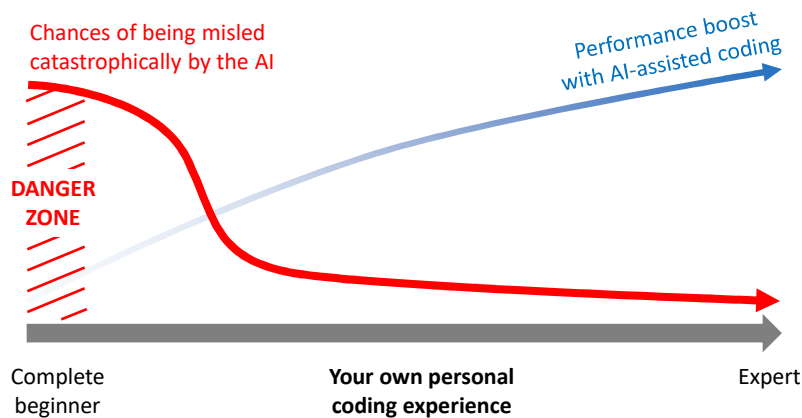
We've trained a model called ChatGPT which interacts in a conversational way. The dialogue format makes it possible for ChatGPT to answer followup questions, admit its mistakes, challenge incorrect premises, and reject inappropriate requests. ChatGPT is a sibling model to InstructGPT, which is trained to follow an instruction in a prompt and provide a detailed response.

[TRY CHATGPT](#)



<https://chatgpt.com/>

At this stage, I don't want you to rely on it, especially if you're just getting started and don't know enough to recognize when it's wrong. Please don't ask it write full programs for you or answer homework problems. Later in the semester, when you starting learning enough basic Python to judge it more effectively, we'll use AI much more.



However, a few things you might find helpful at this early stage:

- (1) Ask it to explain a line of code to you
→ "What does this command do?"
- (2) Ask it to explain programming syntax, suggest an alternative syntax, or a more compact way to perform the same task
- (3) Debugging, debugging, debugging.
→ Give ChatGPT your code and ask it to debug it

Just as an example, here's what chatGPT offers if we give it the example code for reading a file from 8 slides back.

E Can you explain how the following Python code works?

```
count = 0 # Declare a variable to count lines
file = open("mygenomefile", "r") # Open a file for reading (r)
for raw_line in file: # Loop through each line in the file
    line = raw_line.rstrip("\n") # Remove newline
    words = line.split(" ") # split the line into a list of words

    # Print the appropriate word:
    print ("The first word of line {0} of the file is {1}".format(count, words[0]))
    count += 1 # shorthand for count = count + 1

file.close() # Last, close the file.
print ("Read in {0} lines\n".format(count))
```

This Python code reads a file called "mygenomefile" line by line, and for each line it does the following:

1. Removes the newline characters ("\n") from the end of the line using `rstrip()`.
2. Splits the line into a list of words using `split()`.
3. Prints the first word of the line, along with the line number (starting from 0).
4. Increments the `count` variable by 1.

After all the lines have been processed, the code closes the file and prints the total number of lines read.

Here is a breakdown of each line of the code:

Regenerate response

Copy code

etc...
(for
several
pages)

E Can you write a more compact version of the program?

Certainly! Here is a more compact version of the program that achieves the same result:

```
count = 0
with open("mygenomefile", "r") as f:
    for line in f:
        words = line.split()
        print(f"The first word of line {count} of the file is {words[0]}")
        count += 1
print(f"Read in {count} lines")
```

Here is a breakdown of the changes made:

- The `open()` function is called using the `with` statement, which automatically closes the file after the block of code is executed.
- The `raw_line` variable is not needed, so it was removed and the `line` variable was used directly.
- The `rstrip()` method is not needed, because the `for` loop already removes newline characters.
- The `format()` method is replaced with f-strings, which provide a more concise and readable way to insert values into strings.

I hope this helps! Let me know if you have any questions.

A note about proper use and attribution of other people's code:

Most code is either commercial (which you usually can't access or redistribute) or, if it's in the public domain, available under a [license](#), e.g. as for most of the code on github.

Common open source licenses include **CC-BY-4.0**, **BSD**, and the **MIT** license (my own lab often uses the MIT license). These are very permissive and allow you to use the code (with attribution) and license your own project in turn however you like. Others are for **non-commercial use only**, and still others are strong "**copyleft**" licenses (like **GPL** licenses) that require you to use the identical license for any code you distribute as was on the code you reused.

Be absolutely sure to *acknowledge code* that you use & check that you're licensed to use it (especially if you go work in industry after grad school!)

You can read more about software licenses here:

<https://opensource.guide/legal/#which-open-source-license-is-appropriate-for-my-project>
& specifically for Github:
<https://docs.github.com/en/repositories/managing-your-repositorys-settings-and-features/customizing-your-repository/licensing-a-repository>

Myth

vs.

Reality

In bioinformatics, 95% of your time is spent on serious coding

95% of your time is spent converting gene IDs from one format to another. OMG, can't they pick a convention!?

Why learn to code at all?
Doesn't AI replace humans?

ChatGPT lies (misleads?) pretty often.
How will you know?

Once you've got data, just run a few lines of code and it's analyzed.
Boom!

Computational research usually takes longer than the data collection.

With bioinformatics, I can just dream up hypotheses about genes and test them with public data

Mostly true!