

A Python programming primer for biochemists

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

BCH339N Systems Biology/Bioinformatics
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Science news of the day (2015 edition):

U.K.'s 100,000 Genomes Project gets £300 million to finish the job by 2017

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By Tania Rabesandratana | 1 August 2014 12:30 pm | 0 Comments

England's giant sequencing endeavor, the 100,000 Genomes Project, is getting a cash injection from public and private sources to meet its 2017 deadline, Prime Minister David Cameron announced today.



The project, launched by the U.K. government in 2012 and run by a state-owned company called Genomics England, aims to sequence 100,000 whole genomes of patients in the National Health Service's (NHS) records. The goal is to match genomic and clinical data to develop personalized therapies for cancer and rare diseases and to turn NHS into "the first mainstream health service in the world to offer genomic medicine as part of routine care," according to the project's website.

So far, a few hundred genomes have been sequenced in Genomics England's pilot efforts across the country. The funding package announced today will allow the project to ramp up its activities to sequence about 10,000 samples next year and 100,000 by the end of 2017.

Most of the money comes from a deal with Illumina, a U.S. company that manufactures DNA

Science news of the day (2015 edition):

BGI Plans to Launch Two NGS Systems Based on Complete Genomics Technology this Year

Jan 14, 2015 | [Monica Heger](#)

 Premium

SAN FRANCISCO (GenomeWeb) – BGI is planning to launch two next-generation sequencing systems this year based on Complete Genomics' technology, BGI CEO Jun Wang said during a presentation today at the JP Morgan conference.

In addition, he said that two BGI spinoff companies – BGI Tech and BGI Dx (formerly called BGI Health) – have now merged into one company that plans to go public in 2016. BGI Tech and BGI Dx raised ¥1.4 billion (\$226 million) and ¥2 billion (\$323 million), respectively, in private equity financing rounds, and following the merger raised an additional ¥2 billion in private equity financing. Wang first said in 2013 that BGI Tech had plans to go public, but did not have a timeline for doing so. The company had sold shares in order to purchase Complete Genomics, and the timing depended in part on its shareholders, [Wang said at the time](#).

During his presentation today, Wang also discussed several of BGI's clinical sequencing projects, including work in reproductive health, cancer, and complex diseases.

Finally, one of BGI's signature projects, the Million Genomes Project, which aims to sequence one million human, one million plant and animal, and one million bacterial genomes, seems to have expanded in scope. Today, Wang described the Million Omics Database project, which he said would include all 'omics data from one million people, including genomic, transcriptomic, epigenomic, metabolomic, and microbiome data.

Science news of the day (2016 update):

Forbes / Pharma & Healthcare

JAN 10, 2016 @ 05:00 PM 110,300 VIEWS

A Single Blood Test For All Cancers? Illumina, Bill Gates And Jeff Bezos Launch Startup To Make It Happen



Matthew Herper

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I cover science and medicine, and believe in the power of technology.

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Illumina CEO Jay Flatley

What if a simple blood test could detect any cancer early, when it was still easy to treat?

It sounds like science fiction. But [Illumina](#) (ILMN -0.59%), the \$2.4 billion (market cap) biotechnology company that has pioneered cheap, efficient sequencing of DNA, says it could be a reality in a few years. It is launching a new startup, GRAIL (because such a test would be a holy grail for cancer doctors), with \$100 million in funding. Illumina will hold a majority share. Other backers include

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

Most bioinformatics researchers use a scripting language, such as Python, Perl, or Ruby.

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 giving an introduction to Python. This will give you a sense for the language and help us 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 L. Model, O'Reilly Media

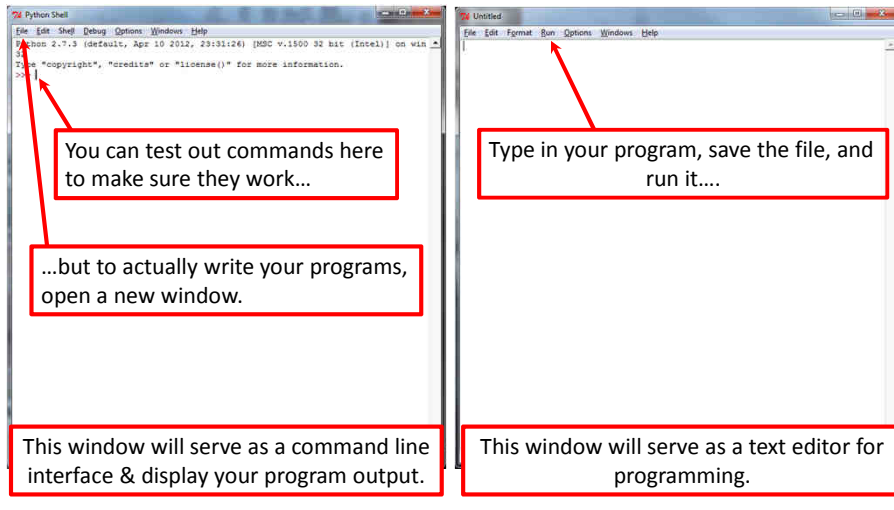
Good intro videos on Python:

CodeAcademy: <http://www.codecademy.com/tracks/python>
 & the Kahn Academy:
<https://www.khanacademy.org/science/computer-science>

A bit more advanced: *Programming Python*, 4th ed.
 Mark Lutz, O'Reilly Media

By now, you should have installed Python on your computer, following the instructions in Rosalind Homework problem #1.

Launch IDLE:



Let's start with some simple programs in Python:

A very simple example is:

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

Let's call it hello.py

Save & run the program. The output looks like this:

```
Hello, future bioinformatician!
```

A slightly more sophisticated version:

```
name = raw_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!

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).**

I recommend using a tab (rather than spaces) so you're always consistent.

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

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

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 the list
    sum = sum + grade # calculate the sum
mean = sum / 5 # now calculate the average grade
print ("The average grade is "),mean # print the results
```

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

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
file = open("mygenomefile", "r")
for raw_line in file:
    line = raw_line.rstrip("\r\n")
    words = line.split(" ")

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

file.close()
print "Read in {0} lines\n".format(count)

```

Stands for "read"

Declare a variable to count lines

Open a file for reading (r)

Loop through each line in the file

\r = carriage return
\n = newline

split the line into a list of words

shorthand for count = count + 1

Increment counter by 1

Last, close the file.

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

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.

PUTTING IT ALL TOGETHER

```

seq_filename = "Ecoli_genome.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 nucleotide.has_key(nuc):
            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} %".format(n, nucleotide[n], fraction)

```

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

The format of the file is ~77,000 lines of A's, C's, G's and T's:
 AGCTTTTCATTCTGACTGCAACGGGCAATATGTCTCTGTGTGGATTAAAAAAGAGTGTG
 TGATAGCAGCTTCTGAAGTGGTTACCTGCCGTGAGTAAATTTAAATTTTATTGACTTAGG
 TCACTAAATACTTTAACCAATATAGGCATAGCGCACAGACAGATAAAAATTACAGAGTAC
 ACAACATCCATGAAACGCATTAGCACCACCATTACCACCACCATTACCATTACCACAGGT
 etc...

Running the program produces the output:

The nucleotide A occurs 1142136 times, or 24.6191332553 %
 The nucleotide C occurs 1179433 times, or 25.423082884 %
 The nucleotide T occurs 1140877 times, or 24.5919950785 %
 The nucleotide G occurs 1176775 times, or 25.3657887822 %

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