Introduction to



with Application to Bioinformatics

- Day 2

Review Day 1

Give an example of the following:

- A number of type float
- A variable containing an integer
- A Boolean/A list/A string
- What character represents a comment?
- What happens if I take a list plus a list?
- How do I find out if x is present in a list?
- How do I find out if 5 is larger than 3 and the integer 4 is the same as the float 4?
- How do I find the second item in a list?
- An example of a mutable sequence
- An example of an immutable sequence
- Something iterable (apart from a list)
- How do I do to print 'Yes' if x is bigger than y?
- How do I open a file handle to read a file called 'somerandomfile.txt'?
- The file contains several lines, how do I print each line?

Variables and Types

A number of type **float**:

3.14

A variable containing an integer:

a = 5

x = 349852

A boolean:

True

A list:

[2,6,4,8,9]

A string:

'this is a string'

Literals

All literals have a type:

```
• Strings (str) 'Hello' "Hi"
```

• Integers (int) 5

• Floats (float) 3.14

• Boolean (bool) True or False

```
In [ ]: | type(3.14)
```

Variables

Used to store values and to assign them a name.

```
In [ ]: a = 3.14
```

Lists

A collection of values.

Operations

What character represents a **comment**?

#

What happens if I take a list plus a list?

The lists will be concatenated

How do I find out if x is present in a list?

How do I find out if 5 is larger than 3 and the integer 4 is the same as the float 4?

$$5 > 3$$
 and $4 == 4.0$

Basic operations

```
Type Operations

int +-/**\%//...
float +-/*\%//...
string +
```

```
In []: 

a = 2

b = 5.46

c = [1,2,3,4]

d = [5,6,7,8]
```

Comparison/Logical/Membership operators

| Operation | Meaning | Operation | Meaning |
|-----------|-----------------------|-----------|-----------------------------------|
| < | less than | | connects two statements, both |
| <= | less than or equal | and | conditions having to be fulfilled |
| > | greater than | | connects two statements, either |
| >= | greater than or equal | or | conditions having to be fulfilled |
| == | equal | not | reverses and/or |
| != | not equal | Operation | Meaning |
| | | in | value in object |
| | | not in | value not in object |

```
In [ ]:    a = [1,2,3,4,5,6,7,8]
    b = 5
    c = 10
    b not in a
```

Sequences

```
How do I find the second item in a list?
list_a[1]

An example of a mutable sequence:
[1,2,3,4,5,6]

An example of an immutable sequence:
'a string is immutable'

Something iterable (apart from a list):
'a string is also iterable'
```

Indexing

Lists (and strings) are an ORDERED collection of elements where every element can be access through an index.

a[0]: first item in list a

REMEMBER! Indexing starts at 0 in python

Mutable / Immutable sequences and iterables

Lists are mutable object, meaning you can use an index to change the list, while strings are immutable and therefore not changeable.

An iterable sequence is anything you can loop over, ie, lists and strings.

New data type: tuples

- A tuple is an immutable sequence of objects
- Unlike a list, nothing can be changed in a tuple
- Still iterable

```
In [ ]: myTuple = (1,2,3,4,'a','b','c',[42,43,44])
myTuple[0] = 42
print(myTuple)
print(len(myTuple))
for i in myTuple:
    print(i)
```

If/ Else statements

```
How do I do if I want to print 'Yes' if x is bigger than y?
if x > y:
  print('Yes')
```

Files and loops

```
How do I open a file handle to read a file called 'somerandomfile.txt'?
          fh = open('somerandomfile.txt', 'r', encoding = 'utf-8')
          fh.close()
         The file contains several lines, how do I print each line?
          for line in fh:
            print(line.strip())
          fh = open('../files/somerandomfile.txt','r', encoding = 'utf-8')
          for line in fh:
             print(line.strip())
          fh.close()
In [ ]:
         numbers = [5,6,7,8]
          while i < len(numbers):</pre>
             print(numbers[i])
             i += 1
```

Questions?

 \rightarrow Any unfinished exercises from Day 1

How to approach a coding task

Problem:

You have a VCF file with a larger number of samples. You are interested in only one of the samples (sample1) and one region (chr5, 1.000.000-1.005.000). What you want to know is whether this sample has any variants in this region, and if so, what variants.

Always write pseudocode!

Pseudocode is a description of what you want to do without actually using proper syntax

What is your input?

A VCF file that is iterable

```
##fileformat=VCFv4.1
##FILTER<<ID=PASS, Description="All filters passed">
##ALT<<ID=PASS, Description="All filters passed">
##ALT<<ID=DNON REF, Description="Represents any possible alternative allele at this location">
##FILTER<<ID=LowQual, Description="VoSLOD < 0.0">
##FILTER<<ID=LowQual, Description="Low quality">
##FILTER<<ID=LowQual, Description="Low quality">
##Source=SelectVariants
##source=SelectVariants
##bottools mergeVersion=1.5+htslib-1.5
#CHROM POS ID REF ALT QUAL FILTER INFO FORMAT sample1 sample2 sample3
1 10492 . C T 550.31 PASS AN=26;AC=2 GT:AD:DP 0/0:0,25:25 0/1:14,23:37 1/1:31,0:31
```

Basic Pseudocode:

- Open file and loop over lines (ignore lines with #)
- Identify lines where chromosome is 5 and position is between 1.000.000 and 1.005.000
- Isolate the column that contains the genotype for sample 1
- Extract the genotypes only from the column
- Check if the genotype contains any alternate alleles
- Print any variants containing alternate alleles for this sample between specified region

```
##fileformat=VCFV4.1
##filtrER<<TD=PASS,Description="All filters passed">
##ALT=<ID=PASS,Description="Represents any possible alternative allele at this location">
##FILTER<TD=LOW_VQSLOD,Description="VQSLOD < 0.0">
##FILTER<TD=LOW_VQSLOD,Description="UQSLOD < 0.0">
##FILTER<TD=LOW_VQSLOD,Description="Low quality">
##FILTER<TD=LOW_VQSLOD,Description="Low quality">
##FILTER<TD=Low_VQSLOD,Description="Low quality">
##FILTER<TD=Low_VQSLOD,Description="Low quality">
##FILTER<TD=Low_VQSLOD,Description="Low quality">
##Source-SelectVariants
##bcftools_mergeVersion=1.5+htslb=1.5
#CHROM POS ID REF ALT QUAL FILTER INFO FORMAT sample1 sample2 sample3
1 10492 . C T 550.31 PASS AN=26;AC=2 GT:AD:DP 0/0:0,25:25 0/1:14,23:37 1/1:31,0:31
```

- Open file and loop over lines (ignore lines starting with #)

```
In [ ]: fh = open('C:/Users/Nina/Documents/courses/Python_Beginner_Course/genotypes.vcf', 'r', encoding = 'utf-8')
for line in fh:
    if not line.startswith('#'):
        print(line.strip())
        break
fh.close()
# Next, find chromosome 5
```

- Identify lines where chromosome is 5 and position is between 1.000.000 and 1.005.000

```
##fileformat=VCFv4.1
##FILTER=<ID=PASS, pescription="All filters passed">
##FILTER=<ID=PASS, pescription="Represents any possible alternative allele at this location">
##FILTER=<ID=LOW_VQSLOD, Description="VQSLOD < 0.0">
##FILTER=<ID=LOW_Qual, Description="Low quality">
##FILTER=<ID=LOW_Qua
```

```
##fileformat=VCFv4.1
##FILTER=<ID=PASS,Description="All filters passed">
##FILTER=<ID=PASS,Description="Represents any possible alternative allele at this location">
##FILTER=<ID=LOW_VQSLOD,Description="VQSLOD < 0.0">
##FILTER=<ID=LOW_QUALD,Description="Low quality">
##FILTER=<ID=LowQual,Description="Low quality">
##FILTER=<ID=LowQual,Description="Low quality">
##FILTER=<ID=LowQual,Description="Low quality">
##FILTER=<ID=LowQual,Description="Low quality">
##FILTER=<ID=LowQual,Description="Low quality">
##FILTER=
##Source=SelectVariants
##botftools mergeVersion=1.5+htslib=1.5
##CHROM POS ID REF ALT QUAL FILTER INFO FORMAT sample1 sample2 sample3
1 10492 . C T 550.31 PASS AN=26;AC=2 GT:AD:DP 0/0:0,25:25 0/1:14,23:37 1/1:31,0:31
```

- Isolate the column that contains the genotype for sample1

```
##fileformat=VCFv4.1
##FILTER=<ID=PASS,Description="All filters passed">
##ALT=<ID=PASS,Description="Represents any possible alternative allele at this location">
##FILTER=<ID=LOW_VQSLOD,Description="VQSLOD < 0.0">
##FILTER=<ID=LOW_QVGLOD,Description="Low quality">
##FILTER=<ID=LowQual,Description="Low quality">
##FILTER=<ID=LowQual,Description="Low quality">
##FILTER=<ID=LowQual,Description="Low quality">
##FILTER=<ID=LowQual,Description="Low quality">
##FILTER=<ID=LowQual,Description="Low quality">
##FILTER=
##Source=SelectVariants
##bottools mergeVersion=1.5+htslib=1.5
##CHROM POS ID REF ALT QUAL FILTER INFO FORMAT sample1 sample2 sample3
1 10492 . C T 550.31 PASS AN=26;AC=2 GT:AD:DP 0/0:0,25:25 0/1:14,23:37 1/1:31,0:31
```

- Extract the genotypes only from the column

- Check if the genotype contains any alternate alleles

```
##fileformat=VCFv4.1
##FILTER=<ID=PASS,Description="All filters passed">
##ALT=<ID=PASS,Description="Represents any possible alternative allele at this location">
##FILTER=<ID=LOW_VQSLOD,Description="VQSLOD < 0.0">
##FILTER=<ID=LOW_QVGLOD,Description="Low quality">
##FILTER=<ID=LowQual,Description="Low quality">
##FILTER=<ID=LowQual,Description="Low quality">
##FILTER=<ID=LowQual,Description="Low quality">
##FILTER=<ID=LowQual,Description="Low quality">
##FILTER=<ID=LowQual,Description="Low quality">
##FILTER=
##Source=SelectVariants
##bottools mergeVersion=1.5+htslib=1.5
##CHROM POS ID REF ALT QUAL FILTER INFO FORMAT sample1 sample2 sample3
1 10492 . C T 550.31 PASS AN=26;AC=2 GT:AD:DP 0/0:0,25:25 0/1:14,23:37 1/1:31,0:31
```

- Print any variants containing alternate alleles for this sample between specified region

→ Notebook Day_2_Exercise_1 (~50 minutes)

Comments for Exercise 1

```
In [ ]:
            fh = open('../downloads/genotypes small.vcf', 'r', encoding = 'utf-8')
            wt = 0
            het = 0
            hom = 0
            for line in fh:
                if not line.startswith('#'):
                    cols = line.strip().split('\t')
                    chrom = cols[0]
                    pos = cols[1]
                    if chrom == '2' and pos == '136608646':
                        for geno in cols[9:]:
                            alleles = geno[0:3]
                            if alleles == '0/0':
                                wt += 1
                            elif alleles == '0/1':
                                het += 1
                            elif alleles == '1/1':
                                hom += 1
            freq = (2*hom + het)/((wt+hom+het)*2)
            print('The frequency of the rs4988235 SNP is: '+str(freq))
            fh.close()
```

Although much shorter, but maybe not as intuitive...

Shorter than the first version, but easier to follow than the second version

More useful functions and methods

What is the difference between a function and a method?

A method always belongs to an object of a specific class, a function does not have to. For example:

print('a string') and print(42) both works, even though one is a string and one is an integer

'a string '.strip() works, but [1,2,3,4].strip() does not work. strip() is a method that only works on strings

What does it matter to me?

For now, you mostly need to be aware of the difference, and know the different syntaxes:

A function:

functionName()

A method:

<object>.methodName()

```
In [ ]: len([1,2,3])
len('a string')

'a string '.strip()
[1,2,3].strip()
```

Functions

| Built-in Functions | | | | | |
|--------------------|-------------|--------------|--------------|----------------|--|
| abs() | delattr() | hash() | memoryview() | set() | |
| all() | dict() | help() | min() | setattr() | |
| any() | dir() | hex() | next() | slice() | |
| ascii() | divmod() | id() | object() | sorted() | |
| bin() | enumerate() | input() | oct() | staticmethod() | |
| bool() | eval() | int() | open() | str() | |
| breakpoint() | exec() | isinstance() | ord() | sum() | |
| bytearray() | filter() | issubclass() | pow() | super() | |
| bytes() | float() | iter() | print() | tuple() | |
| callable() | format() | len() | property() | type() | |
| chr() | frozenset() | list() | range() | vars() | |
| classmethod() | getattr() | locals() | repr() | zip() | |
| compile() | globals() | map() | reversed() | import() | |
| complex() | hasattr() | max() | round() | | |

<u>Python Built-in functions (https://docs.python.org/3/library/functions.html#)</u>

| Built-in Functions | | | | | |
|--------------------|-------------|--------------|--------------|----------------|--|
| abs() | delattr() | hash() | memoryview() | set() | |
| all() | dict() | help() | min() | setattr() | |
| any() | dir() | hex() | next() | slice() | |
| ascii() | divmod() | id() | object() | sorted() | |
| bin() | enumerate() | input() | oct() | staticmethod() | |
| bool() | eval() | int() | open() | str() | |
| breakpoint() | exec() | isinstance() | ord() | sum() | |
| bytearray() | filter() | issubclass() | pow() | super() | |
| bytes() | float() | iter() | print() | tuple() | |
| callable() | format() | len() | property() | type() | |
| chr() | frozenset() | list() | range() | vars() | |
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| ascii() | divmod() | id() | object() | sorted() | |
| bin() | enumerate() | input() | oct() | staticmethod() | |
| bool() | eval() | int() | open() | str() | |
| breakpoint() | exec() | isinstance() | ord() | sum() | |
| bytearray() | filter() | issubclass() | pow() | super() | |
| bytes() | float() | iter() | print() | tuple() | |
| callable() | format() | len() | property() | type() | |
| chr() | frozenset() | list() | range() | vars() | |
| classmethod() | getattr() | locals() | repr() | zip() | |
| compile() | globals() | map() | reversed() | import() | |
| complex() | hasattr() | max() | round() | | |

From Python documentation

sum(iterable[, start])

Sums *start* and the items of an *iterable* from left to right and returns the total. *start* defaults to \overline{o} . The *iterable*'s items are normally numbers, and the start value is not allowed to be a string.

```
In [ ]: sum([1,2,3,4],5)
help(sum)
```

| Built-in Functions | | | | |
|--------------------|-------------|--------------|--------------|----------------|
| abs() | delattr() | hash() | memoryview() | set() |
| all() | dict() | help() | min() | setattr() |
| any() | dir() | hex() | next() | slice() |
| ascii() | divmod() | id() | object() | sorted() |
| bin() | enumerate() | input() | oct() | staticmethod() |
| bool() | eval() | int() | open() | str() |
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| bytearray() | filter() | issubclass() | pow() | super() |
| bytes() | float() | iter() | print() | tuple() |
| callable() | format() | len() | property() | type() |
| chr() | frozenset() | list() | range() | vars() |
| classmethod() | getattr() | locals() | repr() | zip() |
| compile() | globals() | map() | reversed() | import() |
| complex() | hasattr() | max() | round() | |

Methods

Useful operations on strings

| String Methods | | |
|----------------|------------------|--|
| str.strip() | str.startswith() | |
| str.rstrip() | str.endswith() | |
| str.lstrip() | str.upper() | |
| str.split() | str.lower() | |
| str.join() | | |

str.**strip**([chars])

Return a copy of the string with the leading and trailing characters removed. The *chars* argument is a string specifying the set of characters to be removed. If omitted or None, the *chars* argument defaults to removing whitespace. The *chars* argument is not a prefix or suffix; rather, all combinations of its values are stripped:

```
>>> ' spacious '.strip()
'spacious'
>>> 'www.example.com'.strip('cmowz.')
'example'
```

str. lstrip([chars])

Return a copy of the string with leading characters removed. The *chars* argument is a string specifying the set of characters to be removed. If omitted or None, the *chars* argument defaults to removing whitespace. The *chars* argument is not a prefix; rather, all combinations of its values are stripped:

```
>>> ' spacious '.lstrip()
'spacious '
>>> 'www.example.com'.lstrip('cmowz.')
'example.com'
```

str.rstrip([chars])

Return a copy of the string with trailing characters removed. The *chars* argument is a string specifying the set of characters to be removed. If omitted or None, the *chars* argument defaults to removing whitespace. The *chars* argument is not a suffix; rather, all combinations of its values are stripped:

```
>>> ' spacious '.rstrip()
' spacious'
>>> 'mississippi'.rstrip('ipz')
'mississ'
```

```
str. split(sep=None, maxsplit=-1)
```

Return a list of the words in the string, using *sep* as the delimiter string. If *maxsplit* is given, at most *maxsplit* splits are done (thus, the list will have at most *maxsplit*+1 elements). If *maxsplit* is not specified or -1, then there is no limit on the number of splits (all possible splits are made).

If sep is given, consecutive delimiters are not grouped together and are deemed to delimit empty strings (for example, '1,,2'.split(',') returns ['1', '', '2']). The sep argument may consist of multiple characters (for example, '1<>2<>3'.split('<>') returns ['1', '2', '3']). Splitting an empty string with a specified separator returns [''].

For example:

```
>>> '1,2,3'.split(',')
['1', '2', '3']
>>> '1,2,3'.split(',', maxsplit=1)
['1', '2,3']
>>> '1,2,,3,'.split(',')
['1', '2', '', '3', '']
```

If sep is not specified or is None, a different splitting algorithm is applied: runs of consecutive whitespace are regarded as a single separator, and the result will contain no empty strings at the start or end if the string has leading or trailing whitespace. Consequently, splitting an empty string or a string consisting of just whitespace with a None separator returns [].

For example:

```
>>> '1 2 3'.split()
['1', '2', '3']
>>> '1 2 3'.split(maxsplit=1)
['1', '2 3']
>>> ' 1 2 3 '.split()
['1', '2', '3']
```

```
In [ ]:    a = ' split a string into a list '
    a.split()
```

str.join(iterable)

Return a string which is the concatenation of the strings in *iterable*. A TypeError will be raised if there are any non-string values in *iterable*, including bytes objects. The separator between elements is the string providing this method.

In []: ' '.join('a string already')

str. **startswith**(prefix[, start[, end]])

Return True if string starts with the *prefix*, otherwise return False. *prefix* can also be a tuple of prefixes to look for. With optional *start*, test string beginning at that position. With optional *end*, stop comparing string at that position.

str.endswith(suffix[, start[, end]])

Return True if the string ends with the specified *suffix*, otherwise return False. *suffix* can also be a tuple of suffixes to look for. With optional *start*, test beginning at that position. With optional *end*, stop comparing at that position.

```
In [ ]: 'long string'.startswith('ng',2)
   'long string'.endswith('string')
```

str.upper()

Return a copy of the string with all the cased characters [4] converted to uppercase. Note that s.upper().isupper() might be False if s contains uncased characters or if the Unicode category of the resulting character(s) is not "Lu" (Letter, uppercase), but e.g. "Lt" (Letter, titlecase).

str.lower()

Return a copy of the string with all the cased characters [4] converted to lowercase.

```
In [ ]: 'LongRandomString'.lower()
'LongRandomString'.upper()
```

Useful operations on Mutable sequences

| Operation | Result |
|----------------|---|
| | appends x to the end of the |
| s.append(x) | sequence |
| s.insert(i, x) | x is inserted at pos i |
| | retrieves the item $\it i$ from $\it s$ |
| s.pop([i]) | and also removes it |
| | retrieves the first item from s |
| s.remove(x) | where $s[i] == x$ |
| | reverses the items of s in |
| s.reverse() | place |

Summary

- Tuples are immutable sequences of objects
- Always plan your approach before you start coding
- A method always belongs to an object of a specific class, a function does not have to
- The official Python documentation describes the syntax for all built-in functions and methods
- → Notebook Day_2_Exercise_2 (~30 minutes)

IMDb

Download the 250 imdb file from the course website

This format of this file is:

- Line by line
- Columns separated by the | character
- Header starting with #

Votes | Rating | Year | Runtime | URL | Genres | Title

Find the movie with the highest rating

Votes | Rating | Year | Runtime | URL | Genres | Title 126807| 8.5|1957|5280|https://images-na.ssl-images-amazon.com/images/M_V1_.jpg|Drama,War|Paths of Glory 71379| 8.2|1925|4320|https://images-na.ssl-images-amazon.com/images/N_V1_.jpg|Adventure,Comedy,Drama,Family|The Gold Rush

```
# Votes | Rating | Year | Runtime | URL | Genres | Title
126807| 8.5|1957|5280|https://images-na.ssl-images-amazon.com/images/M_V1_.jpg|Drama,War|Paths of Glory
71379| 8.2|1925|4320|https://images-na.ssl-images-amazon.com/images/N_V1_.jpg|Adventure,Comedy,Drama,Family|The Gold Rush
```

For the genre Adventure

Find the top movie by rating

Votes | Rating | Year | Runtime | URL | Genres | Title 126807| 8.5|1957|5280|https://images-na.ssl-images-amazon.com/images/M_Vl_.jpg|Drama,War|Paths of Glory 71379| 8.2|1925|4320|https://images-na.ssl-images-amazon.com/images/N_Vl_.jpg|Adventure,Comedy,Drama,Family|The Gold Rush

Answer

Top movie:

The LOTR: The Return of the King with 8.9

```
In [ ]:
           fh = open('../downloads/250.imdb', 'r', encoding = 'utf-8')
            top = [0, '']
            for line in fh:
                if not line.startswith('#'):
                    cols = line.strip().split('|')
                    genre = cols[5].strip()
                    glist = genre.split(',')
                                                    # one movie can be in several genres
                    if 'Adventure' in glist:
                                                    # check if movie belongs to genre Adventure
                        rating = float(cols[1].strip())
                        if rating > top[0]:
                            top = [rating,cols[6]]
            fh.close()
            print(top)
```

Find the number of genres

Answer

Watch out for the upper/lower cases!

The correct answer is 22

New data type: set

• A set contains an unordered collection of unique and immutable objects

```
Syntax:
For empty set:
  setName = set()

For populated sets:
  setName = {1,2,3,4,5}
```

Common operations on sets

```
set.add(a)
len(set)
a in set
```

```
In [ ]:
    x = set()
    x.add(100)
    x.add(25)
    x.add(3)
    #for i in x:
    #    print(i)

mySet = {1,2,3,4}
mySet.add(5)
mySet.add(4)
print(mySet)
```

Find the number of genres

Votes | Rating | Year | Runtime | URL | Genres | Title 126807| 8.5|1957|5280|https://images-na.ssl-images-amazon.com/images/M_Vl_.jpg|Drama,War|Paths of Glory 71379| 8.2|1925|4320|https://images-na.ssl-images-amazon.com/images/N_Vl_.jpg|Adventure,Comedy,Drama,Family|The Gold Rush

Modify your code to use sets