An introduction to python and its applications in bioinformatics

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Lab Master Class
Jan 2021

The print function and ‘Hello World’

```
(base) nageorge@hydra:~$ python
```

The print function and ‘Hello World’

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Python 3.7.7 (default, Mar 26 2020, 15:48:22)
[GCC 7.3.0] :: Anaconda, Inc. on linux
Type "help", "copyright", "credits" or "license" for more information.
```

The print function and ‘Hello World’

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>>> print('Hello World')
```

The print function and ‘Hello World’

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>>> print('Hello World')
Hello World
```

Variable assignment

```
>>> lab_group = "Hug_lab"
```

Variable assignment

```
>>> lab_group = "Hug_lab"
>>> print(lab_group)
Hug_lab
```

Variable assignment

```
>>> lab_group = "Hug_lab"
>>> print(lab_group)
Hug_lab
>>> lab_group
'Hug_lab'
```

List generation and the len function

```
>>> lab_members = ['Laura', 'Fiona', 'Veronica', 'Dan', 'Panuya', 'Brian', 'Emilie', 'Grant', 'Rosalind', 'Nikhil', 'Lisa']
```

List generation and the len function

```
>>> lab_members = ['Laura', 'Fiona', 'Veronica', 'Dan', 'Panuya', 'Brian', 'Emilie', 'Grant', 'Rosalind', 'Nikhil', 'Lisa']
>>> lab_members
['Laura', 'Fiona', 'Veronica', 'Dan', 'Panuya', 'Brian', 'Emilie', 'Grant', 'Rosalind', 'Nikhil', 'Lisa']
```

List generation and the len function

```
>>> lab_members = ['Laura', 'Fiona', 'Veronica', 'Dan', 'Panuya', 'Brian', 'Emilie', 'Grant', 'Rosalind', 'Nikhil', 'Lisa']
>>> lab_members
['Laura', 'Fiona', 'Veronica', 'Dan', 'Panuya', 'Brian', 'Emilie', 'Grant', 'Rosalind', 'Nikhil', 'Lisa']
>>> len(lab_members)
11
```

List generation and the len function

```
>>> lab_members = ['Laura', 'Fiona', 'Veronica', 'Dan', 'Panuya', 'Brian', 'Emilie', 'Grant', 'Rosalind', 'Nikhil', 'Lisa']
>>> lab_members
['Laura', 'Fiona', 'Veronica', 'Dan', 'Panuya', 'Brian', 'Emilie', 'Grant', 'Rosalind', 'Nikhil', 'Lisa']
>>> len(lab_members)
11
>>> len('str')
3
```

Indexing in python

```
>>> lab_members
['Laura', 'Fiona', 'Veronica', 'Dan', 'Panuya', 'Brian', 'Emilie', 'Grant', 'Rosalind', 'Nikhil', 'Lisa']
```

Indexing in python

```
>>> lab_members
['Laura', 'Fiona', 'Veronica', 'Dan', 'Panuya', 'Brian', 'Emilie', 'Grant', 'Rosalind', 'Nikhil', 'Lisa']
>>> print("The principal investigator of this lab is: " + lab_members[1])
```

Indexing in python

```
>>> lab_members
['Laura', 'Fiona', 'Veronica', 'Dan', 'Panuya', 'Brian', 'Emilie', 'Grant', 'Rosalind', 'Nikhil', 'Lisa']
>>> print("The principal investigator of this lab is: " + lab_members[1])
The principal investigator of this lab is: Fiona
```

??????

Indexing in python

```
>>> lab_members
['Laura', 'Fiona', 'Veronica', 'Dan', 'Panuya', 'Brian', 'Emilie', 'Grant', 'Rosalind', 'Nikhil', 'Lisa']
```

0 1 2 3 4 5 6 7 8 9 10

Indexing in python

```
>>> print("The principal investigator of this lab is: " + lab_members[0])
```

Indexing in python

```
>>> print("The principal investigator of this lab is: " + lab_members[0])
The principal investigator of this lab is: Laura
```

Index ranges and non-inclusivity

```
>>> lab_members
['Laura', 'Fiona', 'Veronica', 'Dan', 'Panuya', 'Brian', 'Emilie', 'Grant', 'Rosalind', 'Nikhil', 'Lisa']
```

Index ranges and non-inclusivity

```
>>> lab_members
['Laura', 'Fiona', 'Veronica', 'Dan', 'Panuya', 'Brian', 'Emilie', 'Grant', 'Rosalind', 'Nikhil', 'Lisa']
>>> lab_members[0:4]
```

Index ranges and non-inclusivity

```
>>> lab_members
['Laura', 'Fiona', 'Veronica', 'Dan', 'Panuya', 'Brian', 'Emilie', 'Grant', 'Rosalind', 'Nikhil', 'Lisa']
>>> lab_members[0:4]
['Laura', 'Fiona', 'Veronica', 'Dan']
```

The for loop

```
>>> for lab_member in lab_members:
```

The for loop

```
>>> for lab_member in lab_members:
...     print(lab_member + " is a cool lab member")
```

The for loop

```
>>> for lab_member in lab_members:
...     print(lab_member + " is a cool lab member")
...
Laura is a cool lab member
Fiona is a cool lab member
Veronica is a cool lab member
Dan is a cool lab member
Panuya is a cool lab member
Brian is a cool lab member
Emilie is a cool lab member
Grant is a cool lab member
Rosalind is a cool lab member
Nikhil is a cool lab member
Lisa is a cool lab member
```

The for loop’s iteration variable

```
>>> for chicken13 in lab_members:
...     print(chicken13 + " is a cool lab member")
```

The for loop's iteration variable

```
>>> for chicken13 in lab_members:
...     print(chicken13 + " is a cool lab member")
...
Laura is a cool lab member
Fiona is a cool lab member
Veronica is a cool lab member
Dan is a cool lab member
Panuya is a cool lab member
Brian is a cool lab member
Emilie is a cool lab member
Grant is a cool lab member
Rosalind is a cool lab member
Nikhil is a cool lab member
Lisa is a cool lab member
```

The if else conditional statements and the “>” comparison operator

```
>>> if len(lab_members) > 10:
```

The if else conditional statements and the “>” comparison operator

```
>>> if len(lab_members) > 10:
...     print("Since when did our lab get so big?")
```

The if else conditional statements and the “>” comparison operator

```
>>> if len(lab_members) > 10:
...     print("Since when did our lab get so big?")
... else:
...     print("Is our lab considered big?")
```

The if else conditional statements and the “>” comparison operator

```
>>> if len(lab_members) > 10:
...     print("Since when did our lab get so big?")
... else:
...     print("Is our lab considered big?")
...
Since when did our lab get so big?
```

Counters, another comparison operator “==” and... basically everything else we’ve discussed

```
>>> name = 'LAURA'
>>> letters = ['L','A','U','R','A']
>>> counter = 0
```

Counters, another comparison operator “==” and... basically everything else we’ve discussed

```
>>> name = 'LAURA'
>>> letters = ['L','A','U','R','A']
>>> counter = 0
>>> for character in name:
...     if character == letters[1]:
...             counter = counter + 1
...
```

Counters, another comparison operator “==” and... basically everything else we’ve discussed

```
>>> name = 'LAURA'
>>> letters = ['L','A','U','R','A']
>>> counter = 0
>>> for character in name:
...     if character == letters[1]:
...             counter = counter + 1
...
>>> print(counter)
2
```

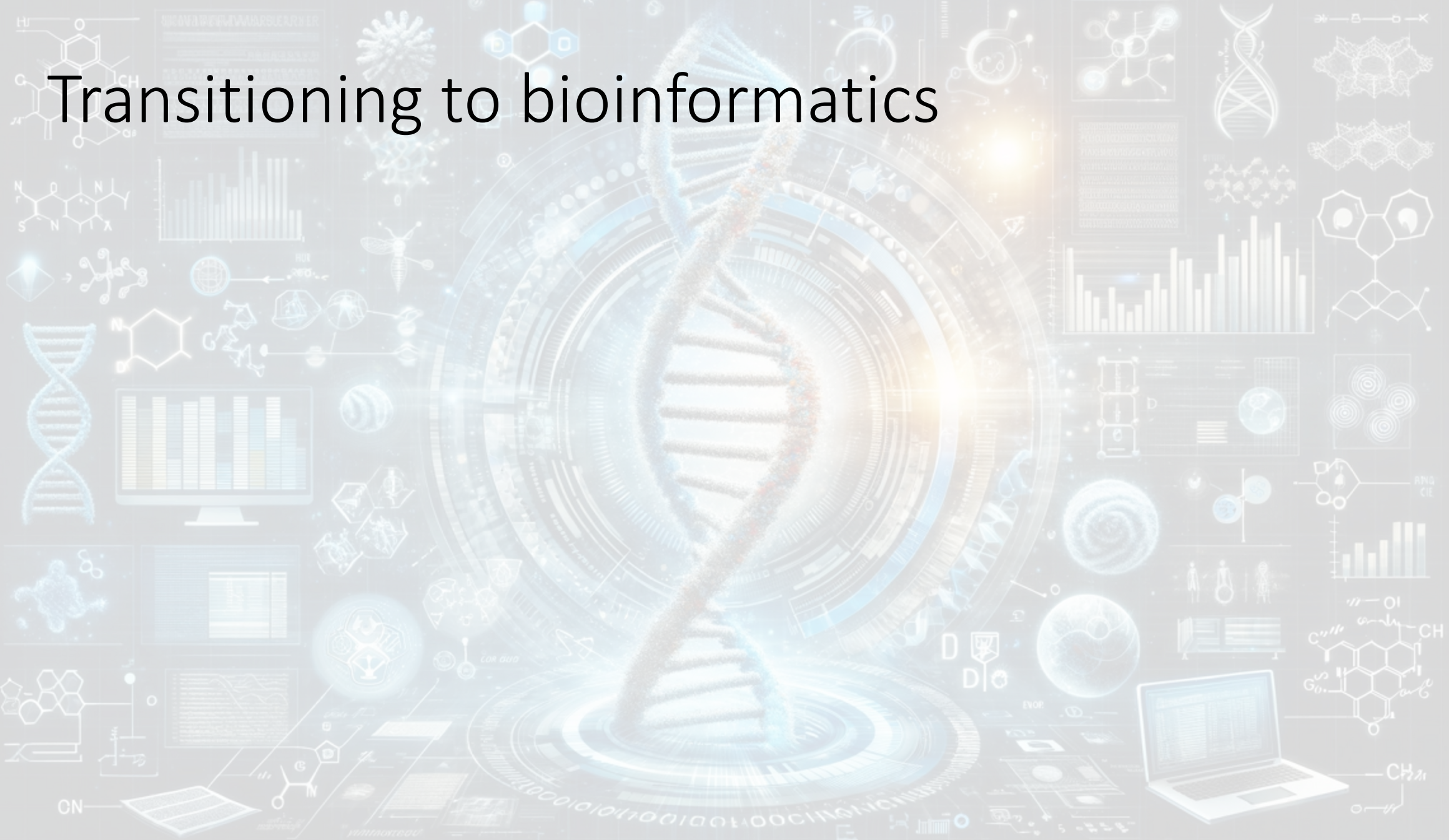
The range function with a for loop

```
>>> for i in range(17):
...     print(i)
...
```

The range function with a for loop

```
>>> for i in range(17):
...     print(i)
...
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
```

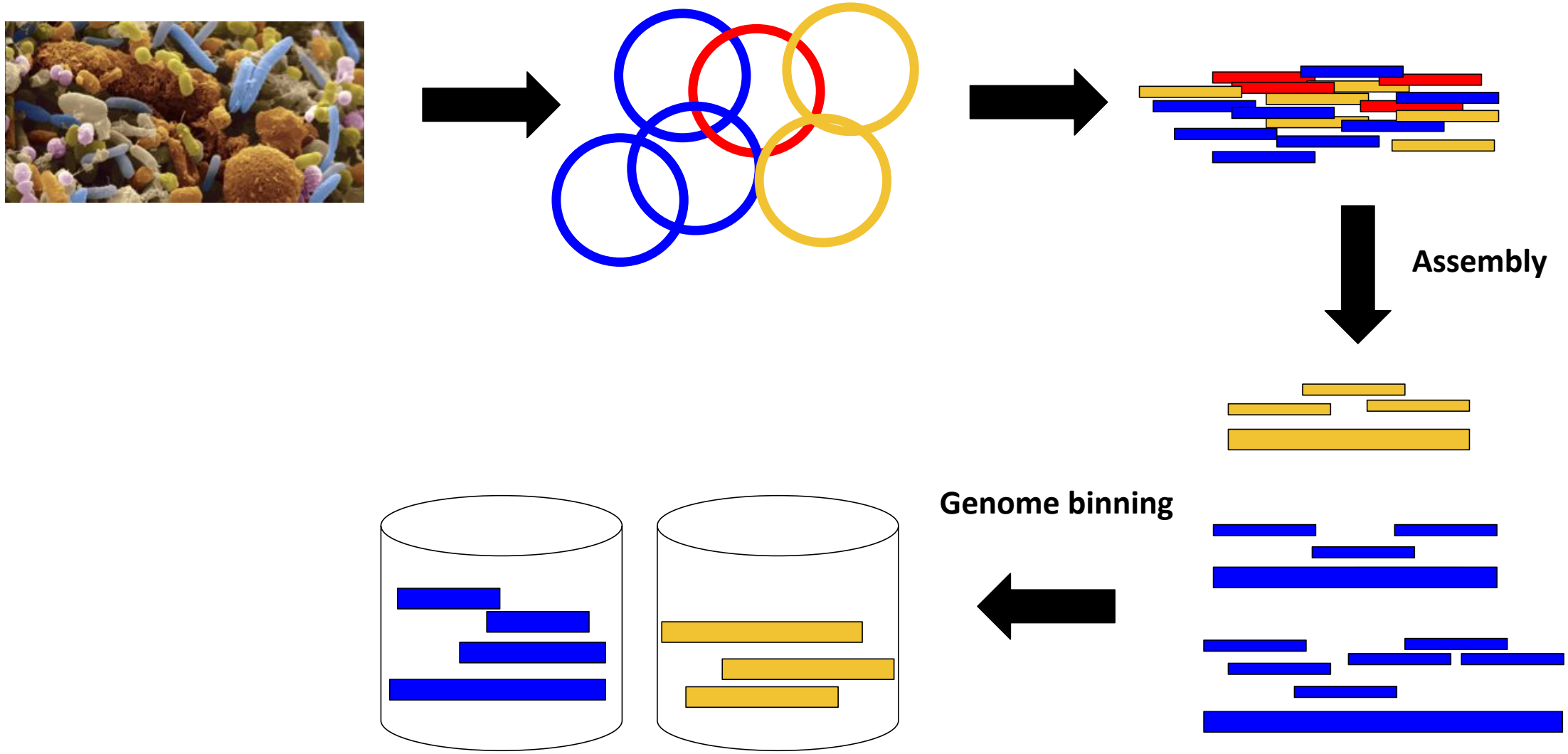
Transitioning to bioinformatics



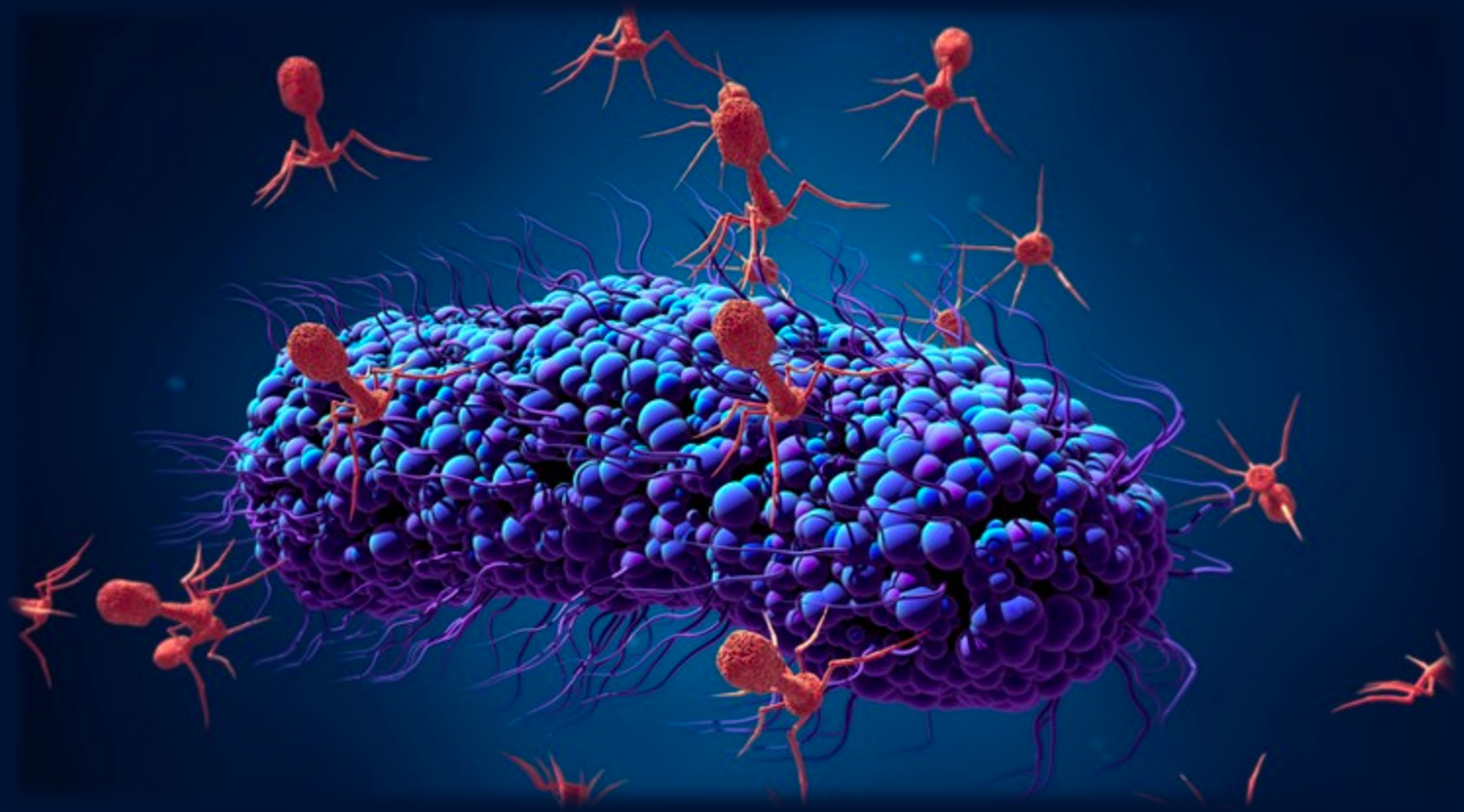
K-mers

- A k-mer is pattern (or part of a sequence) of length k
- E.g. ATA is a 3-mer

Work in our lab involving k-mers



Work in our lab involving k-mers



K-mer detection

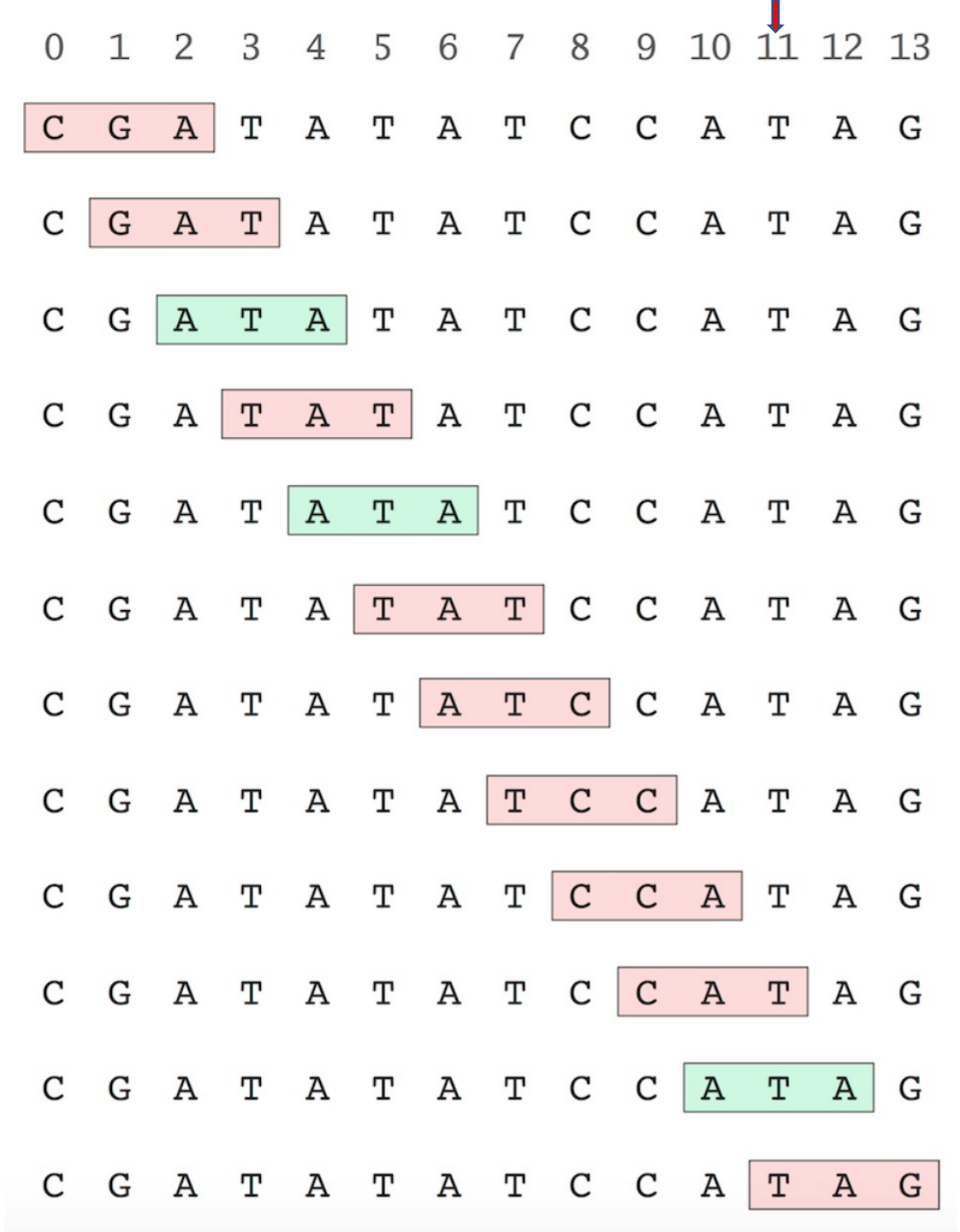
How many times does the 3-mer “ATA” exist in the string below?

CGATATATCCATAG

K-mer detection

How many times does the 3-mer “ATA” exist in the string below?

CGATATATCCATAGTGCTAATTTAATAGCTATGCCCTAAGTATAAGGGCTACGA

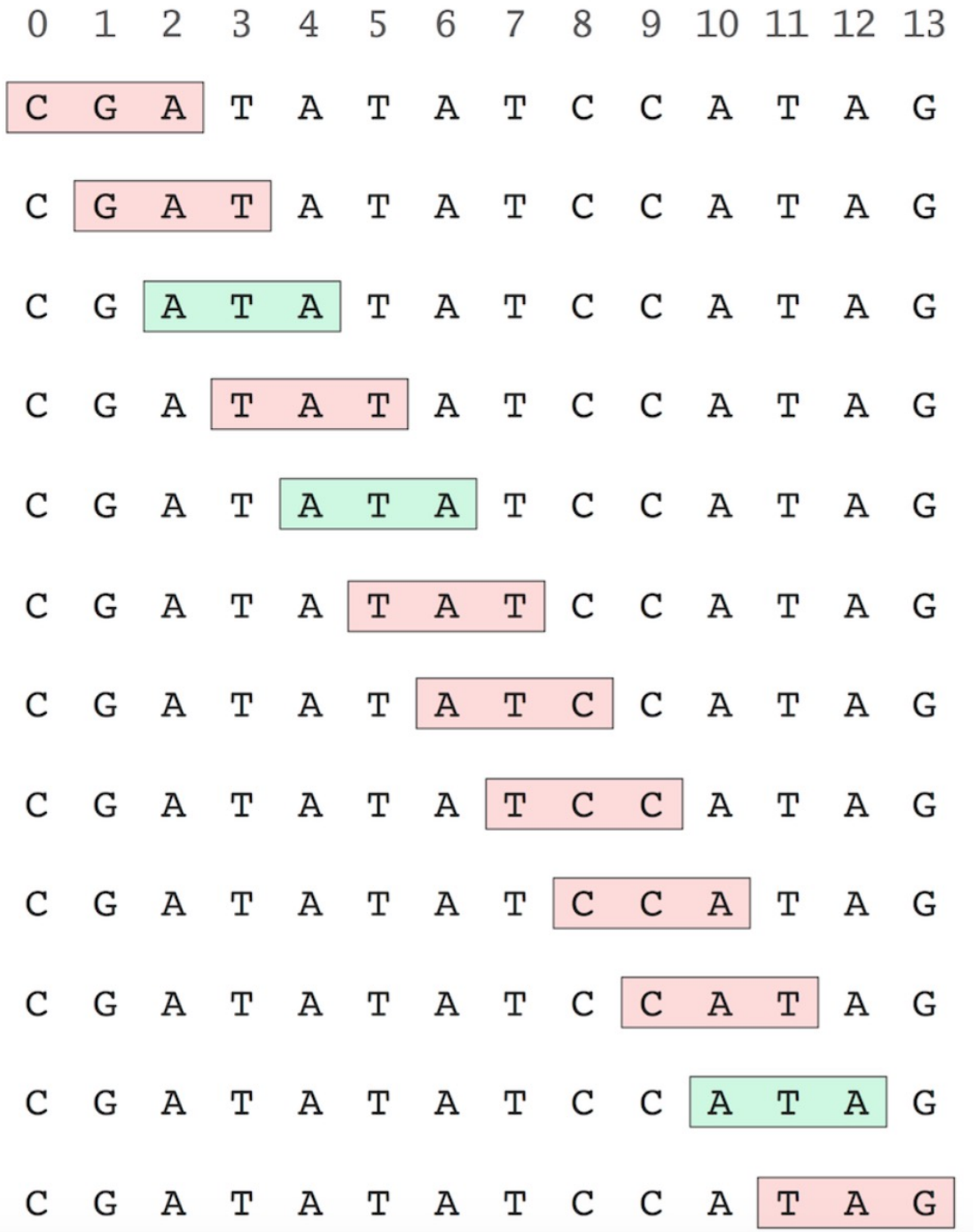


Sequence: CGATATATCCATAG
(14 characters)

3-mer: ATA

Note that the 11th position in the sequence is last position at which a 3-mer can be captured

I.e., the last position a k-mer can be called in a sequence = the length of the sequence – the length of the k-mer



Sequence: CGATATATCCATAG

3-mer: ATA

- We need a way of iterating across the sequence
- We need to compare pieces of the sequence to the k-mer
- We need a counter to keep track of matches to the k-mer

K-mer detection

```
#!/opt/anaconda3/bin/python

kmer = 'ATA'
sequence = 'CGATATATCCATAG'
```

K-mer detection

```
#!/opt/anaconda3/bin/python

kmer = 'ATA'
sequence = 'CGATATATCCATAG'

counter = 0
```

K-mer detection

```
#!/opt/anaconda3/bin/python

kmer = 'ATA'
sequence = 'CGATATATCCATAG'

counter = 0
for i in                                :
```

K-mer detection

```
#!/opt/anaconda3/bin/python

kmer = 'ATA'
sequence = 'CGATATATCCATAG'

counter = 0
for i in [redacted]:
    if [redacted] == kmer:
        counter = counter + 1
```

K-mer detection

```
#!/opt/anaconda3/bin/python

kmer = 'ATA'
sequence = 'CGATATATCCATAG'

counter = 0
for i in range((len(sequence))-(len(kmer))+1):
```

The range function

```
>>> for i in range(17):
...     print(i)
...
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
```

K-mer detection

```
#!/opt/anaconda3/bin/python

kmer = 'ATA'
sequence = 'CGATATATCCATAG'

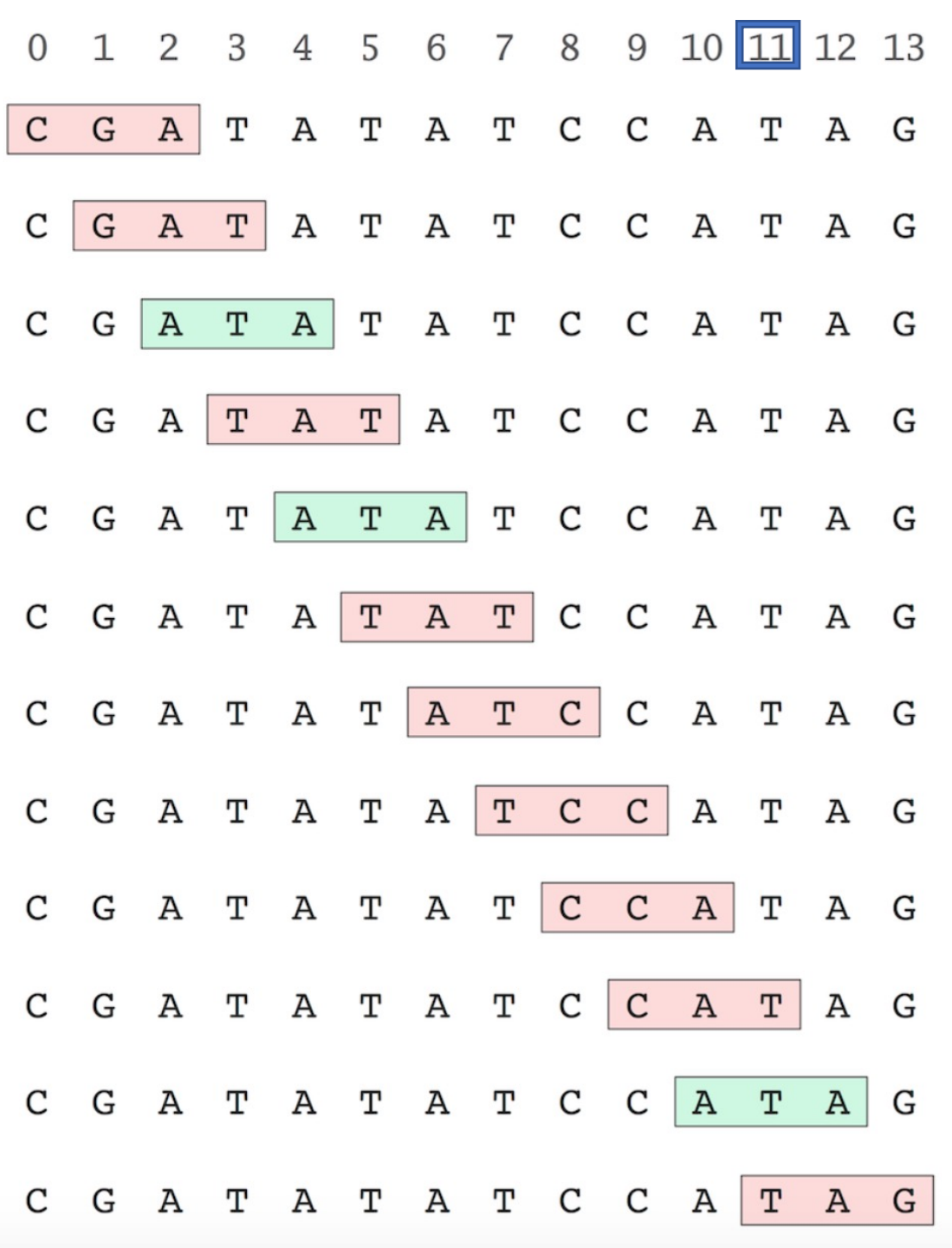
counter = 0
for i in range((len(sequence))-(len(kmer))+1):
```

K-mer detection

```
#!/opt/anaconda3/bin/python

kmer = 'ATA'
sequence = 'CGATATATCCATAG'

counter = 0
for i in range((len(sequence))-(len(kmer))+1):
```



K-mer detection

```
#!/opt/anaconda3/bin/python

kmer = 'ATA'
sequence = 'CGATATATCCATAG'

counter = 0
for i in range((len(sequence))-(len(kmer))+1):
    if sequence[i:i+(len(kmer))] == kmer:
        counter = counter + 1
```

K-mer detection

```
#!/opt/anaconda3/bin/python

kmer = 'ATA'
sequence =
```

0	1	2	3	4	5	6	7	8	9	10	11	12	13
C	G	A	T	A	T	A	T	C	C	A	T	A	G

```
counter = 0
for i in range((len(sequence))-(len(kmer))+1):
    if sequence[i:i+(len(kmer))] == kmer:
        counter = counter + 1
```

if sequence[0:3] == kmer:

K-mer detection

```
#!/opt/anaconda3/bin/python

kmer = 'ATA'
sequence = 'CGATATATCCATAG'

counter = 0
for i in range((len(sequence))-(len(kmer))+1):
    if sequence[i:i+(len(kmer))] == kmer:
        counter = counter + 1
print(counter)
```

K-mer detection (as a python script)

```
➜ PhD_student_thoroughly_confuses_lab_with_poor_explanation_of_python ./kmer_counting2.py
3
```

K-mer detection (with friendly user output)

```
➜ PhD_student_thoroughly_confuses_lab_with_poor_explanation_of_python ./kmer_counting2.py
The kmer ATA occurs 3 times in the sequence CGATATATCCATAG
```

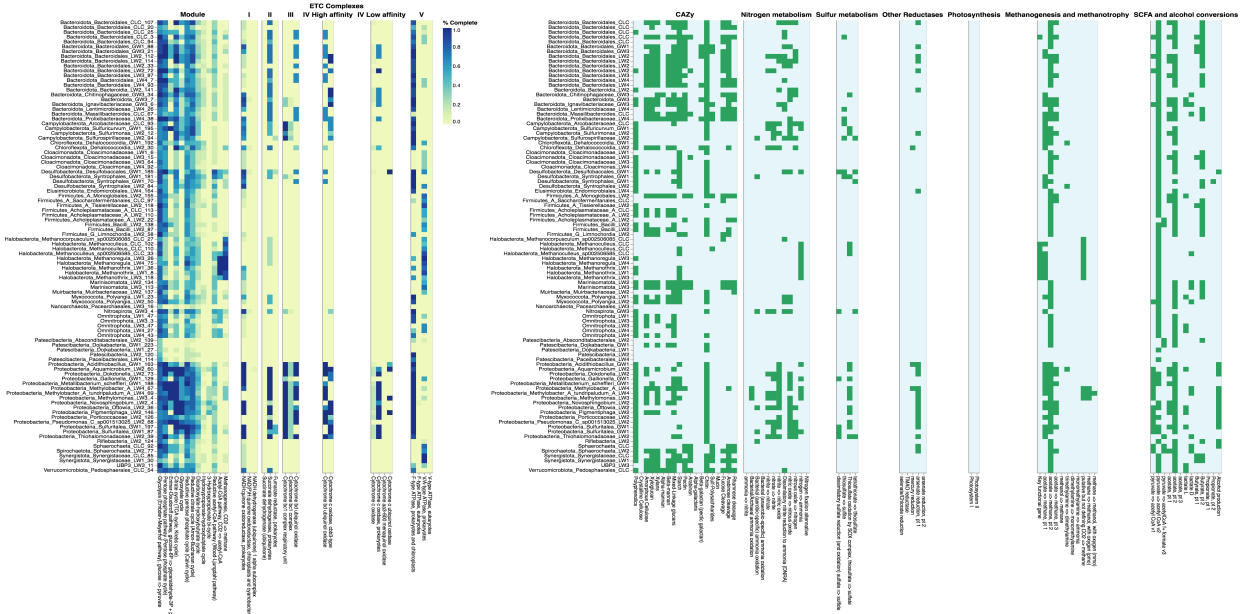
K-mer detection (with arguments passed from the command line)

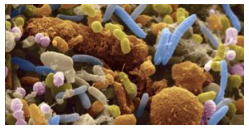
```
➜ PhD_student_thoroughly_confuses_lab_with_poor_explanation_of_python ./kmer_counting.py ATA CGATATATCCATAG
The kmer ATA occurs 3 times in the sequence CGATATATCCATAG
```

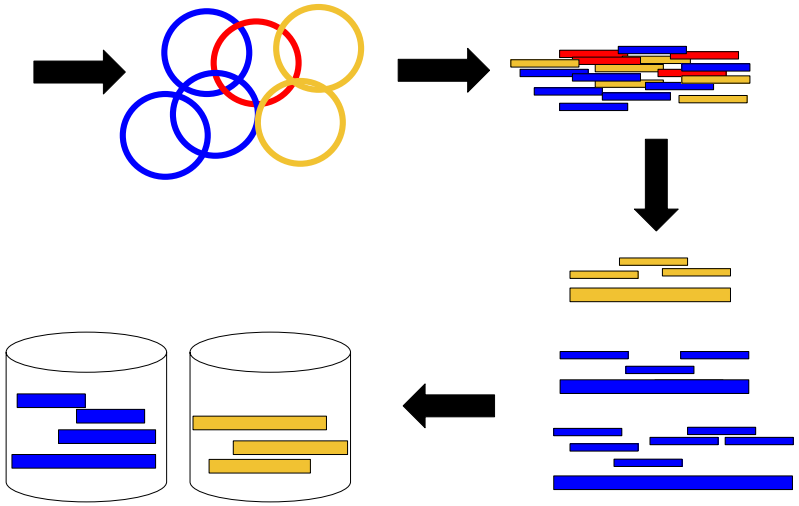
K-mer detection (with arguments passed from the command line)

```
➜ PhD_student_thoroughly_confuses_lab_with_poor_explanation_of_python ./kmer_counting.py ATA CGATATATCCATAGTGCTAATTTAATAGCTATGCCCTAAGTATAAGGGCTACGA

The kmer ATA occurs 5 times in the sequence CGATATATCCATAGTGCTAATTTAATAGCTATGCCCTAAGTATAAGGGCTACGA
```







max	34.000000	27386.000000	3906.000000	31292.000000	42588.000000	73880.000000

```
In [11]: data.columns

Out[11]: Index(['Unnamed: 0', 'date', 'state', 'hospitalized_with_symptoms',
       'intensive_care', 'total_hospitalized', 'home_quarantine',
       'total_confirmed_cases', 'new_confirmed_cases', 'recovered', 'deaths',
       'total_cases', 'swabs_made', 'note_it', 'note_en'],
      dtype='object')
```

relating the variables with scatterplots

```
In [15]: sns.relplot(x="total_confirmed_cases", y="hospitalize", data=data)

Out[15]: <seaborn.axisgrid.FacetGrid at 0x180efd13e80>
```

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Python 3.9.1 documentation

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A collection of exercises to accompany Bioinformatics Algorithms: An Active-Learning Approach by Phillip Compeau & Pavel Pevzner. A full version of this text is hosted on stepic.org

Algorithmic Heights

A collection of exercises in introductory algorithms to accompany "Algorithms", the popular textbook by Dasgupta, Papadimitriou, and Vazirani.


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