A Python programming primer for biologists

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

Systems Biology/Bioinformatics
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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

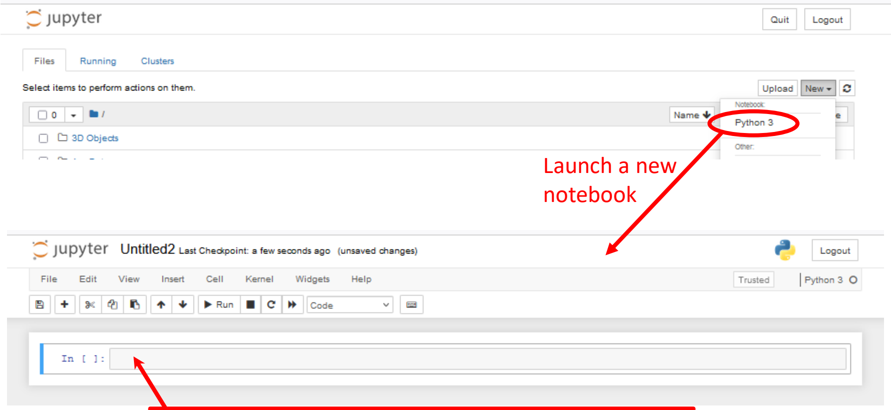
Practical Python, a self-paced online intro course:

- 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:

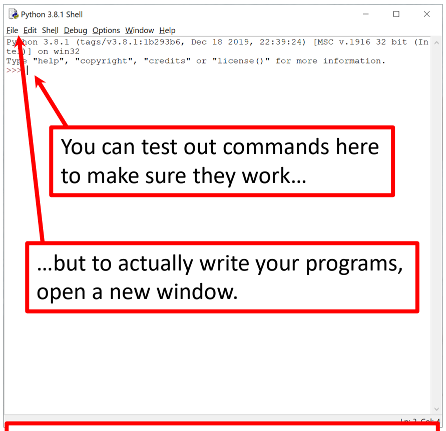


Launch a new notebook

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:

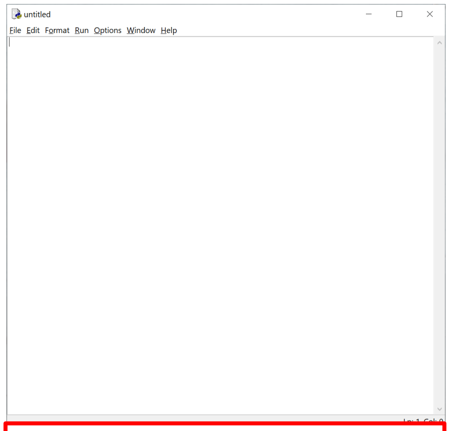
Launch IDLE:



```
Python 3.8.1 (tags/v3.8.1:1b293b6, Dec 18 2019, 22:39:24) [MSC v.1916 32 bit (In
tel)] on win32
Type "help", "copyright", "credits" or "license()" for more information.
>>> 
```

You can test out commands here to make sure they work…

…but to actually write your programs, open a new window.



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

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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:            # i
        sum = sum + grade      # i
                                # e

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	**Python 3**
>>> 2 / 3 0	>>> 2 / 3 0.666666

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

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

Stands for “read”

\r = carriage return
\n = newline

Increment counter by 1

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.

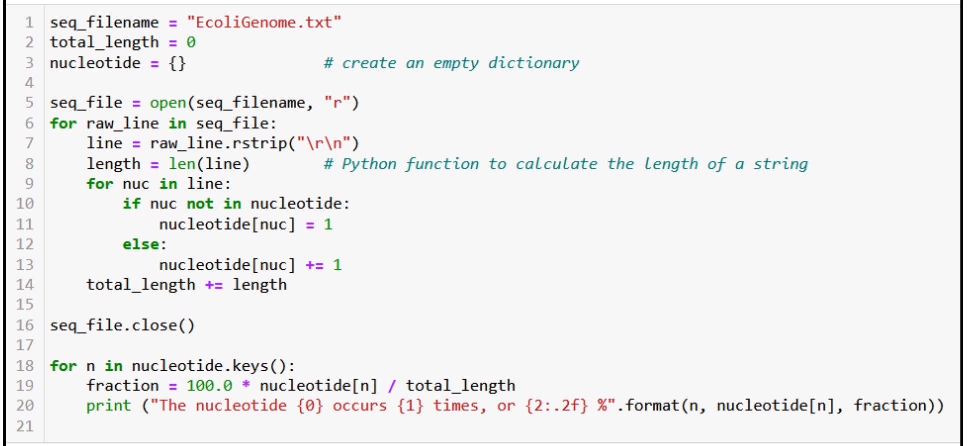
WRITING FILES

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



```
seq_filename = "EcoliGenome.txt"
total_length = 0
nucleotide = {}                # create an empty dictionary

seq_file = open(seq_filename, "r")
for raw_line in seq_file:
    line = raw_line.rstrip("\r\n")
    length = len(line)         # Python function to calculate the length of a string
    for nuc in line:
        if nuc not in nucleotide:
            nucleotide[nuc] = 1
        else:
            nucleotide[nuc] += 1
    total_length += length

seq_file.close()

for n in nucleotide.keys():
    fraction = 100.0 * nucleotide[n] / total_length
    print ("The nucleotide {0} occurs {1} times, or {2:.2f} %".format(n, nucleotide[n], fraction))

```

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 ~77,000 lines of A’s, C’s, G’s and T’s:

```
AGCTTTTCATTCTGACTGCAACGGGCAATATGTCTCTGTGTGGATTAAAAAAAGAGTGTC
TGATAGCAGCTTCTGAACTGGTTACCTGCCGTGAGTAAATTAAAATTTTATTGACTTAGG
TCACTAAATACTTTAACCAATATAGGCATAGCGCACAGACAGATAAAAATTACAGAGTAC
ACAACATCCATGAAACGCATTAGCACCACCATTACCACCACCATCACCATTACCACAGGT
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:

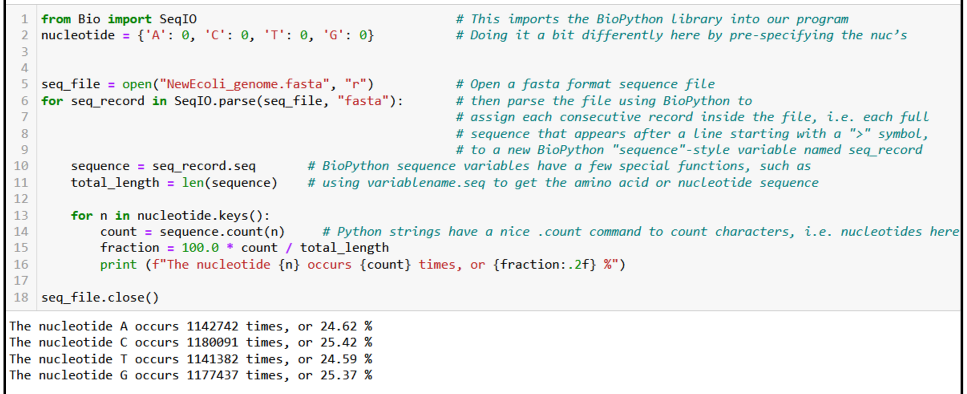
Numpy for numerical analyses (https://numpy.org/)
Scipy for scientific computation (https://scipy.org/)
BioPython for biological data analysis (https://biopython.org/)
Matplotlib for data visualization (https://matplotlib.org/)
Scikit-image for image processing (https://scikit-image.org/)

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:



```python
from Bio import SeqIO                                   # This imports the BioPython library into our program
nucleotide = {'A': 0, 'C': 0, 'T': 0, 'G': 0}           # Doing it a bit differently here by pre-specifying the nuc’s


seq_file = open("NewEcoli_genome.fasta", "r")           # Open a fasta format sequence file
for seq_record in SeqIO.parse(seq_file, "fasta"):       # then parse the file using BioPython to
                                                        # assign each consecutive record inside the file, i.e. each full
                                                        # sequence that appears after a line starting with a ">" symbol,
                                                        # to a new BioPython "sequence"-style variable named seq_record
    sequence = seq_record.seq       # BioPython sequence variables have a few special functions, such as
    total_length = len(sequence)    # using variablename.seq to get the amino acid or nucleotide sequence

    for n in nucleotide.keys():
        count = sequence.count(n)     # Python strings have a nice .count command to count characters, i.e. nucleotides here
        fraction = 100.0 * count / total_length
        print (f"The nucleotide {n} occurs {count} times, or {fraction:.2f} %")

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

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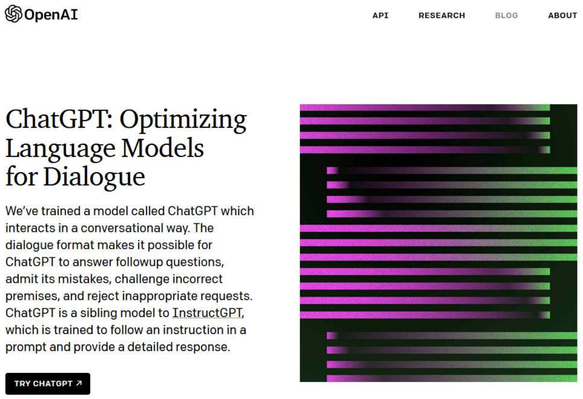
Finally, let’s give you a new programming super-power with ChatGPT

ChatGPT 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.



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.

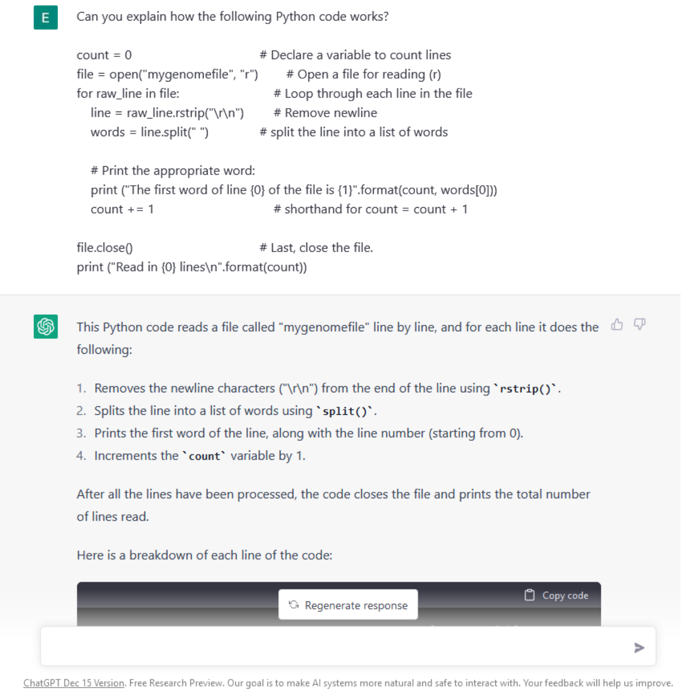
https://chat.openai.com/

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.

However, a few things you might find helpful at this 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 it your code (if there’s not too much to it) and ask it to debug.

Just as an example, here’s what chatGPT offers if we give it the example code for reading a file from 5 slides back.



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("\r\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:

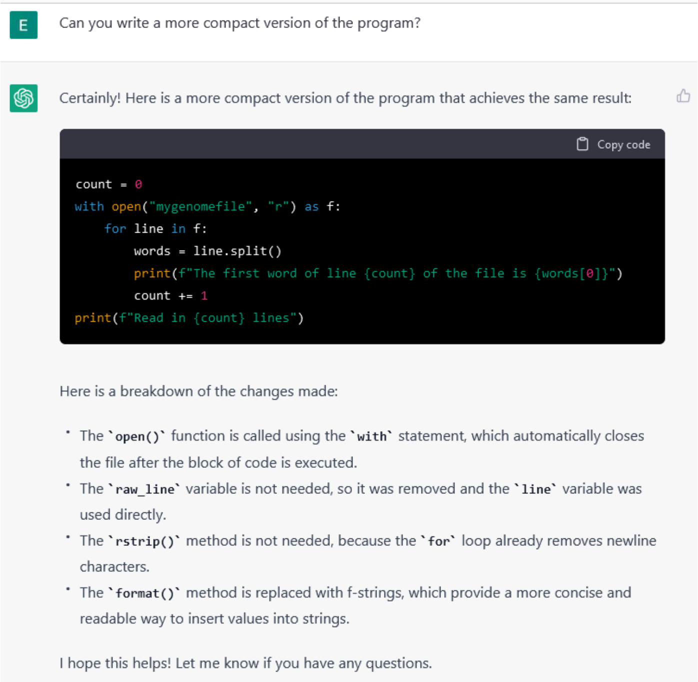
1. Removes the newline characters ("\r\n") from the end of the line using `` `rstrip()` ``.
2. Splits the line into a list of words using `` `split()` ``.
3. Prints the first word of the line, along with the line number (starting from 0).
4. Increments the `` `count` `` variable by 1.

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:

ChatGPT Dec 15 Version. Free Research Preview. Our goal is to make AI systems more natural and safe to interact with. Your feedback will help us improve.

etc…
(for
several
pages)



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 last note about programming and proper 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